

## 2D heat and mass transfer modeling of methane steam reforming for hydrogen production in a compact reformer

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### ABSTRACT

Compact reformers (CRs) are promising devices for efficient fuel processing. In CRs, a thin solid plate is sandwiched between two catalyst layers to enable efficient heat transfer from combustion duct to the reforming duct for fuel processing. In this study, a 2D heat and mass transfer model is developed to investigate the fundamental transport phenomenon and chemical reaction kinetics in a CR for hydrogen production by methane steam reforming (MSR). Both MSR reaction and water gas shift reaction (WGS) are considered in the numerical model. Parametric simulations are performed to examine the effects of various structural/operating parameters, such as pore size, permeability, gas velocity, temperature, and rate of heat supply on the reformer performance. It is found that the reaction rates of MSR and WGS are the highest at the inlet but decrease significantly along the reformer. Increasing the operating temperature raises the reaction rates at the inlet but shows very small influence in the downstream. For comparison, increasing the rate of heat supply raises the reaction rates in the downstream due to increased temperature. A high gas velocity and permeability facilitates gas transport in the porous structure thus enhances reaction rates in the downstream of the reformer.

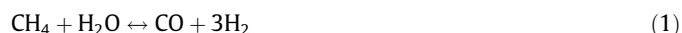
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### 1. Introduction

Hydrogen is an ideal energy carrier to support sustainable energy development [1]. Using a fuel cell, hydrogen can be efficiently converted into electricity with water as the by-product. To make the hydrogen energy and fuel cell commercially feasible, it is critical to produce hydrogen efficiently and economically at a large scale.

In the long term, hydrogen can be produced in a clean way by solar thermochemical water splitting, photocatalytic water splitting or water electrolysis driven by solar cells/wind turbines [2,3]. However, the present energy efficiencies of both thermochemical and photocatalytic hydrogen production methods are too low to be economically viable (i.e. efficiency for photocatalytic hydrogen production is usually less than 1% [2]). Water electrolytic hydrogen production can be a promising technology for large scale hydrogen production but the cost is still high, due to the use of expensive catalyst, i.e. Pt. For comparison, steam reforming of hydrocarbon fuels (i.e. methane) is efficient and can be a feasible way for hydrogen production for the near term [4]. In general, hydrogen production from methane is based on one of the following processes: methane steam reforming (MSR), partial oxidation (POX), and autothermal reforming (ATR) [5]. MSR is the most com-

mon method for hydrogen production from methane at a large scale. In MSR reaction (Eq. (1)), methane molecules react with steam molecules to produce hydrogen and carbon monoxide in the catalyst layer of reformers. Meanwhile, steam can react with carbon monoxide to produce additional hydrogen and carbon dioxide (Eq. (2)), which is called water gas shift reaction (WGS).



WGS is exothermic while MSR is highly endothermic. As the MSR reaction rate is usually higher than WGS, heat is required for hydrogen production by MSR and WGS. The heat supply can be achieved by using a compact reformer (CR). A typical CR consists of a solid thin plate sandwiched between two catalyst layers, as can be seen from Fig. 1 (adapted from [6]). The small thickness of the thin plate allows efficient heat transfer from the combustion duct to the fuel reforming duct to facilitate chemical reactions in the catalyst layer. High power density resulted from the compactness nature of the CRs makes them suitable for stationary and transportation applications [7,8]. Although some preliminary studies have been performed for CRs, there is insufficient numerical modeling on CRs for hydrogen production by methane steam reforming, especially on how the various parameters affect the reformer performance. It is still not very clear how the change in inlet temperature and rate of heat supply can influence the coupled

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## Nomenclature

$B_g$	permeability of electrode ( $\text{m}^2$ )	$S_x, S_y$	source terms in momentum equations ( $\text{kg m}^{-2} \text{s}^{-2}$ )
$C_p$	heat capacity ( $\text{kJ kg}^{-1} \text{K}^{-1}$ )	$S_T$	source term in energy equation ( $\text{W m}^{-3}$ )
$D_i^{\text{eff}}$	effective diffusion coefficient of species $i$ ( $\text{m}^2 \text{s}^{-1}$ )	$S_{\text{Sp}}$	source term in species equations ( $\text{kg m}^{-3} \text{s}^{-1}$ )
$D_{i,k}$	Knudsen diffusion coefficient of $i$ ( $\text{m}^2 \text{s}^{-1}$ )	$\Delta S$	entropy change ( $\text{kJ mol}^{-1} \text{K}^{-1}$ )
$D_{i,j}$	binary diffusion coefficient of $i$ and $j$ ( $\text{m}^2 \text{s}^{-1}$ )	$T$	operating temperature (K)
$F$	Faraday constant ( $\text{C mol}^{-1}$ )	$U$	velocity in $x$ direction ( $\text{m s}^{-1}$ )
$k$	thermal conductivity ( $\text{W m}^{-1} \text{K}^{-1}$ )	$U_0$	gas velocity at the inlet ( $\text{m s}^{-1}$ )
$L$	thickness of electrolyte (m)	$V$	velocity in $y$ direction ( $\text{m s}^{-1}$ )
$M_i$	molecular weight of species $i$ ( $\text{kg mol}^{-1}$ )	$X_i$	molar fraction of species $i$ (-)
$P$	operating pressure (atm)	$Y_i$	mass fraction of species $i$ (-)
$R$	universal gas constant ( $\text{kJ mol}^{-1} \text{K}^{-1}$ )	$\mu$	viscosity ( $\text{kg m}^{-1} \text{s}^{-1}$ )
$R_{\text{MSR}}$	rate of methane steam reforming reaction ( $\text{mol m}^{-3} \text{s}^{-1}$ )	$\varepsilon$	electrode porosity (-)
$R_{\text{WGSR}}$	rate of water gas shift reaction ( $\text{mol m}^{-3} \text{s}^{-1}$ )	$\xi$	electrode tortuosity (-)
$r_p$	mean pore radius of electrode (m)	$\Omega_D$	dimensionless diffusion collision integral (-)
$S_m$	source term in continuity equation ( $\text{kg m}^{-3} \text{s}^{-1}$ )	$\rho$	density of the gas mixture ( $\text{kg m}^{-3}$ )

