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MODELING OF A MICRO-CHANNEL WATER-GAS SHIFT REACTOR

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ABSTRACT

Hydrogen purification through water-gas shift (WGS) is a favored option in fuel processing for hydrogen fuel cells. A three-dimensional single channel model is developed to simulate the behavior of a water-gas shift micro reactor. The flow regime is assumed to be steady and laminar; furthermore, it is presumed that the walls are isothermal. A water-gas shift reaction rate model is utilized to simulate the surface reaction on Pt/TiO₂ catalyst. The gas feed composition is taken as the efflux of a typical auto-thermal reforming (ATR) reactor. A parametric study is conducted to investigate the effect of gas feed temperature, gas space velocity and channel length on water-gas shift micro reactor performance. The study resulted in an optimum water-gas shift micro reactor design. It should be noted that a water-gas shift micro reactor is an essential part of a reactor train to remove carbon monoxide from a hydrogen rich mixture. Such a mixture can be used as fuel for a PEM fuel cell in portable devices. The results of these simulations revealed that the optimum reactor consists of a square cross section channel with 100 μm hydraulic diameter, 20 mm length, space velocity of 1000 h⁻¹ and gas feed temperature of 270°C. The carbon monoxide mole fraction in the efflux is in a range suitable for a typical preferential oxidation (PROX) reactor.

INTRODUCTION

The rapid pace in industrial development during the last decades has led to a quest for new energy resources; this is a direct result of the fact that hydrocarbon fuels emissions are harmful to humans and are destroying the environment. Greenhouse gas emissions (particularly CO₂) concentrations have increased significantly due to combustion exhaust gases. Certain crucial steps should be taken to manage greenhouse gas emissions in the atmosphere, such as: enhancement of energy efficiency, consuming energy that is obtained from low carbon (or carbon-free) sources, and the seizure of carbon for instance storage of carbon dioxide in geologic formations [1]. Therefore, renewable energy sources will be more interesting for the future generations.

Fuel cells are efficient devices for energy conversion with extremely low pollutant emissions in comparison with conventional power generation devices. Due to the simple process in the conversion of chemical energy to electrical energy in proton exchange membrane (PEM) fuel cells, their utilization for portable devices is more interesting than other types of fuel cells. The preferred fuel for a PEM fuel cell is hydrogen; however, hydrogen does not exist naturally, and it should be produced from other sources such as hydrocarbon fuels through steam reforming (SR), partial oxidation reforming (POR) or auto-thermal reforming (ATR). During these processes carbon monoxide (CO) is also generated, while its amount should be reduced to below 10 PPM for using in PEM fuel cells. Thus a series of reactions must be applied to the generated hydrogen-rich mixture to decrease the amount of CO and increase the hydrogen concentration.

The water-gas shift (WGS) is an important industrial reaction with several applications, such as fuel processing for fuel cells. The water-gas shift (WGS) is a process during which carbon monoxide and water vapor react to produce carbon dioxide and hydrogen.



At low temperatures formation of products would be much greater than the high temperature products; nonetheless, the reaction would be a slow one. Hence the water-gas shift reactor is the bulkiest component of a fuel processor. Moreover, for mobile applications size and weight are of crucial importance; consequently, a compact and efficient fuel processor is preferred. Therefore, a micro reactor would make an attractive option.

Numerous authors simulated water gas-shift reactor to study its behavior and performance. Nevertheless, most of them concentrated on the unsteady behavior of one or two dimensional models. Additionally, some authors have

concentrated on the water-gas shift reaction kinetics and have developed models for various catalyst types.

Giunta *et al.* [2] used a one dimensional heterogeneous model for simulation of a fixed-bed water-gas shift reactor. In that study commercial Cu/Zn/Ba/Al₂O₃ is used as the catalyst. Catalyst deactivation due to thermal factors (sintering) was considered. The simulation results show that isothermal condition yields to higher conversion than adiabatic condition. Also, using smaller pellet size results in smaller reactor size.

In another study Choi and Stenger [3] investigated the water-gas shift kinetic and suggested an equation for the reaction rate. They utilized a micro reactor with commercial Cu/ZnO/Al₂O₃ catalyst in the temperature range of 120-250°C. The investigation shows that management and control of reactor temperature and water addition results in constant CO concentration at the outlet.

Adams and Barton [4] used a dynamic, heterogeneous and two-dimensional simulation to study a packed bed water-gas shift reactor. This model is applicable to a wide range of temperature and size.

