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Numerical study of methane TPOX within a small scale Inert Porous Media based reformer

*Miguel A.A. Mendes**, *José M.C. Pereira*, *José C.F. Pereira*

Universidade de Lisboa, Instituto Superior Técnico, Mech. Eng. Dept., LASEF, Av. Rovisco Pais 1, 1049-001 Lisbon, Portugal

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ABSTRACT

Methane Thermal Partial Oxidation (TPOX) within a small scale Inert Porous Media (IPM) based reactor was investigated numerically in order to explore the operating conditions and possible procedures for maximizing the reforming efficiency and minimizing the soot formation. A quasi-1D model of the TPOX reactor was validated and further used to study the process. The model considers detailed chemistry and solves the energy balances for both gas and solid phases, including radiative heat transfer in the solid phase. The parametric results of the reactor operation show that the optimal air–fuel ratio is a compromise between soot formation and reforming efficiency. Moreover, a high preheating temperature of the reactants is found to be always beneficial for the process, and the effect of power input is negligible for the reforming efficiency. The numerical investigations also suggest that shorting the IPM length, as well as mixing small amounts of water vapor with the reactants, appear to be effective procedures for improving the operation performance of the TPOX reactor.

1. Introduction

Power generation from fossil fuels has been widely considered as one of the main contributors for global warming, while at the same time the reserves of these non-renewable energy sources are rapidly depleting worldwide. Therefore, there is an increasing interest in developing power generation systems based on clean and sustainable energy sources. However, around 80% of the total energy consumption in the world is based yet on fossil fuel reserves. Consequently, in order to gradually convert the actual power generation systems from conventional to renewable, a smooth transition is required to meet the actual energy demand [1].

Emerging power generation technologies, such as Solid-Oxide Fuel Cells (SOFCs), are particularly attractive, when compared to conventional technologies, due to their potential for efficient use of hydrocarbon fuels and reduced emissions. SOFCs present very high efficiencies at elevated working temperatures (500–1000 °C) being therefore attractive for use in commercial and industrial Combined Heat and Power (CHP) applications [2–4]. Although other fuel cell types, such as, Molten-Carbonate Fuel Cells (MCFCs) or High-Temperature Polymer Electrolyte Membrane Fuel Cells (HT-PEMFC), also present a great potential for CHP [5,6]. In addition, SOFCs are fuel flexible and are able to operate either on pure hydrogen or hydrocarbon fuels. Therefore, systems based on SOFC technology have the potential to provide a transition solution from fossil fuels to more clean and sustainable energy carriers, such as bio-fuels and hydrogen. However, SOFC operation directly on hydrocarbon fuels is very limited and fuel reforming processes are generally required in order to convert hydrocarbon

* *Corresponding author.*
E-mail addresses: miguel_a_mendes@hotmail.com, miguel.mendes@iwtt.tu-freiberg.de (M.A.A. Mendes).
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Nomenclature

$\dot{m}''$	axial mass flux, kg/m^2 s
A	reactor cross-sectional area, m^2
a_v	surface area to volume ratio, m^{-1}
C_p	specific heat capacity at constant pressure, J/kg K
d_p	characteristic pore dimension, m
h_k	enthalpy of k species, J/kg
H_v	volumetric convective heat transfer coefficient, W/m^3 K
k	thermal conductivity, W/m K
MW_k	molar weight of k species, kg/kmol
Nu	Nusselt number
Q_r	radiative heat flux, W/m^2
Q_w	wall heat loss per unit of length, W/m
Re	Reynolds number
T	temperature, K
t	time coordinate, s
u	axial mean velocity of gas phase, m/s
v_k	diffusion velocity of k species, m/s
x	axial coordinate, m
Y_k	mass fraction of k species

Greek symbols

β	solid extinction coefficient, m^{-1}
$\dot{\omega}_k$	production rate of k species, kmol/m^3 s
ϵ	solid emissivity
λ	mass ratio of air to fuel
μ	dynamic viscosity, kg/m s
ω	solid scattering albedo
ϕ	porosity
ρ	mass density, kg/m^3
τ	residence time, s

Subscript

g	gas phase
s	solid phase

fuels into synthesis-gas (consisting mainly of H_2 and CO) [7]. Owing to the carbon deposition and anode deactivation problems, external reforming is generally preferred over internal reforming, specially on practical small scale systems.

