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Subspace-based model identification of a hydrogen plant startup dynamics

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ABSTRACT

This work addresses the problem of determining a data-driven model for the startup of a hydrogen production unit, and demonstrates the approach both on a detailed first principles simulation model and by application to real data. To this end, first a detailed first principles model of the hydrogen plant is developed in Honeywell's UniSim design by adapting the plant standard operating procedure (SOP). Illustrative simulations are next presented to establish the meaningfulness of approximating process nonlinearity with a (higher order) linear time invariant (LTI) model. Then an LTI data-driven model of the hydrogen unit startup process using subspace identification based methods is identified. The framework is then implemented and successfully validated data on simulated data and on data from an industrial hydrogen unit.

1. Introduction

Hydrogen is an indispensable chemical component extensively used in petroleum and chemical industries. An economic way to commercially produce hydrogen is to utilize steam methane reforming (SMR) (Kroschwitz and Seidel, 2006). SMR process operation (like most other operations) undergoes scheduled startup and shutdown procedures which is sometimes initiated due to the need for regular maintenance and sometimes by unforeseen circumstances. Startups/shutdowns are implemented using standard operating procedures (SOPs). These procedures present various constraints and challenges such as constraints on the reformer exit temperature and firebox pressure (Du et al., 2014). Further, a typical startup involves a series of operations such as ramping various flows, introducing certain flows, along with making discrete decisions such as starting up certain parts of the unit. Thus, the startup time is not fixed and varies based on the decisions taken at various stages. Startups and shutdowns are fairly resource intensive operations, and stand to gain from optimizing the startup procedure via operating procedure synthesis (OPS).

A key requirement for OPS is a good model for the startup process. There exist several modeling approaches that are well suited for small scale processes (see Batres et al., 2002 for an excellent review) but difficult to implement to large chemical units. Out of these approaches, dynamic simulation based strategies are most prominent. In these approaches, dynamic simulations are used to select the best startup scenarios. The detailed models allow a good description of the startup dynamics and are valuable from a process analysis standpoint. One of the key contributions of the present work is the development of a detailed first principles model for the hydrogen unit startup, with appropriate adaption of the plant startup SOP. Note however that such detailed first principles models pose computational challenges when directly embedded in optimization problems, and thus existing SOP synthesis approaches utilize heuristics in an attempt to determine optimal profiles (e.g., see Scenna et al., 1998; Yang et al., 2010; Zhao et al., 2014; Reepmeyer et al., 2004). Performance of a more rigorous optimization necessitates the use of simpler models that can capture the startup/shutdown dynamics, and yet be amenable for online implementation. One of the contributions of the present work is the recognition of the startup/shutdown process as a batch like process that opens up the possibility of adapting data-driven batch modeling techniques to identify models that capture the startup process dynamics reasonably well, and yet are not too computationally complex.

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While a variety of a data-driven modeling techniques exist for modeling and control of batch processes, not all of these are suitable for the problem at hand. One approach that has found wide variety of applications is partial least squares (PLS), which models the process in a projected latent space (Flores-Cerrillo and MacGregor, 2002). PLS models are in essence time-varying linear models, linearized around mean past trajectories, and thus require the batches to be of same length, or to find an appropriate alignment variable. As indicated earlier, the inherent variabilities of the startup procedure do not result in startups of equal length.

In one recently proposed approach (Aumi et al., 2013) the models were based on the 'current measurements' of the process instead of the 'time'. These developments were followed by contributions in the area of integration of these data-driven models with model predictive control formulations (Aumi and Mhaskar, 2012; Aumi et al., 2013). More recently a subspace identification based batch control approach was proposed in Corbett and Mhaskar (2016) where an LTI state-space model of the batch process is identified, and does not require the training batches to be of equal length. The problem of optimizing hydrogen startups thus stands to gain from these recent results. Note that while the approach in Corbett and Mhaskar (2016) has subsequently been adapted to detailed simulations of an electric arc furnace (Rashid et al., 2016) and particle size distribution (PSD) control (Garg and Mhaskar, in press), it has not been applied yet on a process of the present complexity, using real data, and to model startups.