Ding and Chan [5] developed a two dimensional unsteady model to study the performance of a water-gas shift reactor. The simulation results demonstrated that most of the carbon monoxide and hydrogen consumption occurred in the first 50% length of the reactor. In addition, at higher temperatures more CO conversion was achieved. Moreover, the research was conducted to explore the effect of gas space velocity. Temperature range of 873-973 K and gas space velocity range of 107 to 213 h⁻¹ is proposed to be the optimum operating condition for the simulated reactor.

Sun *et al.* [6] exploited Langmuir–Hinshelwood (LH) kinetic rate model at ambient pressure for noble metal catalysts. They used this model to simulate a water-gas shift reactor for fuel processing from natural gas. The simulation results revealed that LH kinetic rate model yields to more acceptable results than power law kinetic rate equations. They also established that reactors with noble metal catalysts are of less size than reactors that employ copper-zinc as catalyst by an order of 10.

In this paper, a three-dimensional single-channel water-gas shift micro reactor is modeled and the power law kinetics of Pt/TiO₂ catalyst is used. The equation is valid in the temperature range of 200-270°C [7] as it is discussed in detail later on in the paper. The channel walls are assumed to be isothermal and the reactions occur only on the wall surfaces. The effects of some essential parameters on the efficiency of the micro reactor are examined. These parameters are the gas feed temperature, gas space velocity and channel length. The gas feed composition is taken as the efflux of a typical ATR reactor and the operating conditions are set in a range so that the device could be paired with a typical portable PEM fuel cell.

A parametric study is carried out to obtain the optimum operating conditions and geometric parameters of the micro channel so that the maximum CO conversion is achieved.

In order to solve the non-linear coupled mass, momentum and energy equations a CFD code is developed. A finite volume method using the SIMPLE algorithm for pressure–velocity linkage is applied.

2. NUMERICAL MODEL

2.1. Problem statement

In the present study a rectangular single-channel micro reactor with hydraulic diameter of 100 μm and length of 20 mm is simulated. The flow regime is assumed to be laminar, steady and incompressible. Moreover, the gas mixture is assumed as an ideal gas and its properties are calculated at each point based on the local gas composition. The flow Knudsen number at the baseline simulation is 0.0007; since it is smaller than 0.001 the continuum assumption is valid. Fig. 1 represents a schematic model of the single-channel geometry.

A typical auto-thermal reactor efflux [8] gas composition is used, which consist of 7 species: CH₄, O₂, CO, CO₂, H₂, H₂O and N₂. The gas composition at the baseline condition is listed in Table 1.

Table 1. Operating conditions and inlet mole fractions for the baseline case.

Parameter	Value
Space velocity (h ⁻¹)	1,000
Channel length (mm)	16.0
Channel hydraulic diameter (μm)	100.0
Inlet temperature (°C)	270
Inlet pressure (Pa)	101,325
CH ₄ mole fraction (%)	10.0
O ₂ mole fraction (%)	0.0
CO mole fraction (%)	4.0
H ₂ O mole fraction (%)	21.5
H ₂ mole fraction (%)	30.5
CO ₂ mole fraction (%)	17.0
N ₂ mole fraction (%)	balance

To attain optimized operating conditions and channel geometry a parametric study is performed. In these simulations the CO concentration is reduced below 2%, which is in a proper range to be fed to a typical PROX micro-reactor.

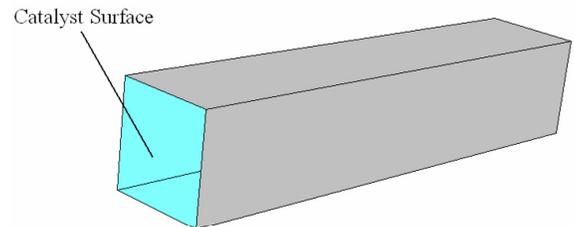


Fig. 1. Schematic model of WGS channel.

2.2. Governing equations

The governing equations for a reacting flow in a three dimensional rectangular duct are the conservations of mass, momentum, energy and chemical species in a Cartesian

coordinate system. Because of the fact that the continuum assumption is valid, the Navier-Stokes equations are applicable.

