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Multi-resolution model of an industrial hydrogen plant for plantwide operational optimization with non-uniform steam-methane reformer temperature field

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ABSTRACT

Hydrogen is consumed in large quantities in the chemical industry. The most common industrial process for hydrogen production is steam-methane reforming, which is carried out using an energy-intensive furnace. The plant energy efficiency depends strongly on the spatial temperature distribution within the furnace; the narrower the distribution, the higher the efficiency that can be achieved. However, currently available studies on plantwide optimization of hydrogen plants ignore this crucial aspect. Adequate resolution of the spatial temperature distribution is necessary to determine the furnace operating temperature, which, in turn, determines the plant efficiency. In this work, a multi-resolution model of a hydrogen plant is developed. It includes a high-resolution model of the furnace, and low-resolution models, adequate for the purpose of plantwide optimization, of other unit operations. The developed model is used to determine the optimal process conditions after furnace temperature homogenization as part of a plant start-up or setpoint changeover procedure.

1. Introduction

Hydrogen (H_2) is an important chemical that is used in many catalytic processes for the synthesis of commodity chemicals such as methanol and ammonia. It is also consumed in large amounts for processing crude oil in refineries. The recent trend of increasingly sour (high sulfur content) crude oil feedstocks, stringent petroleum product specifications and environmental regulations, and greater demand for ammonia-based fertilizers imply that demand for H_2 will continue to rise (Olivieri and Vegliò, 2008). The bulk (~80%) of the H_2 consumed in these industries is provided by steam reforming of natural gas (Simpson and Lutz, 2007) and a typical modern reforming-based plant of capacity 112,000 N m^3/h (100 MMSCFD) of H_2 consumes a substantial amount (~10^5 GJ/day or ~10^{14} BTU/day) of energy (Peng, 2012). For a plant of this capacity, operating savings of up to $600,000/year can be realized from a 1% increase in energy efficiency (Latham et al., 2011). Consequently, it becomes imperative to operate such plants as efficiently as possible in the face of increasing global competition and regulatory constraints.

Fig. 1 shows the process flowsheet of a reforming-based H_2 plant, where the endothermic reforming reactions take place inside hundreds of catalyst-packed reformer tubes placed vertically in a physically large-scale refractory-lined furnace, also called steam-methane reformer (SMR), and separation of high-purity H_2 product is accomplished through pressure swing adsorption (PSA). The widespread use of this process can be attributed to its high theoretical energy efficiency (energy content of H_2 product per unit energy consumed); typical commercial plants are designed for 80–90% thermal efficiency (Peng, 2012) and through elaborate heat recovery, the efficiency may approach 95% (Dybkjær, 1995). However, many H_2 plants operate below their design efficiencies due to the non-ideal behavior of some process units, observed during plant operations but not explicitly accounted for during the design calculations or during operational optimization. The key to achieving further efficiency improvements lies in minimizing these non-idealities through use of advanced sensors and model-based optimization. Specifically, in a H_2 plant, a key non-ideality is the distribution of the wall temperatures of the reformer tubes. While the temperatures of the tube walls increase, inevitably, along the length of each tube (downwards), in an ideal scenario, the axial tube temperature profile in the furnace is the same, i.e., at a given axial position (furnace height), the tube wall temperatures (TWTs) for all the tubes would be identical. However, in practice, the difference between the maximum and minimum tube wall temperatures at a given axial position (height) varies between 30 K and 110 K (Slavejkov et al., 2006; Kumar et al., 2016b). TWTs along the tube lie in the range of 900–1200 K. Axial temperature

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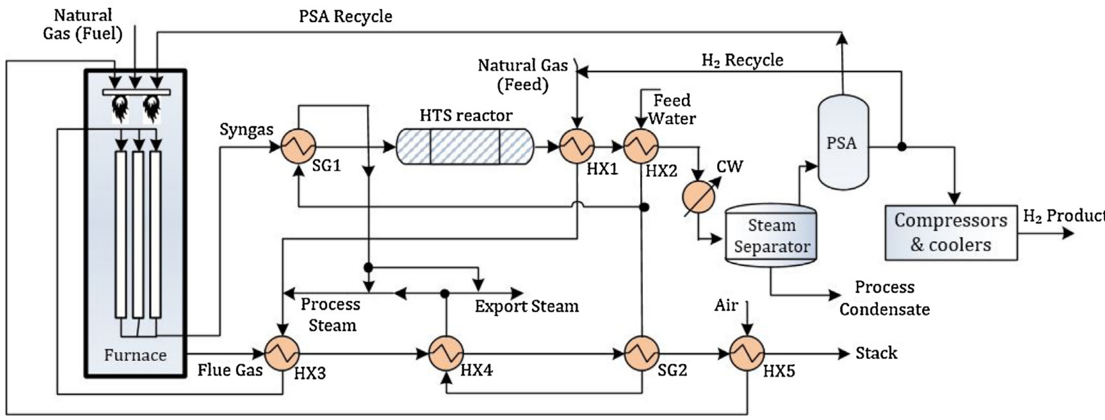

Fig. 1. Schematic of a reforming-based hydrogen production plant.