There are three main reforming technologies used for synthesis-gas production from liquid and gaseous hydrocarbon fuels: steam reforming, catalytic or thermal partial oxidation and autothermal reforming [8]. Among these, Thermal Partial Oxidation (TPOX) offers several advantages [9,10], such as: no need for external heat sources and additional feeds; absence of catalysts which eliminates the catalyst deactivation problems; good dynamic response; and hydrocarbon flexibility. However, at the same time it presents comparatively low hydrogen yield and tendency to produce soot.

Performing the TPOX within Inert Porous Media (IPM) based reformers is a practical solution to prevent flame stability problems, which are promoted by the slow reaction rates at low adiabatic flame temperatures existing in the TPOX process [11,12]. The high heat recirculation from the hot products to the reactants, provided by the solid matrix, originates local super-adiabatic combustion temperatures, which increase the reaction rates and the stability of the TPOX process improving its operational characteristics [12]. Comprehensive reviews on IPM combustion can be found in Refs. [13–15].

Several recent studies have investigated TPOX of hydrocarbons within IPM, and different techniques have been successfully applied in order to stabilize the reforming process, see, *e.g.*, Refs. [11,12,16–18]. Studies regarding transient TPOX within IPM can be found in Refs. [16,17]. These works applied the filtration combustion principle, which involves a traveling combustion wave freely propagating within a IPM, where the pore size of the solid matrix is typically sub-critical. Therefore, the IPM must be preheated to high temperatures in order to initialize the combustion wave propagation. On the other hand, stationary techniques for TPOX within IPM can be found in Refs. [11,12,18]. In these techniques, the combustion zone is steadily stabilized inside a porous matrix of supercritical pore size, and the nature of stabilization phenomenon is completely different from the one existing in transient approaches. In Ref. [18], experimental investigations of methane–air TPOX process within a small scale IPM based reformer were performed for different ranges of inlet temperature, power input and air–fuel ratio. The TPOX process was steadily stabilized by employing a reactor formed by a diffuser-like upstream section followed by a downstream cylindrical section, similar to the one presented in Ref. [12], and the IPM consisted of a packed bed of Al_2O_3 rings. Temperature profiles were measured along the reactor central axis, and concentrations of synthesis-gas species (H_2, CO, CO_2, CH_4, C_2H_2) were measured at the reactor outlet.

To the authors knowledge, there are no studies in the literature regarding the optimization of the TPOX process within IPM based reactors similar to the ones used in Refs. [12,18].

The objective of the present study is to investigate possible solutions in order to maximize the reforming efficiency and minimize the soot formation on the methane TPOX process within a small scale IPM based reactor. For this purpose a quasi-1D combustion model have been used, which was validated against the experimental results from Ref. [18]. The numerical model considers detailed chemical kinetics and solves the gas and solid phase energy balances, including radiative heat transport in the solid phase. With the help of this numerical model, a wide range of operating conditions as well as different procedures were explored in order to evaluate which conditions and procedures maximize the reforming efficiency and minimize the soot formation on this particular TPOX reactor.

The present paper is organized in the following form: First, the numerical model of the methane TPOX reactor is described. Further, simulation results are presented, including model validation, parametric study, and different procedures for improving the process. Finally, the main conclusions are summarized.

2. Numerical model

This section describes the numerical model used in order to simulate the methane TPOX process within a small scale IPM based reactor, experimentally tested in Ref. [18]. The TPOX