The continuum equation for 3D steady-state flow is given by

$$\nabla \cdot (\rho \vec{V}) = 0 \quad (1)$$

The Navier-Stokes equations, stated below, represent the conservation of momentum for the given conditions.

$$\vec{V} \cdot \nabla (\rho \vec{V}) = -\nabla p + \nabla \cdot (\mu \nabla \vec{V}) \quad (2)$$

The mass balance for the i^{th} species is presented in Eq. (3), and the molar production rate is indicated by Eq. (4) in which r is the WGS rate and ξ_i is the stoichiometric coefficient of the i^{th} species in the water-gas shift reaction.

$$\nabla \cdot (\rho \vec{V} Y_i) = \nabla \cdot (D_{eff,i} \rho \nabla Y_i) + \omega_i MW_i \quad (3)$$

$$\omega_i = \xi_i r \quad (4)$$

Eq. (3) is applied for 6 species and the nitrogen mass fraction is calculated from the following equation.

$$Y_{N_2} = 1 - \sum_{i,j \neq N_2} Y_i \quad (5)$$

Eq. (6) states the conservation of energy:

$$\nabla \cdot (\rho c_p \vec{V} T) = \nabla \cdot (k \nabla T) + \rho_{cat} \Delta H r \quad (6)$$

In Eq. (6) the reaction enthalpy is a function of temperature. However, the reaction occurs on the reactor wall which is assumed to be at a constant temperature.

Since the chemical reactions occur only on the internal walls of the micro channel, the source terms in Eqs. (3) and (6) are zero for internal computational cells.

In Eqs. (1-3) and (6), the fluid density is computed from the ideal gas equation for a multi-component mixture, which is:

$$\rho_{mix} = \frac{P_{work} MW_{mix}}{R_u T_{work}} \quad (7)$$

The effective mass diffusion coefficient is computed from the following equation,

$$D_{eff,i} = \frac{1 - \chi_i}{\sum_{j \neq i} \frac{\chi_j}{D_{ij}}} \quad (8)$$

where D_{ij} is the binary diffusion coefficient for the species pair i and j .

The constant pressure specific heat, dynamic viscosity and thermal conductivity of the gas mixture are computed with

$$c_{p,eff} = \sum_i c_{p,i} Y_i \quad (9)$$

$$\mu_{eff} = \sum_i \mu_i Y_i \quad (10)$$

$$k_{eff} = \sum_i k_i \chi_i \quad (11)$$

2.3. Boundary conditions

In order to solve the governing equations the following boundary conditions are considered. At the micro reactor inlet, velocity, pressure, temperature and composition of the gas mixture

are given. The reactor walls are permeable due to surface reactions; thus, source terms are used for species at the walls. Considering the Knudsen number, the flow regime is continuum and so the no-slip condition is applied at the micro reactor walls. Furthermore, the walls are assumed to be isothermal. The outflow mixture is discharged to a PROX reactor at ambient pressure and the gradients of all other dependent variables are set to zero at the micro reactor outlet.

2.4. Chemical kinetics

Various authors have reported kinetic rate equations for the water-gas shift reaction for diverse catalysts and operating conditions.

Phatak *et al.* [9] presented a kinetic rate on Pt supported on ceria and alumina which have the operating temperature range of 180-345°C and is applicable at ambient pressure. Also Radhakrishnan *et al.* [10] reported a kinetic rate equation for Pt/Re catalysts supported on ceria-zirconia for hydrogen purification which is generated from natural gas. In another investigation Jacobs *et al.* [11] proposed a kinetic rate equation for Pt/CeO₂ fuel processing catalysts for fuel cell applications.

In this paper the WGS kinetic rate on 0.5 wt% Pt/TiO₂ catalyst is used, which is developed by Kalamaras *et al.* [7] and given by Eq. (12). The kinetic rate is an empirical power law which is fitted to experimental reaction rates and is valid in the temperature range of 200-270°C.

$$r = k \times P_{CO}^a \times P_{H_2O}^b \times P_{CO_2}^c \times P_{H_2}^d \times (1 - \beta) \quad (12)$$

$$k = k_0 \times e^{\frac{-E_a}{R_u \times T_{work}}}$$

In this equation r is the reaction kinetic rate (mol s⁻¹ g_{cat}⁻¹); k is the rate constant; P_i is the partial pressure of species i (atm); a , b , c , and d are the reaction orders with respect to CO, H₂O, CO₂, and H₂; β is the approach to equilibrium which is presented in Eq. (13); k_0 is the pre-exponential factor; E_a is the apparent activation energy of reaction (kJ/kmol); R_u is the universal gas constant (kJ/kmol K); and T_{work} is the reaction temperature (K).

$$\beta = \frac{P_{CO_2} \times P_{H_2}}{K_{equil} \times P_{CO} \times P_{H_2O}} \quad (13)$$

$$K_{equil} = \exp\left\{\frac{5693.5}{T} + 1.077 \ln T + 5.44 \times 10^{-4} T - 1.125 \times 10^{-7} T^2 - \frac{49170}{T^2} - 13.148\right\} \quad (14)$$

While the reaction occurs on reactor walls, the wall temperature is used to define kinetic parameters. Reaction orders are tabulated in Table 2. The catalyst specific area is assumed to be 41 m²/g [7].

