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CFD modeling and control of a steam methane reforming reactor

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HIGHLIGHTS

- Computational fluid dynamics modeling of steam methane reforming reactor.
- Model calibration and comparison with industrial plant data.
- Integration of computational fluid dynamics modeling and boundary feedback control.
- The use of feedback control improves closed-loop dynamics and feed disturbance rejection.

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ABSTRACT

This work initially focuses on developing a computational fluid dynamics (CFD) model of an industrial-scale steam methane reforming reactor (reforming tube) used to produce hydrogen. Subsequently, we design and evaluate three different feedback control schemes to drive the area-weighted average hydrogen mole fraction measured at the reforming tube outlet ($\bar{x}_{H_2}^{outlet}$) to a desired set-point value ($\bar{x}_{H_2}^{set}$) under the influence of a tube-side feed disturbance. Specifically, a CFD model of an industrial-scale reforming tube is developed in ANSYS Fluent with realistic geometry characteristics to simulate the transport and chemical reaction phenomena with approximate representation of the catalyst packing. Then, to realize the real-time regulation of the hydrogen production, the manipulated input and controlled output are chosen to be the outer reforming tube wall temperature profile and $\bar{x}_{H_2}^{outlet}$ respectively. On the problem of feedback control, a proportional (P) control scheme, a proportional-integral (PI) control scheme and a control scheme combining dynamic optimization and integral feedback control to generate the outer reforming tube wall temperature profile based on $\bar{x}_{H_2}^{set}$ are designed and integrated into real-time CFD simulation of the reforming tube to track $\bar{x}_{H_2}^{set}$. The CFD simulation results demonstrated that feedback control schemes can drive the value of $\bar{x}_{H_2}^{outlet}$ toward $\bar{x}_{H_2}^{set}$ in the presence of a tube-side feed disturbance and can significantly improve the process dynamics compared to the dynamics under open-loop control.

1. Introduction

The steam methane reforming (SMR) process, which produces bulk hydrogen gas from methane through catalytic reactions, is the most common commercial method for industrial hydrogen production. A general industrial-scale SMR process can be described by the schematic of Fig. 1. The steam methane reformer (for simplicity, it is denoted as "reformer" in the following text) is the core unit in a SMR process which has a process (tube) side and a furnace side that interact through heat exchange through the walls of reforming reactors (for simplicity, they are denoted as the "reforming tubes"). In the furnace side, combustion of the furnace-side feed, usually a mixture of methane, hydrogen, carbon dioxide, carbon monoxide and air, heats the reforming tubes via radiative heat exchange; inside the reforming tubes, catalytic reactions take place, converting steam and methane into hydrogen and carbon oxides (including CO and CO_2). A traditional top-fired, co-current furnace usually includes top burners which are fed with the furnace-side feed, refractory walls enveloping the combustion products, flue gas tunnels transporting the flue gas out of the reformer, and reforming tubes.

For the last 50 years, extensive work has been performed on

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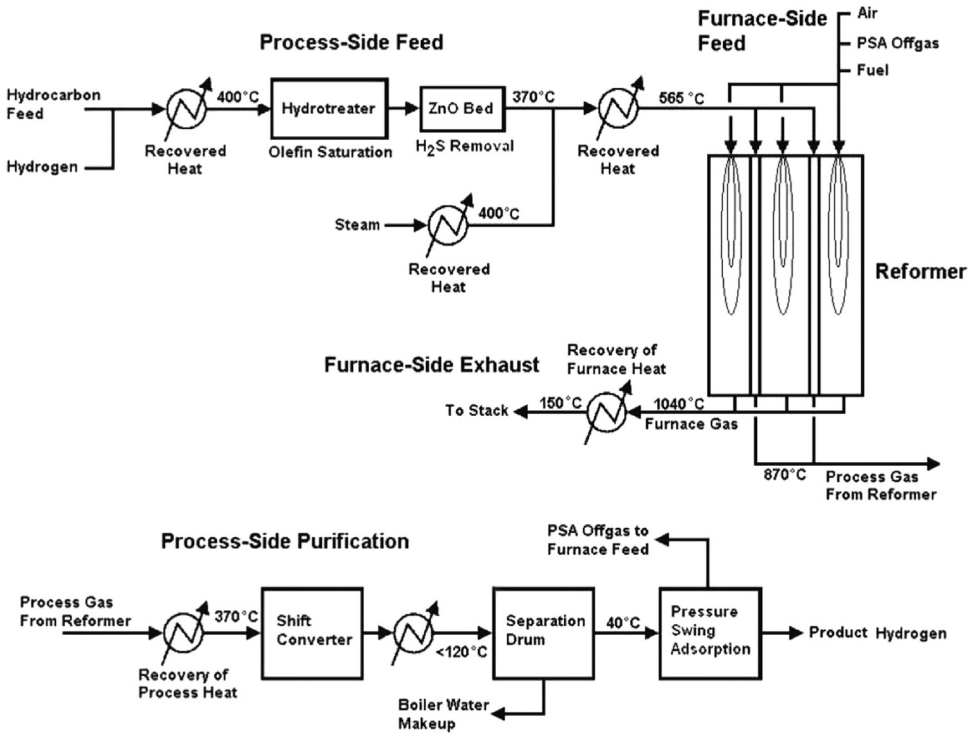

