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A large-scale benchmark for the CFD modeling of non-catalytic reforming of natural gas based on the Freiberg test plant HP POX

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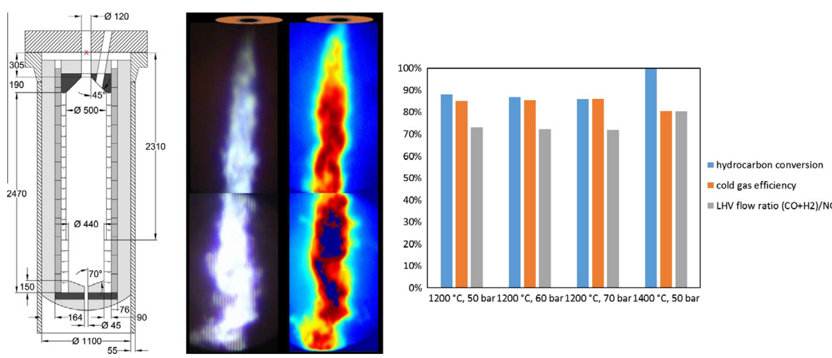
HIGHLIGHTS

- Natural gas reforming at high pressures and temperatures was studied experimentally.
- A semi-industrial test plant with comprehensive instrumentation was used.
- A new optical system allows the flame zone to be studied directly.
- Measurements were carried out at different pressures and temperatures.
- The data set provides a challenging benchmark for numerical modeling.

GRAPHICAL ABSTRACT



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ABSTRACT

The non-catalytic reforming of natural gas to syngas was studied with test runs at the semi-industrial scale test plant HP POX. The product gas composition, and gas and wall temperatures across the reactor were considered at 50, 60 and 70 bar(g), while the reactor temperature was varied between 1200 and 1400 °C. In addition, the flame structure was studied using optical measurements. The experiment was designed to provide a challenging benchmark for numerical modeling. For that reason, the reactor geometry, boundary conditions, and the experimental data are provided in such a way that the results can easily be reproduced using CFD.

1. Introduction

Non-catalytic reforming via partial oxidation is one promising technology for the production of syngas from natural gas or other gaseous or liquid feedstocks. Due to high process temperatures and pressures, the access to the reaction chamber of the gasifier for measuring e.g. temperatures and gas composition is typically limited. In addition, industrial plants are large-scale facilities with a thermal capacity in the range of between 300 and 1000 MW, which are normally not equipped with instrumentation for process analysis. This is one of the reasons why numerical models have become more and more attractive in recent years to gain a deeper understanding of the physical processes in such systems.

The modeling approach for high-pressure, high-temperature gasifiers is based on kinetic models (see e.g. [1–7]) on the one hand, or on multi-dimensional CFD models [7–12] on the other hand. While the kinetic models provides a fast analysis of the reactor's

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basic characteristics, CFD can provide more specific information about the multi-dimensional flow, species and temperature distributions. The CFD approach requires more information about the reactor, for example the detailed geometries of the reactor chamber and the burner as well as the complete mass and energy balance.

At high pressures and temperatures, several physical phenomena influence the partial oxidation characteristics, such as radiation or turbulence-chemistry interaction. For that reason, a validation of the CFD model is necessary. Obviously, the validation of the numerical model should be performed by the use of results from high-pressure, high-temperature test runs that are close to the operating conditions of large-scale facilities.

In the literature, experimental results are mainly available for lab-scale systems, and are limited in terms of operating temperature or pressure, see e.g. [13–17]. For large-scale facilities, most of the experimental data cannot be reproduced due to restrictions concerning operating data or reactor details. One exception is the work of Guo et al. [10], where detailed information is provided about the reactor geometry. Nevertheless, the experimental data available for large-scale facilities are mostly limited to data on the outlet gas compositions, with a lack of data about the flame structure or the temperature distribution inside the reactor.

To overcome this limitation, experimental data sets for the high-pressure, high-temperature gasification were obtained from test runs in the HP-POX test plant at the TU Bergakademie Freiberg. The HP POX is a semi-industrial test facility with comprehensive instrumentation, including a novel optical system for the direct investigation of the flame zone (see Section 2.1).

In order to provide a general validation case for the numerical modeling of partial oxidation processes under high-pressure, high-temperature conditions, and on length-scales that are relevant for industrial processes, new HP-POX test runs were carried out based on a modified geometry, and comprehensive measurements were involved. For example, the gas temperature was monitored along the reactor, and the outer wall temperature was determined at several positions on the reactor wall. In addition, the flame temperature and shape were observed using the optical probe system Optisos®. Gas compositions at the outlet were provided, and were cross-checked using hot-gas probes, taken at a position inside the reactor chamber, but close to the reactor outlet.