Table 2. Kinetic parameters.

Catalyst	a	b	c	d	K_0	E_{app} (J/mol)
0.5% Pt/TiO ₂	0.5	1.0	0.0	-0.7	0.31	45219.6

2.5. Solution method

To solve the non-linear coupled governing equations, a computational fluid dynamics (CFD) code was developed. The code is based on the finite volume method using the SIMPLE algorithm for the coupling of pressure and velocity domains [12]. To linearize the convective terms the power-law scheme is utilized, and a central difference scheme is applied to linearize the diffusive terms [13]. The algebraic system of equations is solved with the Jacobian point-to-point iteration method, except for pressure correction equation which is solved by using the Gauss-Seidel iteration method [14]. The reaction rate equation is also linearized for each species.

To save computational time, first the governing equations are solved without considering the reaction and property changes. After a number of iterations, this solution is used as an initial guess for the reactive flow calculations. Moreover, thermo-physical properties of the gas mixture are updated every 50 iterations to reduce numerical fluctuations. In order to stabilize numerical calculations of the reactive flow field, under-relaxation factors are used for all equations and these factors are gradually increased up to 0.99. This will promote stability of the numerical calculations, while secures accuracy of the numerical results.

3. RESULTS AND DISCUSSION

The present model is developed to investigate the behavior of a water-gas shift surface micro reactor for fuel cell applications. No compatible data, either numerical or experimental, was found in the literature for direct validation of our numerical results. A parametric study is done to investigate the effects of certain parameters on CO conversion. Consequently, an optimum state for the geometry and operating conditions of the WGS micro reactor is defined.

3.1. Grid Study

In order to estimate a suitable number of grid points for discretization of the computational domain, a grid study is first performed. Calculations are carried out for three cases with the same geometry and operating conditions but with different grid points: a fine grid of $592 \times 10 \times 10$ nodes, a medium grid of $470 \times 8 \times 8$ nodes and a coarse grid of $374 \times 6 \times 6$ nodes.

In Fig. 2 variation of averaged CO mole fraction at y - z surfaces along the micro channel are depicted for these three cases. Since the difference between the fine grid and the medium grid simulation results are negligible, the medium grid is recognized to be suitable for the micro channel simulation.

3.2. Baseline Simulation

In this section a single micro channel is considered with the operating conditions and geometry characteristics are tabulated in Table 1.

Contours of mole fraction of carbon monoxide and hydrogen are depicted in Fig. 3. It should be noted that as a result of high aspect ratio of the channel, the length scale in x -direction is different than that of y - and z - directions in these figures. It goes without saying that CO consumption is equal to H_2 formation. This

result is compatible with the fact that the water-gas shift reaction is molar balanced and so the molecular weight of the mixture will remain constant through the micro channel. Hence, the NO , CH_4 and O_2 mole fractions are constant along the channel.

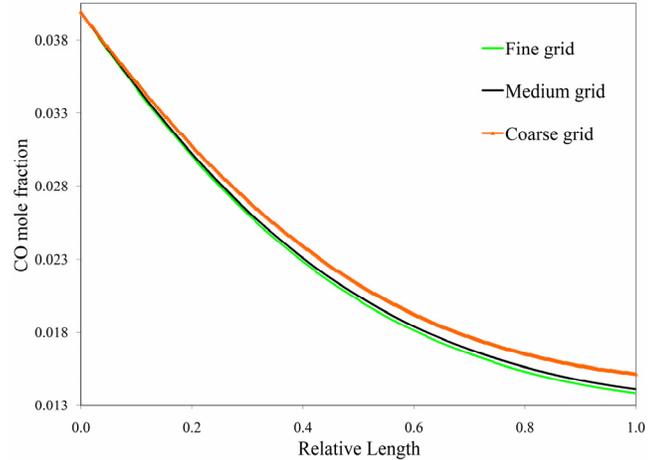


Fig. 2. Grid study of the simulation results for species mole fractions along the micro channel for the baseline conditions (CO).

As seen in these figures, the H_2 generation and CO removal mainly occur in the primary half of the micro channel length. Reduction of water and carbon monoxide mole fractions along the micro channel results in reduction of the water-gas shift reaction rate. Consequently, the CO conversion will diminish at the end of the channel in comparison with the first half its length.