Motivated by these considerations, in this work we address the problem of determining a data driven model for the startup of a hydrogen plant. The paper is organized as follows. First necessary background on hydrogen production process and system identification are presented in Section 2. Section 3 presents the modifications necessary to adapt a detailed first principles model in UniSim design to enable simulating the startup and shutdown phase. Although the primary focus of the proposed approach is to identify reduced order data-driven model of the process, the development of a detailed first principles model serves two key purposes. Firstly, it enables the generation of startup and shutdown (simulated) data of the process which can be used to test/develop the data-driven modeling approach. Secondly, a detailed simulator capable of mimicking the startup/shutdown can serve as a good analysis tool for control practitioners. Before implementing subspace identification methods to identify a reduced order linear time-invariant model of the process, the suitability of a linear model to explain the dynamics of a finite duration nonlinear process is illustrated through simulations in Section 4.1. Then, an LTI data-driven model of the process using subspace identification based method is identified in Section 4.2. Simulation results illustrate the prediction capabilities of the identified model validated against the detailed first principles simulation model. Next, the approach is implemented on data collected from a Praxair hydrogen unit, and validated in Section 4.3. Finally, a few concluding remarks are presented in Section 5.

2. Preliminaries

This section presents an overview of the hydrogen production process, and subspace identification approaches.

2.1. Process description

Hydrogen is commercially manufactured by steam methane reforming, where natural gas (NG) and superheated steam are fed to a chemical reactor called reformer, which consists of catalyst tubes filled with nickel reforming catalyst as depicted in Fig. 1. Natural gas is first purified by removing any liquid that may have condensed

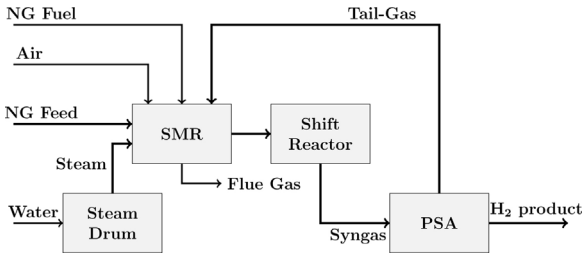

Fig. 1. A schematic of the hydrogen production process.

due to low ambient temperature. It is then split into two streams. Most of the natural gas is compressed as the feed to the reformer. A small amount is used as fuel to provide heat for the reformer. The steam is produced from water by a steam system in the heat recovery block. The NG feed stream is heated using downstream process heat and further processed by removing any unfavorable compounds to the reformer catalyst. Under normal conditions, the pressure of the NG fuel is controlled by an upstream valve, and the flow rate of the NG fuel is controlled by a downstream valve. The majority of the hydrogen is produced in the reformer through the following chemical reactions:

$$C_xH_y + xH_2O \rightleftarrows xCO + \left(x + \frac{y}{2}\right) H_2 \quad (1)$$

$$CO + H_2O \rightleftarrows CO_2 + H_2 \quad (2)$$

Reaction (1) is known as reforming and Reaction (2) is also called shift conversion. Both the reactions are reversible. The overall reaction is endothermic. Reformer exit temperature (RET) is an important process variable for this process and is expected to be kept at a specific value by heating the reformer. This heat is provided by burning the off-gas from the pressure swing adsorber (PSA) and NG fuel stream. The NG fuel stream is used to regulate the reformer exit temperature under nominal operating scenarios. Moreover, the temperature is affected by the flow rates of the combustion air and the superheated steam.

The reformer effluent process gas passes through a reactor, where additional hydrogen is produced by shifting most of the carbon monoxide in the process gas to carbon dioxide and hydrogen through Reaction (2). The reactor effluent stream then passes through the heat recovery and is sent to the PSA, where the hydrogen is produced. The PSA process is based on the physical adsorption phenomena. High volatile compounds with low polarity such as hydrogen are practically non-adsorbable compared to water, nitrogen, carbon monoxide, ammonia, methane, sulfur compounds and hydrocarbons. Most of the impurities in the gas can be selectively adsorbed, resulting in high purity hydrogen. During normal operation, the off-gas out of the PSA is used as the primary fuel that provides heat for the reformer.

The combustion heat resulting from the ignition of air and fuel in burners heat the reformer tubes. A fan is used to supply air to the burners and another one draws the combustion products, which are termed flue gas, out of the reformer firebox. The firebox pressure should not reach its lower and upper limits for safety. If the pressure is too low, the fire can be extinguished. If it is too high, it may impose safety hazards to facility and personnel. The pressure is controlled by adjusting the position of the suction louvers of Fan 2. As the louvers open, the fan draws more flow, resulting in a lower pressure. Conversely, as the louvers close, the fan draws less flow to increase the pressure.

The focus of the present work is modeling of the startup process. A typical startup involves ramping the natural gas fuel to reach a sufficient reformer exit temperature, introduction of natural gas feed and steam, regulation of nitrogen flow in the reactor tubes. It also requires making discrete decisions such as starting up the