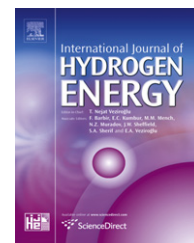


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On reaction coupled transport phenomenon in reformer ducts

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ABSTRACT

In compact steam reformer the probability of component degradation and failure depends strongly on the local temperature gradients coupled by various transport processes and chemical reactions in multi-functional materials. In this paper, the modeling and analysis of coupled mass transport and heat transfer processes are conducted for compact design steam reformer duct, which consists of a porous layer for the reforming reactions of methane, the fuel gas flow duct and solid plate. A fully three-dimensional computational fluid dynamics (CFD) approach is applied to calculate transport processes and effects of thermal conductivities of the involved multi-functional materials on reforming reaction rates and heat transfer/temperature distributions, in terms of surface temperatures/heat fluxes and Nusselt numbers. The steam reformer conditions such as mass balances associated with the chemical reactions and gas permeation to/from the porous layer are implemented in the calculation. The results reveal that a small thermal conductivity of the porous layer and solid plates promote high reforming reaction rates, and the convective heat transfer at the top interface varies more significantly along the main flow reformer duct.

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1. Introduction

It is a fact that proton exchange membrane fuel cells (PEMFCs) essentially need pure hydrogen as a fuel. However, hydrogen does not appear naturally as a gaseous fuel, and it usually has to be generated from whatever fuel source is locally available. For this concern, external fuel processing components, e.g., reformers and the ones to remove CO, should be incorporated into the PEMFC systems. It is true that methane is a convenient feedstock because the existing natural gas pipeline infrastructure makes it readily available and accessible at any point along the distribution chain. Availability of highly compact hydrogen reactors is very significant for PEMFC applications at central stations, substations, or residences.

In the hydrogen reactors, methane can be converted into H₂, CO and CO₂, such as in steam methane reforming (SMR),

partial oxidation (POX) and autothermal reforming (ATR) by employing alumina supported Ni as a catalyst.

There is an increasing interest worldwide in the development of compact fuel processing technologies for fuel cell systems. The overall idea is to catalytically activate both sides of a compact reactor, i.e., one side having combustion for supplying heat, and the other side appearing steam reforming of methane and hydrogen production. In this configuration, the thin porous layers for both sides result in small thermal conduction and species diffusion path lengths that largely eliminate heat and mass transfer restrictions associated with conventional reformers, and it is possible to have an improved utilization of the intrinsic reforming catalyst kinetics, and to achieve an efficient heat transfer. The compact design concept could lead to major applications in fuel cell systems for stationary and transportation applications, see references

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Nomenclature			
a	width of porous layer, m	Y	mass fraction of fuel species
b	width of flow duct, m	x, y, z	Cartesian coordinates
c_p	specific heat, J/(kg K)	<i>Greek symbols</i>	
D	molar diffusion coefficient of fuel gas species, m ² /s	β	permeability of porous layer, m ²
H	enthalpy, kJ/mol	ε	porosity
h	overall height of the duct, m	μ	dynamic viscosity, kg/(m s)
h_d	height of the duct, m	ν	kinematic viscosity, m ² /s
h_p	thickness of porous layer, m	ρ	density, kg/m ³
k	thermal conductivity, W/(m K); reaction rate constant, mol/(m ³ Pa ² s)	τ	tortuosity
M	molecular weight of species, kg/mol	<i>Subscripts</i>	
\dot{m}	mass diffusion flux, kg/(m ² s)	di	diffusion layer
\dot{n}	molar diffusion flux, mol/(m ² s)	eff	effective parameter
Nu	Nusselt number	f	fuel gas mixture
n	total number of species	CH ₄	methane
P	pressure, Pa	CO	carbon monoxide
q	heat flux, W/(m ²)	CO ₂	carbon dioxide
R	internal reforming reaction rate, mol/(m ³ s)	e	equilibrium
\Re	gas constant, kJ/(mol K)	gm	fuel gas mixture
Re	Reynolds number (UD_p/ν)	H ₂	hydrogen
r_e	effective radius, m	H ₂ O	water
S	source term	in	inlet
T	temperature, °C	k	Knudsen diffusion
V	velocity vector, m/s	m	mass transfer
V_i	velocity components in x, y and z directions, respectively, m/s	p	permeation; porous layer
X	molar fraction of fuel species	r	steam reforming reaction
		s	solid wall; shift reaction; species

[1,2]. As revealed in references [3,4], most reformer literature is devoted to its steam reforming reaction kinetics, materials for the components and catalyst forming/distribution and relevant literature review shows that research on thermal management coupled by catalytic chemical reactions is very limited.

In most cases, the characteristic of heat transfer has been modeled after the classical duct flow problem with either uniform wall flux or wall temperature conditions. This assumption is rather gross because the catalytic reforming reaction rates are strongly coupled with fuel gas flows and heat transfer through and over the porous layers. As a consequence, the interface boundary conditions and convective heat transfer coefficients are significantly different from the conventional ones. As expected, the thermal properties of multi-functional materials may have certain effects on the catalytic reaction and the convective heat transfer characteristics.

2. Objectives, problem statement and mathematical modeling

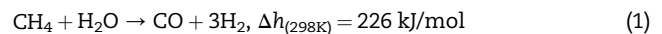
A three-dimensional computational procedure is applied to simulate and analyze steam reforming of methane in a composite domain consisting of a porous active layer, a gas flow duct and solid plates.

There are several transport processes (such as mass, heat and momentum transport) together with chemical reactions

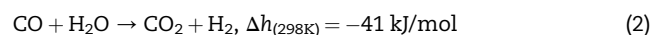
appearing in multi-functional reactors. It is often found that the endothermic and exothermic reactions (hydrocarbon cracking, steam reforming and dehydrogenation) are strongly coupled by heat transfer in the reactors.

A general in-house developed computational fluid dynamics (CFD) code is applied to simulate a methane reforming duct from a typical compact reformer, as shown in Fig. 1. The steam reforming, water gas-shift, and reverse methanation reactions of methane are the major ones with significant reaction rates [3,4], only the following chemical reactions are then considered in this study:

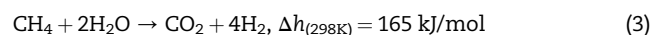
Methane steam reforming reaction:



Water gas-shift reaction:



Reverse methanation reaction:



It should be mentioned that the above processes in Eqs. (1) and (3) are endothermic and the overall reactions consumes the net heat. In general, this heat is supplied depending on the thermal integration methods employed and the associated combustion processes. In this study, the solved governing

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