In Fig. 4 the variations of CO conversion as well as mole fractions of all species along the channel are plotted. The CO removal is the chief objective of the water-gas shift reactor. It is observed that CO mole fraction gradient does not approach zero at the channel exit; thus, this micro channel length will not suffice for complete CO removal and the channel length should be enlarged.

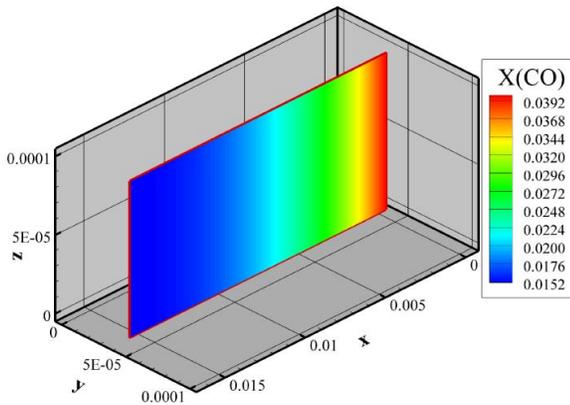
3.3. Parametric Study

Numerous simulations are performed to inspect the influence of significant parameters on CO conversion. These parameters are channel length, gas space velocity and gas feed temperature. To investigate the effect of each parameter on the water-gas shift reactor efficiency, that parameter is varied while the others are held constant. Thus the effect of that variable on carbon monoxide conversion in the water-gas shift reactor is investigated.

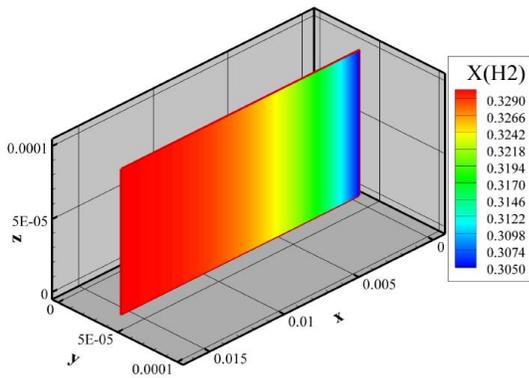
3.3.1. Inlet Gas Temperature

As mentioned before, the present water-gas shift reaction rate equation is justified in the temperature range of 200 - $270^\circ C$; thus, to study the effect of gas feed temperature on CO conversion, the temperature is varied in this range. In Fig. 5 the CO conversion is plotted for three lengths and five different gas

space velocities. It can be conceived that for all gas space velocities, while the temperature is rising, the CO conversion increases significantly. According to the water-gas shift rate equation, while the temperature is rising and other parameters are held constant, the reaction rate increases. Thus, increasing the temperature yields to higher CO conversion. Increasing the temperature may not be the finest solution to achieve higher CO conversion in all applications. Note that at higher temperatures the equilibrium shifts to lower CO removal.



(a)



(b)

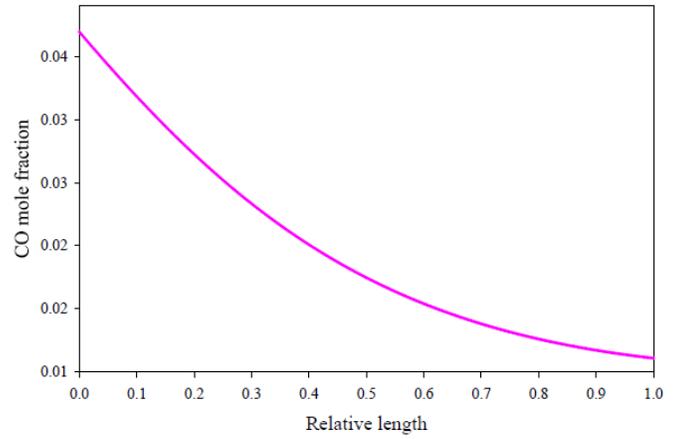
Fig. 3. Contours of species mole fractions along the micro channel for the baseline conditions: (a) Carbon monoxide (b) Hydrogen.