Adapted from Esposito and Dadebo (2011).

discrepancies place a limit on the maximum furnace operating temperature, which affects the overall energy efficiency of the plant. The need for uniformity in the axial TWT profile can also be seen from the perspective of the process intensification principle that states that to ensure maximum operation efficiency of a process, the entire feedstock should be processed in a consistent way (Van Gerven and Stankiewicz, 2009). In an SMR this translates into maintaining an axially uniform TWT within the furnace (i.e., making sure that the tube temperatures at a given height are the same). The relationship between TWT distribution and the plant energy efficiency is discussed in detail later in the paper.

In this work, we provide a methodology for the inclusion of the SMR TWT distribution in the flowsheet optimization of the H_2 plant to determine the optimal values of the plant inputs (manipulated variables) that maximize the plant thermal efficiency. An application of the TWT distribution-aware H_2 plant model for flowsheet optimization after furnace temperature homogenization is presented.

While the above arguments show that it is crucial to adequately model the SMR TWT distribution in an integrated H_2 plant model that is used for plantwide optimization, TWT distribution modeling has been neglected in the literature on H_2 plant and SMR modeling. This can be attributed, apart from the numerical challenges associated with solving the detailed-furnace-based H_2 plant models, to the difficulty of obtaining furnace-wide TWT distribution measurements. Common industrial practice is to use thermocouples or hand-held pyrometers to record TWTs of a few tubes. While installing thermocouples on all the tubes is economically prohibitive, pyrometer-based manual measurement is labor-intensive and prone to errors. Moreover, a correct measurement of the maximum TWT cannot be guaranteed with these devices. To tackle the issue of the TWT distribution measurement, an array of high-precision infrared cameras was installed around the furnace of a real commercial H_2 plant testbed studied in this work. Leveraging the distributed TWT measurements from the cameras, in our previous work, we reported on the usage of data-driven SMR models for real-time temperature homogenization of a simulated SMR (CFD model) (Kumar et al., 2015) and an experimental implementation in the industrial testbed plant (Kumar et al., 2016b). A 44% reduction in the TWT non-uniformity was demonstrated experimentally for the industrial system. Recently, we also demonstrated the feasibility of using a high-resolution physics-based furnace model, capable of resolving the spatial TWT distribution, for furnace temperature optimization (Kumar et al., 2017). Based on favorable computational time, provision of convenient update of model parameters, and prediction capability over a diverse range of furnace operating conditions, the use of the physics-based furnace model was recommended over the data-driven models for furnace temperature homogenization.

In this work, the high-resolution physics-based SMR model is integrated into a complete H_2 plant model and an explicit study of the plantwide benefits of optimization of TWT distribution is provided. This work is also a demonstration of the Smart Manufacturing (SM) paradigm (Davis et al., 2012) wherein greater adoption of advanced sensor-based modeling and data analytics, and cyber-infrastructure in manufacturing plants drives the next generation of innovation for attaining higher operation efficiency. The reader is referred to Korambath et al. (2014, 2016), Davis et al. (2015), and Kumar et al. (2015) for a detailed description of the SM framework and the IT-related details of adaptation of SM to the H_2 plant testbed.

The paper is structured as follows. In the next section a literature review on modeling of hydrogen plants and SMR furnaces is provided. Next, the H_2 plant flowsheet is described followed by a description of the SMR furnace and of the TWT distribution problem. Then, the mathematical models of the units of the H_2 plant and the numerical techniques employed to solve them are provided. Base plant conditions and the results of application of a TWT optimization scheme are presented followed by a study of the impact of variations in plant variables on the TWT distribution. Finally the plantwide optimization scheme is shown and the corresponding results are presented.

We dedicate this paper to Professor Rafiqul Gani in recognition of his inspirational contributions in process design and optimization.

2. Literature review

2.1. Modeling and optimization of hydrogen plants

Incorporation of high-resolution, detailed modeling of spatially distributed process units provides a more realistic estimate of the optimal performance of a chemical plant, as shown by Pattison et al. (2016). In the case of the SMR plant, process units that do not show significant spatially distributed profile such as the heat exchangers and the steam separator can be justifiably treated as a low-resolution lumped system. This suggests the need of a multi-resolution model of a H_2 plant that includes a high-resolution model of the furnace, and low-resolution models, adequate for the purpose of plantwide optimization, of other unit operations of the plant. However, no such work is available in the current literature. Oh et al. (2001) and Rajesh et al. (2001) have studied the trade-offs between maximization of H_2 product and export steam for a fixed feed of natural gas into the reformer tubes. However, a detailed