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# Numerical study on the effects of the macropatterned active surfaces on the wall-coated steam methane reformer performances

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## ABSTRACT

This paper deals with a numerical study on the steam methane reforming reaction performances into a wall-coated steam methane reformer (WC-SMR), intended to produce hydrogen. In this work a new catalytic pattern, purporting to enhance the WC-SMR efficiency, is proposed. A comparison study is made between the new inter-catalytic layers pattern and a conventional one with a continuous catalytic layer pattern. Both WC-SMR models operate at similar conditions and at the same design parameters, except the catalytic zone length which is monitored by taking into account the inter-catalytic layers spacing or not. Our results show that, by adopting a catalytic surface with an inter-catalytic spacing, the methane conversion could be enhanced and thus the hydrogen production is intensified.

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## Introduction

The high demand for energy in the world faces us with major challenges to achieve. One of the key challenges here is how to meet the growth in demand of energy supply while helping to protect the environment. This fact will force us to seek, in the near future, other energy sources than fossil fuels, or at least, to reduce their energetic dependency. Currently, the clean energy carriers and renewable sources take over gradually on the traditional sources such as coal and oil. According to the World Energy Outlook 2014 of the International Energy Agency

(IEA), the fossil fuels will represent only one quarter of global energy demand by 2040 [1]. Among these alternatives way to supply the global energy need, sustainable hydrogen carriers seems to offer friendly environmentally solution for numerous global issues such as climatic warming, the fate of the carbon and the greenhouse effect. Indeed, the hydrogen is inexhaustible, clean and the most abundant substance in the world. Furthermore, it is the most energetic element per unit of mass ( $120 \text{ kJ g}^{-1}$ ). However, most of the existing hydrogen in the earth is completely under oxidized state, forming the water ( $\text{H}_2\text{O}$ ) without fuel value. Also, it can be bound to the carbon in form of light hydrocarbons, like methane ( $\text{CH}_4$ ) with

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**Nomenclature**

$A$	pre-exponential factor, $s^{-1}$
$A_{ij}$	function used in equation (13)
$a, b$	exponential indexes
$C_p$	specific heat, $J\ kg^{-1}\ K^{-1}$
$D$	mass diffusion, $mol\ m^{-2}\ s^{-1}$
$E$	activation energy, $J\ mol^{-1}$
$h$	heat transfer coefficient, $W\ m^{-2}\ K^{-1}$
$Le$	Lewis number, –
$M$	molar mass, $g\ mol^{-1}$
$P$	pressure, Pa
$p_i$	partial pressure, Pa
$r$	reaction rate, $mol\ m^{-2}\ s^{-1}$
$R_g$	universal gas constant, $8.314472, J\ mol^{-1}\ K^{-1}$
$S$	source term, $m^{-3}$
$S_i$	rate of chemical appearance and disappearance, $mol\ m^{-2}\ s^{-1}$
$T$	temperature, K, or $^{\circ}C$
$u$	axial velocity, $m\ s^{-1}$
$v$	transverse velocity, $m\ s^{-1}$
$w$	mass fraction, –
$x$	axial coordinate, m
$y$	transverse coordinate, m, Molar fraction, –
$\Delta H_{298}^{\circ}$	standard enthalpy of formation, $J\ mol^{-1}$
$\Delta T$	temperature difference, K, or $^{\circ}C$

**Greek symbols**

$\mu$	dynamic viscosity, $m^{-1}\ kg\ s^{-1}$
$\rho$	fluid density, $kg\ m^{-3}$
$\nu''$	stoichiometric coefficient of product species, –
$\nu'$	stoichiometric coefficient of reactant species, –
$\lambda$	thermal conductivity, $W\ m^{-1}\ s^{-1}$

**Subscripts**

$f$	fluid, fiber
$g$	gas
$i, j$	reactant and product components
In	inlet
Mix	mixture
w	wall
WGS	water gas shift

high energetic potential. So, the hydrogen needs to be isolated from the substances to which it is bound. Nowadays, the hydrogen is mainly produced from water, biomass and far more from fossil fuels. The methods of hydrogen production from fossil fuels are: (a) Methane Steam Reforming (MSR) [2–5], (b) Autothermal Reforming (ATR) [6–8], and (c) partial oxidation (POX) [9–11]. The largest amount of hydrogen is produced mostly by MSR process especially from natural gas reforming, almost 80% of the overall hydrogen production from fossil fuels [12].

The intensification of MSR process can lead to a significant saving of energy and cost. In fact, this process depends strongly on the heat and mass transfer behaviors of the reactors, because of the endothermic nature of the MSR reaction. In this respect, many researches have been devoted to the intensification of the reforming process, by investigating several

aspects and parameters such as reactor's design, development of new catalysts and optimization of the reactor coating. Thus, Jiwanuruk et al. [13] conducted a three-dimensional numerical study on MSR reaction combined with methane combustion in micro reformer. In such systems, the heat need of endothermic MSR reaction is supplied by the combustion of methane. Authors investigated the arrangement effect among the exothermic and the endothermic systems by comparing two configurations regarding their catalytic coating: checked and parallel catalyst arrangements, and explored also the mixture flow direction on the micro reformer performances. The results show that both configurations give the same conversion rate of methane which is estimated about 68%. However, hot and cold spots are discovered in the parallel case. Concerning the mixture flow direction, the co-current direction allows a slight enhancement about 1% in terms of the methane conversion. Similarly, Karimipourfard et al. [14] explored numerically the “thermal interlocking” between the combustion/reaction of methane in a Steam Methane Reformer (SMR), intended to generate simultaneously synthesis gas and hydrogen. Authors combined two endothermic reactions with an exothermic reaction, and compared the performances reached with those obtained by a conventional SMR. The findings show that, using such thermal interlocking among reactions, the productions are increased while reducing the reformer size and the energy consumption. For their part, Murphy et al. [15] investigated experimentally and numerically the effect of the use of ceramic micro channel reactors for MSR reaction. They compared the performances of their device to an equivalent metallic micro reactor. They found that the heat transfer behavior is fairly similar to conventional micro reactors, but the production costs were reduced. Furthermore, structured patterns and layered configurations of catalyst can have a positive effect in terms of the reactors performances. Thereby, Fazeli et al. [16] conducted a numerical study on a wall-coated catalytic micro channel reactor for hydrogen production from methanol. In their work, the catalytic oxidation of methanol supplied the heat requirement of the steam reforming reaction. They analyzed the heat transfer between both zones by comparing two different configurations, namely, the micro channels equipped by Zigzag and straight catalytic patterns. They showed that the catalyst coated in zigzag pattern offers an efficient behavior, unlike the straight one.

In the same underlying ideas, we propose via a numerical study, to investigate the catalyst coating pattern on the Wall-Coated SMR (WC-SMR), mainly to explore the effect of the discretization of a continuous catalytic wall. To this end, a comparison of two catalytic arrangements, macro-patterning and continuous catalytic layer, in the WC-SMR is carried out. The obtained results show that the presence of the inter-spacing among the discrete catalytic layers can offer an outstanding enhancement of the methane conversion.

**MSR process and kinetic mechanism description**

MSR is the reaction of natural gas or light hydrocarbons with oxidized superheated steam. The MSR process has been used in industry for hydrogen production since the 1930s [17]. Nowadays, it is the most industrial process used on this

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