3.3.2. Space Velocity

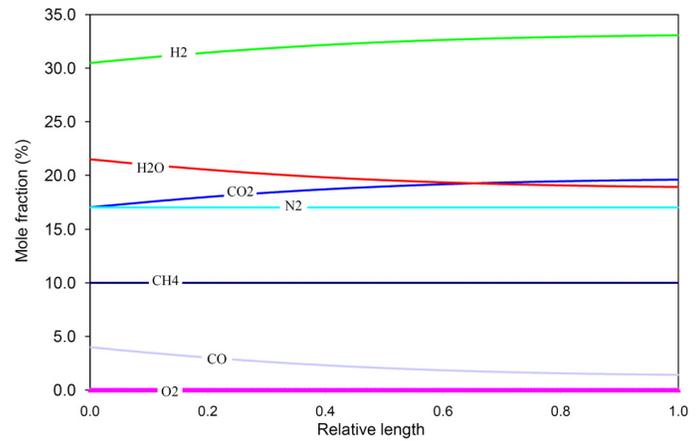
Fig. 6 illustrates the CO conversion for three different lengths and gas space velocities. It is observed that at higher temperatures, decreasing the gas space velocity does not have any significant effect on CO conversion. On the other hand, the effect of increasing the channel length on CO conversion is not altered as the temperature is increased.

The variation of CO conversion is also a function of gas space velocity and is discussed in greater detail in this section. Fig. 5 revealed that as the space velocity declines, the conversion efficiency amplifies. These results are displayed for three different lengths and in the temperature range of 230-270°C. By reducing the space velocity from 5000 h⁻¹ to 1000 h⁻¹, the conversion of CO

improves extensively. This is a sound result because of the fact that, if the gas space velocity is decreased, the residence time will increase, which means that the reaction has more time to complete. It can be seen that at lower temperatures reducing the gas space velocity results in doubling CO conversion, but as the temperature increases the difference between CO conversions for several gas space velocities yield to small values.



(a)



(b)

Fig. 4. (a) CO mole fraction variations (b) species mole fractions variations, along the micro channel for the baseline conditions.

It should be noted that while the gas space velocity decrease the mass flow rate will be reduced and so for a typical application more micro channels are needed. Hence, obtaining the optimum gas space velocity is an important part of the optimization of a water gas shift reactor.

3.3.3. Channel Length

Since the channel length is an essential parameter in the water-gas shift micro reactor efficiency it must be selected carefully. In this section the simulation is performed on all range of the gas feed temperatures and gas space velocities for three lengths: 16, 18 and 20 mm.

length yields to a large fuel processor, which is undesirable for portable applications. Therefore, to optimize a water-gas shift micro reactor both of these effects should be combined to obtain the maximum CO conversion.