transport and reaction kinetics in the reformer, which are important for optimization of the reformer operation conditions. In addition, the study in the literature considers pre-reformed methane gas consisting of  $\text{CH}_4$ ,  $\text{H}_2\text{O}$ ,  $\text{CO}$ ,  $\text{CO}_2$ , and  $\text{H}_2$  gas mixture at the inlet [6]. While it may be more appropriate to use  $\text{CH}_4/\text{H}_2\text{O}$  mixture as the feeding gas to the reformer.

In this paper, 2D numerical model is developed to simulate the performance of a CR for methane reforming. Different from the previous studies using pre-reformed gas mixtures at the inlet, the present study uses a  $\text{CH}_4/\text{H}_2\text{O}$  mixture at the reformer inlet. In real application, the steam to carbon ratio (SCR) is an important parameter as carbon deposition can occur at a low (i.e. less than 1) SCR [9]. As the present study do not consider the carbon deposition behavior in the reformer, a constant SCR of 2.0 is adopted. The effects of the reformer structural/operating parameters on the coupled transport and reaction phenomena are investigated and discussed in detail.

## 2. Model development

A 2D model is developed for hydrogen production from methane reforming in a CR. Heat from the combustion duct is supplied to the Ni-based (i.e. [10]) catalyst layer via the solid thin film layer and it is specified as a boundary condition [6]. Without considering the 3D effect, the coupled transport and chemical reaction phenomena in the computational domain can be shown in Fig. 2, including the solid plate, the reforming duct, and the porous catalyst layer. The 2D model consists of a chemical model and a CFD model. The chemical model is developed to calculate the rates of chemical reactions and corresponding reaction heats. The CFD

model is used to simulate the heat and mass transfer phenomena in the CR.

### 2.1. Chemical model

In operation, methane-containing gas mixture ( $\text{CH}_4$ : 33%;  $\text{H}_2\text{O}$ : 67%) is supplied to the reforming duct. The gas species are then transported from the gas duct into the porous catalyst layer, where MSR reaction (Eq. (1)) and WGSR (Eq. (2)) take place. The formulas proposed by Haberman and Young [11] have been widely used for simulating the rates ( $\text{mol m}^{-3} \text{s}^{-1}$ ) of MSR ( $R_{\text{MSR}}$ ) and WGSR ( $R_{\text{WGSR}}$ ), thus are adopted in the present study.

$$R_{\text{MSR}} = k_{\text{rf}} \left( P_{\text{CH}_4} P_{\text{H}_2\text{O}} - \frac{P_{\text{CO}} (P_{\text{H}_2})^3}{K_{\text{ps}}} \right) \quad (3)$$

$$k_{\text{rf}} = 2395 \exp \left( \frac{-231266}{RT} \right) \quad (4)$$

$$K_{\text{pr}} = 1.0267 \times 10^{10} \times \exp(-0.2513Z^4 + 0.3665Z^3 + 0.5810Z^2 - 27.134Z + 3.277) \quad (5)$$

$$R_{\text{WGSR}} = k_{\text{sf}} \left( P_{\text{CO}} P_{\text{H}_2\text{O}} - \frac{P_{\text{CO}_2} P_{\text{H}_2}}{K_{\text{ps}}} \right) \quad (6)$$

$$k_{\text{sf}} = 0.0171 \exp \left( \frac{-103191}{RT} \right) \quad (7)$$

$$K_{\text{ps}} = \exp(-0.2935Z^3 + 0.6351Z^2 + 4.1788Z + 0.3169) \quad (8)$$

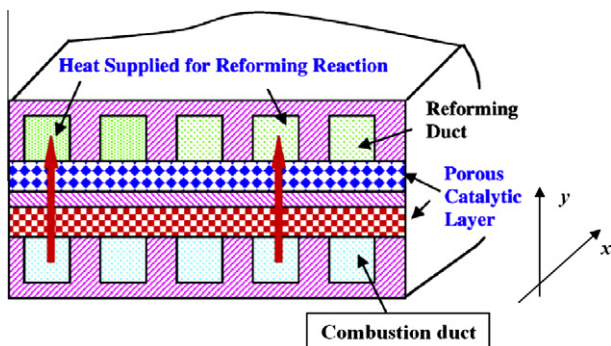


Fig. 1. Schematic of a compact reformer (CR) (adapted from [6]).

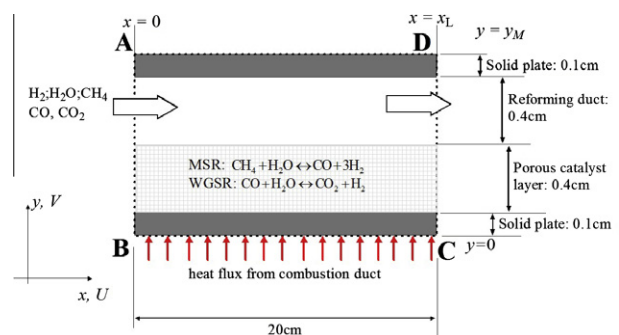


Fig. 2. Computational domain.

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