The experiments were performed at pressures between 50 and 70 bar(g), and at 1200 and 1400 °C. At some of these operating conditions the gas composition at the reactor outlet is far away from the thermo-chemical equilibrium, which is a more challenging benchmark of the numerical model used. Since the experiments were conducted as part of the Virtuhcon research project at TU Bergakademie Freiberg, the new results were named the 'Virtuhcon test case'.

This manuscript is structured as follows: in Section 2 the general experimental setup is discussed along with the different measuring systems. Afterward, the specifics and experimental results of the test case are presented in Section 3.

2. Experimental setup

2.1. The HP-POX test plant

The semi-industrial test plant HP POX was designed and erected by Lurgi GmbH (now a part of the Air Liquide group) at the IEC (Institute of Energy Process Engineering and Chemical Engineering, TU Bergakademie Freiberg). Since 2004, the plant has been operated by IEC's technical and scientific staff, predominantly in week-long test campaigns. Due to its special design and modifiable reactor geometry, the test plant allows test programs to be carried out for the high-pressure autothermal non-catalytic reforming of natural gas (Gas-POX), the high-pressure autothermal catalytic reforming of natural gas (ATR), and the high-pressure gasification of liquid feeds such as fuel oil and heavier residues. More than 8000 h of test operation have been achieved in the last ten years.

One field of research involving the HP POX dealt with the increase in the operating pressure of the syngas production, which results in several benefits, such as a higher specific throughput and lower compression effort for downstream processes. The compositions of raw gas and trace compounds were studied depending on various operational parameters, such as the residence time, steam/carbon ratio, gasification temperature and pressure [6,18].

The core part of the test plant is the gasification reactor. The reactor is equipped with a top-mounted multi-channel burner. Individual burners are designed for various process conditions and feedstock. There are specific requirements concerning the feedstock supply due to the high operating pressures and temperatures: natural gas is provided at 12 bar(g) from the gas pipeline and may be compressed to at most 113 bar(g) and preheated to 380 °C (Gas-POX) or 620 °C (ATR). Process steam (at most 115 bar(g), 400 °C) is generated from deionized water using a high-pressure steam boiler. Oxygen is stored in a liquid state and has to be pumped, vaporized and preheated using a steam-driven heat exchanger (O_2 parameters: at most 110 bar(g), 280 °C – dependent on steam pressure). Liquid feedstock is supplied from thermo-stated tanks (storage temperature at most 160 °C) and may be further preheated in order to decrease viscosity.

The feedstock is processed with oxygen and steam at temperatures of up to 1450 °C and pressures of up to 100 bar(g). At first, oxygen, steam and e.g. natural gas (mainly methane) are fed into the reactor by means of the burner. The conversion of natural gas begins in a non-premixed turbulent flame in the upper free space of the reactor. The conversion of the feedstock is completed in a subsequent post-flame zone. The flame zone is characterized by lean and rich mixtures of oxygen and methane which are closely located to each other. Temperature peaks of above 3000 °C occur due to the local stoichiometric combustion of methane to water steam and carbon dioxide [11]. The subsequent endothermic reforming reactions and the superposed mixing processes reduce the average gas temperature to a range from 1400 to 1000 °C. This represents the reactor exit temperature, and the temperature range varies depending on the operating conditions. The general scheme of the reactor is illustrated in Fig. 1.

In the ATR mode, the reaction chamber is partially filled with common reforming catalysts. In the Gas-POX and oil gasification mode, the volume of the empty reaction chamber (approximately 0.455 m^3) can be reduced using additional refractory bricks (down to a minimum of approximately 0.066 m^3).

The raw gas leaving the reactor is rapidly quench-cooled with water. In the HP-POX plant the reaction chamber and the quenching chamber are placed together in one pressure vessel. It's overall dimensions including the quench chamber comprise a height of 6.25 m, and a diameter of 1.5 m. It should be noted that in industrial applications a waste heat boiler for steam generation instead of a quench is installed. Downstream of the gas sampling and measurement, the product synthesis gas is flared at the flue gas chimney.

The plant has a maximum thermal capacity of 5 MW (corresponding to at most 500 Sm^3/h natural gas, or 500 kg/h liquid feed), and generates up to 1500 Sm^3/h synthesis gas. The equipment allows for the variation of process parameters (pressure, temperature, quenching temperature) exceeding the range commonly employed in industrial practice.

2.2. Measuring systems

Beside the control equipment, the plant is also fitted out with sample points and analysis equipment at various locations. As