



3D numerical study of the performance of different burner concepts for the high-pressure non-catalytic natural gas reforming based on the Freiberg semi-industrial test facility HP POX



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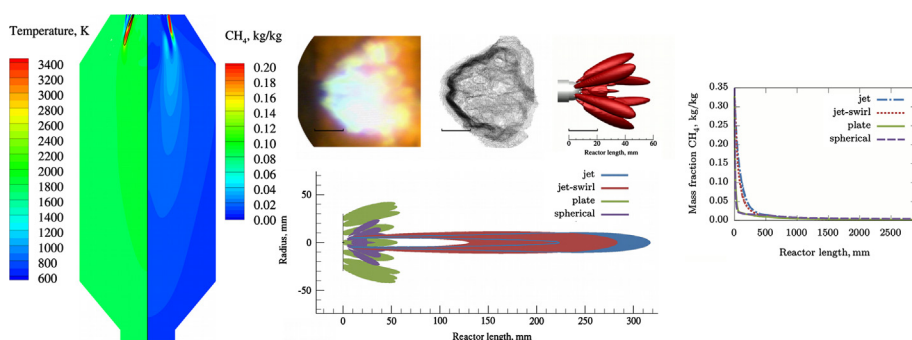
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HIGHLIGHTS

- Numerically and experimental investigations of different HP POX burner concepts.
- Validation of the CFD setup using optical measurements of the flame structure.
- Validation of the CFD setup using global outlet conditions.
- 2D and 3D numerical study of different burner concepts.
- New burner concepts show a potential for improving the reactor performance.

GRAPHICAL ABSTRACT



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ABSTRACT

In this work, new test burner concepts for the non-catalytic partial oxidation of natural gas are evaluated using numerical modeling. The 3D CFD model for reactive flow calculations incorporates a detailed reaction mechanism containing 28 species and 112 reactions, and is extensively validated against data obtained in the semi-industrial test facility HP POX in Freiberg. The validation cases operate at 61 bar (a) and outlet temperatures of approximately 1688 K. The CFD models demonstrate that the optimized burner concepts result in a significantly higher natural gas conversion rate, which allows for a more compact reactor design or, alternatively, for a higher throughput in existing industrial facilities. In addition, the final burner concepts are tested experimentally. Optical measurements demonstrate that the CFD model is capable of reproducing the complex 3D flame structures and reliably predicting the overall performance of the reactor.

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1. Introduction

Three different types of natural gas reforming processes are in use today: allothermal catalytic reforming (steam reforming), non-catalytic partial oxidation, and autothermal catalytic reforming (ATR). Until today, the reforming of natural gas has been

dominated by steam reforming. The increasing expenses for catalysts, a transition to more feedstock flexibility, and higher plant capacities are leading to a growing interest in non-catalytic processes such as partial oxidation. Further efforts are needed to increase the throughput of the process, to reduce the capital expenditure for new facilities, and to increase the product stream quality in order to reduce the downstream gas treatment.

Technology developments can be based either on experimental or on numerical studies. Most experimental studies of gaseous

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partial oxidation are carried out to investigate specific physical phenomena in lab-scale units, see [1–3]. The disadvantage here is that the experiments are not capable of fully reproducing the real conditions in industrial-scale facilities, and therefore they cannot be used for testing new components or new concepts. On the other hand, due to the high costs only a limited number of pilot- or industrial-scale plants are available for experiments and most of them cannot be used for specific technology improvements. Li et al., for example, introduced a 300 kW hot coke oven gasifier with detailed internal temperature measurements and an outlet composition for ambient pressure operation conditions [4]. Xu et al. presented data of a large scale 125 MW high pressure partial oxidation (HP POX) system operating at 54 bar(a) [5]. Recently, Richter et al. introduced the Virtuhcon benchmark for computational fluid dynamics (CFD) modeling, based on several measurements at the 5 MW semi-industrial test facility HP POX in Freiberg [6]. The advantage of the HP POX plant is its flexibility, which allows the testing of different reactor and burner geometries.

Alternatively, numerical models offer a fast, cost-efficient way to analyze reactive systems, which is the basis for accelerated technology developments, also known as rapid prototyping. Depending on the level of detail, the models are based on idealized assumptions, which are not capable of fully reflecting the real physical process. Modeling strategies are based on simplified 0D/1D or on more sophisticated 2D and 3D CFD models. Examples of 0D and 1D approaches are given in [7–11]. Comparisons of such models with experimental data indicate that deviations of several mole percent are feasible and only rudimentary information on distributions are available. One advantage of these approaches is that the quality of a chosen reactor configuration can be assessed quickly including tests of different chemical kinetics.