Fig. 1. Steam methane reforming process diagram (Othmer).

the development of first-principles reformer models. The mathematical modeling methodology of the complete reformer was first proposed and developed in the 1960s (McGreavy and Newmann, 1969). With the improved understanding of both physical and chemical phenomena inside the reformer, more comprehensive mathematical models have been developed considering more detailed and precise radiation mechanisms, combustion models, flue gas flow patterns, SMR reaction kinetics and packed bed reactor models (Latham, 2008). However, solving these complete reformer models is computationally expensive due to the increasing complexity of the fundamental nonlinear partial differential equations describing reformer physico-chemical phenomena. Also, for large reformers with complicated geometry, the geometry characteristics and various boundary conditions (Latham, 2008) make mathematical modeling very difficult.

On the other hand, with the dramatic increase of computing power, computational fluid dynamics (CFD) modeling has become an increasingly important platform for reformer modeling and design, combining physical and chemical models with detailed representation of the reformer geometry. When compared with first-principles modeling, CFD is a modeling technique with powerful visualization capabilities to deal with various geometry characteristics and boundary conditions. Moreover, CFD modeling provides flexibility to modify design parameters without the expense of hardware changes which brings large economic and time savings (Uriz et al., 2013). CFD technology has been successful in carrying out the simulation of industrial furnaces (Baburić et al., 2005; Han et al., 2006; Stefanidis et al., 2006; Noor et al., 2013) and SMR tube reactors, i.e., reforming tubes modeled as packed-bed reactors (Calis et al., 2001; Behnam et al., 2012; Dixon, 2014; Guardo et al., 2004). Specifically, recent attempts to use CFD modeling to characterize the physico-chemical phenomena of transport and reaction processes inside reforming tubes have been done exclusively on a microscopic or bench-scale level, e.g., the effect of catalyst orientation on catalytic performance is investigated with a CFD model of a single catalyst particle (Dixon, 2014), and the validation of CFD simulation results to experimental data is performed with a CFD model of a bench-scale reforming tube (Behnam et al., 2012). In the present work, we focus on an industrial-scale reforming tube, i.e., the external diameter, internal diameter and exposed length of the reforming tube are 14.6 cm, 12.6 cm and 12.5 m respectively. It is noteworthy that the CFD model of the industrial-scale reforming tube in this work is developed based on a unit currently employed in a commercial plant. Therefore, the CFD model has the geometry characteristics of an industrial-scale reforming tube, i.e., the length and inner and outer tube radii, includes an industrially relevant representation of the catalyst network, and incorporates appropriate boundary conditions including the reforming tube outer wall temperature and tube-side feed conditions. A major purpose of the CFD modeling in this work, in addition to its purpose as a means for evaluating various control strategies, is to propose a method of industrial reforming tube modeling with considerable modeling accuracy that can help evaluate various modeling assumptions usually employed.

The production rate of hydrogen fuel from a typical SMR process strongly depends on the operating temperature of the furnace, where the aforementioned reforming tubes are encapsulated, and more specifically the outer reforming tube wall temperature. Because of the endothermic nature of SMR reactions, a higher outer reforming tube wall temperature theoretically results in a higher production rate of hydrogen fuel. On the other hand, operating the reforming tubes at excessively high temperature can lead to disastrous consequences and significant capital loss. Particularly, the formation of carbon on the catalyst surface and on the inner reforming tube surface prevents the reactants from entering the catalyst active sites and reduces the rate of heat transfer to the tube-side gas mixture respectively. As a result, the reaction progress and hydrogen production might be disrupted. Additionally, the expected lifetime of reforming tubes is extremely sensitive to changes in operating temperatures, i.e., an increase in tube wall temperature of 20 K can reduce the tube lifetime by half (Pantoleontos et al., 2012; Latham, 2008). Moreover, reforming tubes are one of the most expensive plant