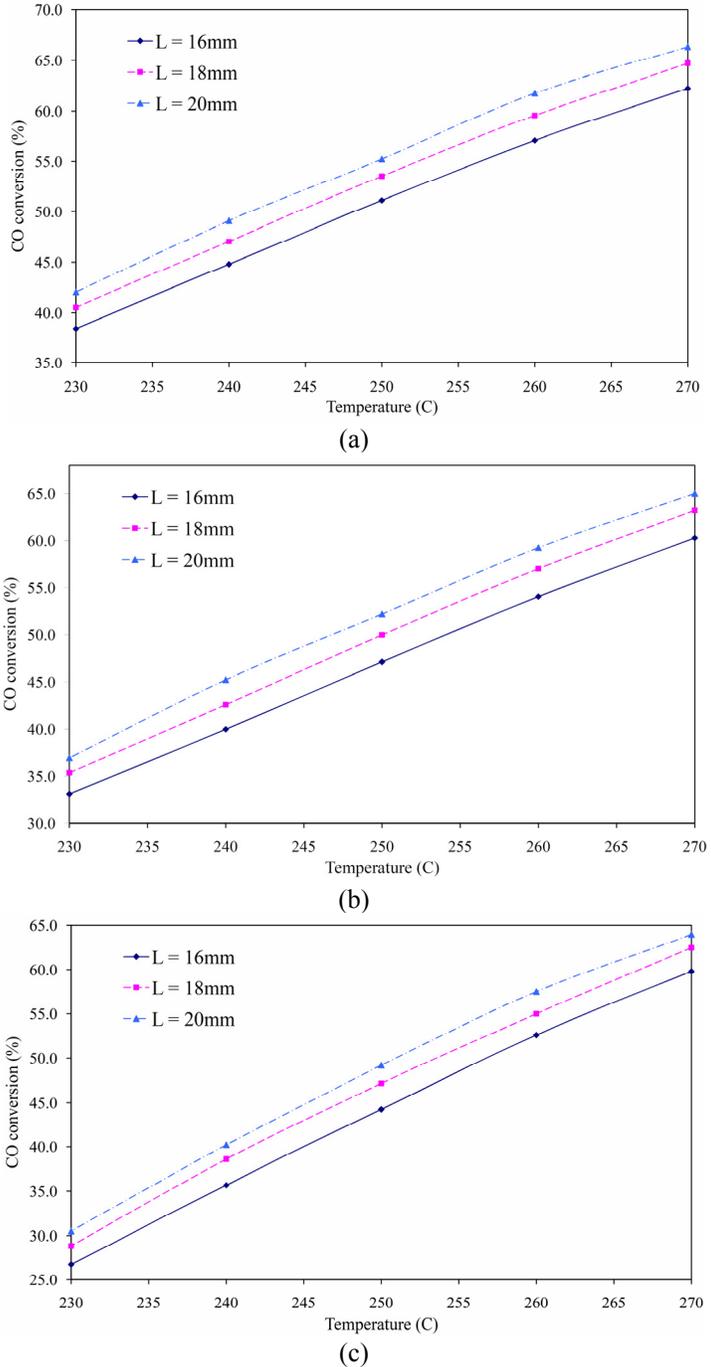


Fig. 6. Effect of inlet gas temperature and channel length on CO conversion for three gas space velocities: (a) 1000 h⁻¹, (b) 3000 h⁻¹, (c) 5000 h⁻¹.

There seems to be a reactor length beyond which no meaningful improvement in conversion occurs. For the present

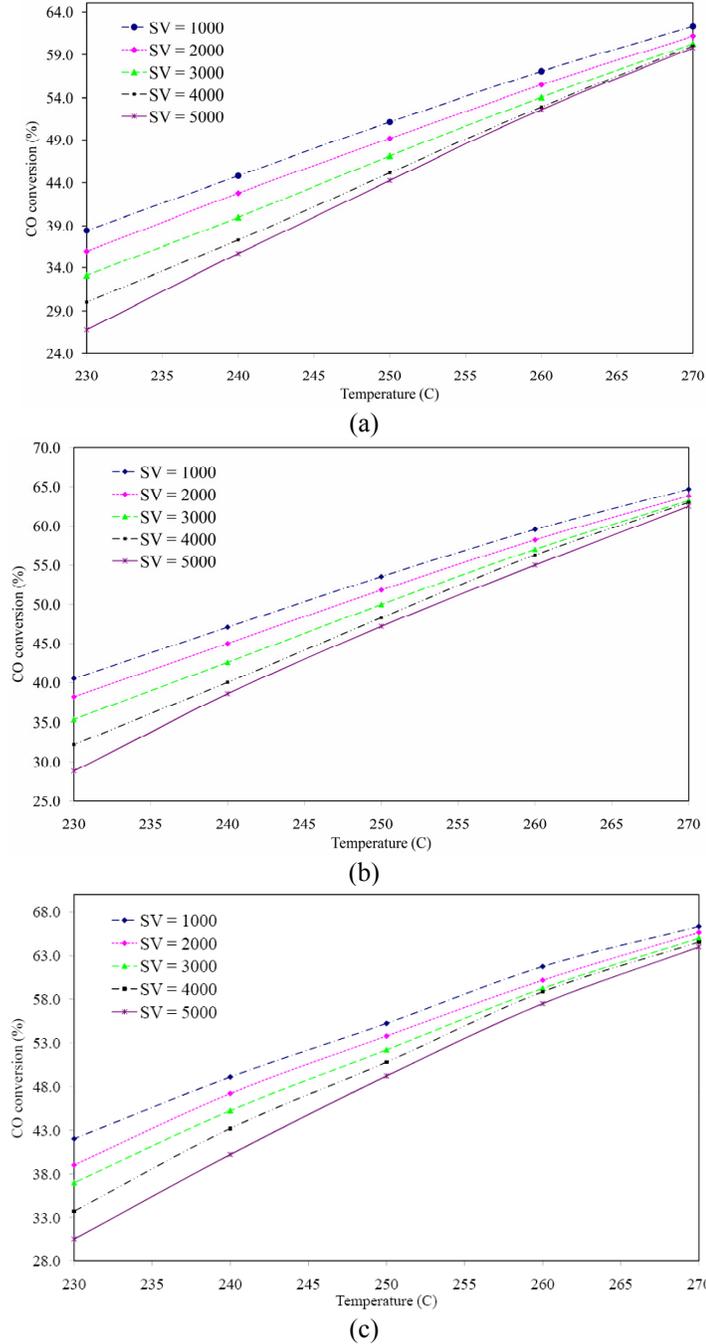


Fig. 5. Effect of inlet temperature and gas space velocity on CO conversion for three channel lengths: (a) 16 mm, (b) 18 mm, (c) 20 mm.