If the focus is on developing new burner designs or more complex reactor geometries, 2D or 3D CFD calculations are necessary to estimate the complex interaction between fluid mechanics, turbulent mixing, and chemical reactions in the reactor. The turbulence chemistry interaction and the homogeneous reaction mechanism are especially significant for reliable CFD modeling, and are intensively discussed in literature. For instance, Vascellari et al. [12], Xu et al. [5] and Guo et al. [13] used 2D axis symmetric CFD simulations in order to critically discuss the performance of two basic turbulence-chemistry interaction (TCI) concepts – the Eddy Dissipation Concept Model (EDC) and the class of presumed probability density function models (PDF) for modeling the non-catalytic reforming of natural gas. Xu et al. [5] demonstrated that both approaches reproduce the experimental data, if some criteria for mesh quality and the volume fraction constant for the EDC model are respected.

In this work, new experimental burner concepts for the non-catalytic reforming of natural gas were developed. All simulations are based on the same boundary conditions. The basic influence of the burner systems themselves regarding the reactor performance is in the focus of this work. This suffices for the question which burner performance best with the same fuel requirements. To do so, 2D and 3D CFD calculations were carried out, and two new burner designs were tested in the semi-industrial test facility HP POX in order to validate the numerical results. The present paper is structured in the following manner. In Sections 2 and 3, all boundary and model conditions are described, as well as the experimental data used to validate the numerical setup. A detailed analysis of the performance of different burner concepts is presented in Section 4.

2. Experimental HP POX configuration

The semi-industrial test plant HP POX, at the Institute of Energy Process Engineering and Chemical Engineering of the TU Ber-

gadamie Freiberg, has been operated since 2004 to study the high-pressure non-catalytic and catalytic reforming of natural gas, heavy oil and higher residuals.

Some features of the plant are the comprehensive instrumentation, an optical system for directly studying the flame zone, and a flexible reactor geometry. The reactor chamber height can be varied between 200 mm and 2300 mm, the reactor diameter can be adjusted between 125 mm and 250 mm, and different burner configurations can be applied. The maximum operating pressure is 101 bar(a), and the maximum reactor temperature at the outlet is 1770 K while the maximum temperature in the flame zone can exceed 3000 K. More detailed information can be found in Richter et al. [6].

2.1. Reactor geometry

The numerical studies in this work are based on selected test runs at the semi-industrial HP POX test plant. The used reactor geometry is given in Fig. 1. The difference to previous test runs (e.g. Ref. [6]) is a decreased reactor volume of 0.041 m³, with the aim of testing different burner concepts in a more compact reactor environment. The final reactor length is approximately 2.9 m, and the reactor diameter is 250 mm in the upper section, and 100 mm in the lower section.

2.2. Burner geometries

This work evaluates three different burner concepts for a non-premixed gas POX reactor system. One concept is a standard multichannel jet burner applied in several industrial systems. The two other burners are new concepts. For these new concepts, test burners specially designed for the semi-industrial test facility HP POX were produced. It should be noted that the designs for industrial-scale concept burners may differ in contrast to the HP POX rig designs, e.g. due to a different cooling system and piping. The geometric outline for the three burners are given in Fig. 2. The standard multichannel jet burner consists of an injection lance with two separated streams for oxygen and steam. The lance inlets are shielded by a gaseous, annular fuel stream. The normalized injection areas from in- to the outside are in the ratio of 1.0/0.352/1.168.

The spherical burner concept uses a different lance configuration than the jet burner, which premixes the oxidizer and steam flows. The oxygen/steam injection ports are located on a spherically formed tip which leads to a more areal distribution of the reactants from the axial central injection location. The lance streams are shielded in the similar manner as in the jet burner configuration, by a gaseous fuel stream. The injection nozzles are situated in the center and on two concentric circles on the burner tip equidistant with a nozzle count of 1/3/6. The opening angles of the two outer circles are tilted by 50° and 90° respectively.

The injection layout for the multichannel plate burner coincides with the jet and spherical burner concepts. Oxygen and steam are provided by the inner injection ports, respectively, and are shielded as well by the gaseous stream. They consist of equidistant annular tilted distributed holes with two different peripheral radii. The outer radius in respect to the inner radius is 1.48 times larger. In addition to the two streams in Fig. 2(c), a third stream for H₂O is located between those but just at four different peripheral locations. Both new concepts, the spherical and plate designs, follow a new strategy by using single injection ports to distribute the flame region over a greater volume.

2.3. Experimental boundary conditions

The performance of the jet and the spherical burners are tested using the semi-industrial test plant HP POX. The boundary condi-

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