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# Numerical investigation on the wall-coated steam methane reformer improvement: Effects of catalyst layer patterns and metal foam insertion

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## ABSTRACT

In this paper, a numerical simulation of improving performances of catalyst wall-coated steam methane reformer for hydrogen production is presented. A comparative analysis of three different configurations of a parallel-plate reformer is carried out. A single catalyst layer of 10 mm length is adopted for the first configuration, while, for the second one, it is divided into five discrete uniform layers and impregnated alternately on the reformer's walls. For the third one, metal foam bounded by the discrete catalyst layers is inserted into the catalyst region. The effects of the catalyst-layer patterns and the metal foam insertion on the thermal behavior and the reaction kinetics are analyzed. The involved transport phenomena are governed by momentum, energy and species equations. The Darcy-Brinkman-Forchheimer model is used in the metal foam region while the Navier–Stokes equations are employed in the clear region. The obtained results show that this combination between the catalyst arrangement and the metal foam insertion, improves the steam methane reformer efficiency. The  $\text{CH}_4$  conversion rate improving is estimated to 44.6%.

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## Introduction

Most of the world's energy system is based on converting primary energy resources in other forms depending on their final use. In fact, since the eighteenth century, fossil fuels have been the driving force of the industrial development. However, these resources present two significant drawbacks. The first problem is their nonrenewable nature, so they will

irremediably run out. Second is that this dependency has negatively affected the environment because of the large emission of global warming gases and other pollutants. To address some of these issues, the interest in alternative renewable-energy resources and energy carriers has considerably grown. Nowadays, hydrogen is considered as a promising carrier of energy. It is produced almost exclusively from fossil fuels, through diverse processes [1], such as methane steam reforming (MSR) or catalytic partial oxidation (POX) of

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**Nomenclature**

A	pre-exponential factor
$A_{ij}$	function used in Eq. (21)
a, b	exponential indexes
$C_f$	inertial coefficient [–]
$C_p$	specific heat, [J kg <sup>-1</sup> K <sup>-1</sup> ]
D	mass diffusion, [mol m <sup>-2</sup> s <sup>-1</sup> ]
d	diameter, [m]
E	activation energy, [J mol <sup>-1</sup> ]
h	heat transfer coefficient, [W m <sup>-2</sup> K <sup>-1</sup> ]
$K_p$	permeability, [m <sup>-2</sup> ]
Le	Lewis number [–]
M	molar mass, [g mol <sup>-1</sup> ]
P	pressure [Pa]
$p_i$	partial pressure [Pa]
PPI	pores Per Inch [–]
R	reaction rate, [mol m <sup>-2</sup> s <sup>-1</sup> ]
$R_g$	universal gas constant, 8.314472 [J mol <sup>-1</sup> K <sup>-1</sup> ]
S	source term, [m <sup>-3</sup> ]
$S_i$	rate of chemical appearance and disappearance, [mol m <sup>-2</sup> s <sup>-1</sup> ]
T	temperature, [K, or °C]
u	axial velocity, [m s <sup>-1</sup> ]
v	transverse velocity, [m s <sup>-1</sup> ]
w	mass fraction [–]
x	axial coordinate [m]
y	transverse coordinate [m], Molar fraction [–]
$\Delta H^\circ_{298}$	standard enthalpy of formation, [J mol <sup>-1</sup> ]
$\Delta T$	temperature difference, [K, or °C]

**Greek symbols**

$\mu$	dynamic viscosity, [m <sup>-1</sup> kg s <sup>-1</sup> ]
$\rho$	fluid density, [kg m <sup>-3</sup> ]
$\epsilon$	porosity [–]
$\nu''$	stoichiometric coefficient of product species [–]
$\nu'$	stoichiometric coefficient of reactant species [–]
$\lambda$	thermal conductivity, [W m <sup>-1</sup> s <sup>-1</sup> ]

**Subscripts**

e	effective
f	fluid, fiber
g	gas
i, j	reactant and product components
Mix	mixture
p	pore
s	solid
w	wall
WGS	water gas shift

hydrocarbon-based fuels [2]. According to Abánades [3], the world's hydrogen production is provided almost by MSR of natural gas. For that purpose, remarkable efforts have been made during the last 20 years to understand and assess the sustainability related to safety, environmental impact and

overall efficiency of hydrogen production through this process. This fact has been confirmed by the high number of studies that focused on optimizing hydrogen production such as developing new reactors and catalysts [4].

Demand for “greener” energies has played an important role in developing systems which combine the use of hydrogen and electricity as clean energies, such as fuel cells (FC), and even more, micro combined heat and power (CHP) systems, which are based on FCs. These generators of the combined energy are a stationary FC system; they produce simultaneously heat and power in a single integrated system [5]. The main advantage of the micro-CHP systems is that the fuel energy is almost fully used. The use of such combined systems results in significant energy and fuel savings, as well as a substantial reduction of CO<sub>2</sub>. According to Liso et al. [6], better performance of the FC-based micro-CHP systems can be obtained by MSR, when compared to other processes such as POX.

To improve these promising systems, many researchers have focused on how to improve the fuel conversion processes. For MSR, one finds mainly two ways to generate the hydrogen: “Direct or indirect” internal reforming systems [7] [8], and the external reforming systems such as the steam methane reformers (SMR) [9]. For the latter way, the main goal of the process intensification is to provide FC stacks with the highest rates of H<sub>2</sub>, lowest carbon emissions, and to lower the unconverted synthesis gas at the SMR outlet. Lee et al. [10] studied numerically the effects of the combustion parameters on the performance of an FC reformer. Their results showed that the reforming performance can be optimized by adjusting the fuel and equivalence ratios. Ni Meng [11] studied numerically a compact reformer for hydrogen production. He conducted parametric simulations to investigate the effects of operating parameters such as porosity, temperature and the rate of the heat supply on the reformer performance.

Improving SMR by using of new configurations and optimal catalyst coating is also a way to increase its efficiency. Lee et al. [12] conducted experimental and numerical investigations of the thermal and mass behavior of an SMR. They proposed a new configuration of packed catalyst for hydrogen production. Their results showed that a bed packed repeatedly with inert and active catalysts is more efficient than a conventional SMR. De Jong et al. [13] analyzed numerically the heat and reaction kinetics processes into an SMR. They evaluated its performance for several configurations. Sigurdsson et al. [14] studied experimentally and numerically the flow distribution into a catalytic parallel-plate SMR. Their study revealed that flow maldistribution exists in the reformer stack. This maldistribution can be improved by increasing the pressure drop characteristics of the catalyst wire-mesh. Kim-Lohsoontorn et al. [15] studied a tubular solid oxide FC (SOFC) by modeling an indirect internal reformer. They proposed a novel catalytic annular-coated wall reformer and compared it with different designs, to determine the most efficient reformer. Dokamaingam et al. [16] modeled a SOFC with an indirect internal reforming process. They compared the catalytic coated-wall reformer with a conventional packed bed one. Their comparison showed that the coated-wall internal reformer gives a better efficiency and a fast methane conversion.

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