In Fig. 6 the simulation results for these lengths are displayed. As expected the conversion is improved while the channel length is increased. This is because the catalyst surface area is increased with the channel length; hence more residence time is available to the reactants. In this sense, it appears that the effect of increasing the micro channel length is somewhat similar to the effect of reducing gas space velocity. Note that the water-gas shift reactor is the bulkiest part of fuel processing for fuel cell and increasing its

conditions this length is found to be about 20 mm; a channel length more than this will not provide a higher CO conversion.

3.4. Optimum Operating Conditions

In order to obtain the optimum operating conditions for a water-gas shift reactor for portable applications, effects of various parameters on CO conversion should be taken into account and compared with each other. Hence as it is observed in Figs. 5 and 6 increasing the temperature to 270°C and reducing the gas space velocity to 1000 h⁻¹ will result in the maximum CO conversion. Also the 20 mm length appears to be sufficient for the present water-gas shift micro reactor. The geometrical and operating specifications for the optimum case are presented in Table 3. The carbon monoxide mole fraction at the exit is suitable for the efflux to be fed to a typical PROX reactor for further treatment [15].

Nonetheless, selection of the optimum case is dependent on the desired application as well as on the other components of a fuel processor. In this case the outlet CO mole fraction at the optimized conditions of the water-gas shift reactor is equal to 1.6% (dry basis). For complete hydrogen generation and purification a reactor train is needed which includes an ATR reactor, a WGS reactor and a PROX reactor.

Table 3. Operating conditions and outlet mole fractions for the optimum case.

Parameter	Value
Space velocity (h ⁻¹)	1,000
Channel length (mm)	20.0
Channel hydraulic diameter (μm)	100.0
Inlet temperature (°C)	270
Inlet pressure (Pa)	101,325
Outlet CO mole fraction (% dry basis)	1.6

4. CONCLUSIONS

In the present investigation a finite volume-based CFD code was developed to study a three-dimensional water-gas shift micro surface reactor for fuel cell applications. The kinetic rate for a 0.5 wt% Pt/TiO₂ catalyst is used in the temperature range of 200-270°C. Effects of the main parameters on CO conversion are investigated; these include gas feed temperature, gas space velocity and channel length. Through numerous simulations the following results are obtained:

- Increasing the temperature in the range of 230-270°C result in more carbon monoxide removal and hydrogen generation.

- Reducing the gas space velocity in the range of 1000-5000 h⁻¹ leads to an increase in carbon monoxide conversion.

- Increasing the channel length in the range of 16-20 mm results in more CO conversion and hydrogen generation; however increasing the channel length beyond 20 mm does not have a significant effect on the water-gas shift micro reactor performance.

In order to optimize the water-gas shift micro reactor several cases in the temperature range of 230-270°C and gas space velocity range of 1000-5000 h⁻¹ for three different channel lengths are considered and simulated. Therefore, the optimum design conditions are obtained as follows: temperature at 270°C, gas space velocity of 1000 h⁻¹ and a channel length of 20 mm. Such an optimized water-gas shift micro reactor will be an integral part of a complete fuel processing device for portable fuel cell applications.

5. NOMENCLATURE

c_p	constant pressure specific heat ($kJ/kg.K$)
D_{ij}	binary diffusion coefficient (m^2/s)
E_a	apparent activation energy ($kJ/kmol$)
ΔH	reaction enthalpy ($kJ/kmol$)
k	thermal conductivity ($W/m.K$)
k	reaction rate constant
k_0	pre exponential factor
K_{equi}	equilibrium constant
MW	molecular weight ($kg/kmol$)
P	pressure (Pa)
R	total reaction rate ($kmol/m^3.s$)
R_u	universal gas constant ($J/kmol.K$)
T	temperature (K)
\vec{V}	velocity vector (m/s)
Y	species mass fraction

Greek symbols

ω	species surface reaction rate ($kmol/m^2.s$)
μ	kinematic viscosity ($N.s/m^2$)
ζ	stoichiometry coefficient
ρ	density (kg/m^3)
χ	species mole fraction
β	approach to equilibrium

Sub or superscripts

<i>a</i>	CO reaction order
<i>b</i>	H ₂ O reaction order
<i>c</i>	CO ₂ reaction order
<i>cat</i>	catalyst
<i>d</i>	H ₂ reaction order
<i>eff</i>	effective
<i>equi</i>	equilibrium
<i>i</i>	<i>i</i> th species or reaction
<i>j</i>	<i>j</i> th species or reaction
<i>mix</i>	gas mixture
<i>work</i>	working operation

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