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Lattice Boltzmann Modeling of Methane Steam Reforming Reactions in Solid Oxide Fuel Cells

Mehdi Rahimi Takami^a, Davood Domiri Ganji ^{a,*}, Mojtaba Aghajani Delavar ^a, Shahriar Bozorgmehri ^b

^a Department of Mechanical Engineering, Babol Noshirvani University of Technology, Babol, Iran ^b Renewable Energy Department, Niroo Research Institute (NRI), Tehran, Iran ^{*}Corresponding author E-mail address: ddg_davood@yahoo.com

Article Information	Abstract
Article History:	The present study evaluated the rate of methane steam reforming (MSR) in a solid
Received: 2020-05-03	oxide fuel cell (SOFC). In this regard, a numerical model is applied to investage the effects of different parameters on the reactants concentration and temperature
Received in revised form: 2020-07-27 Accepted: 2020-07-28	distributions in the SOFCs. The developed model is based on the Lattice Boltzmann method (D2Q9) and validated with experimental results. Parametric effects, including current density, anode porosity, steam to carbon ratio (S/C), and Reynolds number of the inlet flow in the anode channel, are surveyed as a new parameter.
Keywords	Also, the results of reactant concentrations are illustrated in two-dimensions. These results showed that the porosity and Reynolds number of flow have the lowest and
Solid oxide fuel cell Methane steam reforming Lattice Boltzmann method Reaction rate Concentration distribution	highest impact on the reaction rate of MSR, respectively. The lowest MSR rate at the center of the SOFC happened when the Reynolds number of the input flow equals 5, and the highest MSR rate occured when the Reynolds number is 15 or the steam to carbon ratio equaled to 1.

1. Introduction

In recent years, SOFCs have attracted a lot of attention and been greatly developed because of their advantages such as flexibility in fuel [1, 2], modularity, high efficiency, and versatility [3, 4]. In these fuel cells, natural gas can be used as a fuel due to high operating temperature and the presence of nickel as a catalyst [5, 6], which makes them more efficient for producing electricity compared to internal combustion engines in areas that are rich in natural gas. Although, using methane can cause problems like carbon deposition [7] and a temperature gradient [8], which decrease the cell lifetime.

A large number of studies have been conducted on the

effect of reforming on cell performance. Lanzini and Leone [9] studied direct internal reforming by using two different types of biogas and then presented a new energy model. Mogensen et al. [10] reviewed the studies of reforming reaction kinetic and examined their effect on the results of the simulation. Thattai et al. [11] evaluated direct internal reforming in SOFCs comparing the kinetics of power-law and Langmuir-Hinshelwood.

The above-mentioned studies and other studies [12-15] examined the effect of reforming on SOFCs performance. The rate of MSR reaction plays an important role in temperature and concentration distributions and provides an informative parameter for study. Fan et al. [16] studied the effect of current density on the MSR reaction rate in a SOFC experimentally, and Park et al. [17] analyzed the effect of the operating temperature, fuel, and air inlet temperatures on the rate of chemical reactions and concentration distributions. Ahmed and Foger [18] conducted a comparative analysis of the kinetics effects of various reforming reactions on distributing temperature and concentration, and Chalusiak et al. [19] presented a numerical analysis of SOFC transient performance by direct internal reforming to increase the efficiency of the process.

In this study, the MSR reaction rate on a conventional SOFC is simulated for different gas conditions and temperatures. Biert et al. [20] investigated the differences between the MSR reaction rates predicted by the two kinetic models, and Wang et al. [21] studied the effects of mass transfer models on the MSR reaction rate. They both showed that the obtained results from different models are the same.

The numerical method used in the presented studies was the conventional CFD method. Since the accuracy of simulating the diffusion phenomenon is important in modeling of a fuel cell, the Lattice Boltzmann method (LBM) has been used in some studies to simulate mass transfer [22–27]. Joshi et al. [22] studied the impact of dimensionless flux and porosity on mass transport and concentration polarization. Xu et al. [23] compared the results of the LBM model and conventional CFD methods with experimental results. Paradis et al. [24] investigated the effect of electrochemical reactions on the mass diffusion. The results of these studies have shown that the LBM method, as a mesoscale method, is more accurate compared to macro-scale methods.

This method has also been used to study, carbon deposition [28], electrochemical performance [29], temperature distribution [30], and concentration distribution [31] In the researches of Xu and Dang [28] and Chiu et al. [31] the MSR reaction was considered and simulated, but the rate of reforming reactions were not investigated. Due to the use of porous media and the ability of LBM to simulate this media and the diffusion phenomenon in it, research has also been performed in other applications [32–34]. In some studies [22, 25, 26, 28, 31], the simulation was performed only for porous media, and this media was reconstructed. But in other studies [30 32, 33, 34], two different distribution functions were used in the simulation to avoid increasing the number of meshes.

The effects of parameters, such as operating temperature, current density, and inlet temperature on the reaction rate have been investigated in the literature, but the effect of the Reynolds number of inlet flow, porosity, and the S/C of inlet flow on MSR reaction rate has not been studied. Moreover, the rate of reforming reactions have not been investigated using LBM, even though this method is much more accurate than the CFD conventional methods [22–24].

In this study, a FORTRAN code was established by using LBM to simulate and investigate the MSR rate. Furthermore, the effect of current density, Reynolds number of inlet flow, porosity, and S/C on the reaction rate and concentration and temperature distributions were studied. Due to the high accuracy of the LBM method to simulate diffusion phenomena, the results are more reliable for the MSR reaction rate, which is highly dependent on the concentration of gases and temperature. For this purpose, a numerical model has been developed to simulate a solid oxide fuel cell and the changes in the concentration and temperature, as well as the reaction rate of the MSR for different conditions.

2. Model development

Three models should be solved simultaneously to

simulate the performance of SOFC: the thermodynamic, LBM, and electrochemical models.

As shown in Fig. 1, the thermodynamic model consists of chemical and diffusion submodels. In the chemical submodel, reactions are simulated, and their rate is obtained. By using the diffusion submodel, the diffusion coefficients of the momentum, heat, and mass are calculated. The results of the thermodynamic model are used as input in the LBM model. The output of this model is the distribution of concentration and temperature in the geometry of the study, which is used to calculate the I-V curve in the electrochemical model. The convergence criterion is such that the maximum error value for the parameters of velocity, temperature, and concentration in 10 consecutive repetitions should be less than 0.01 percent.



Fig. 1. Flowchart of the numerical model.

2.1. Thermodynamic model

2.1.1. Chemical model

Finding the governing equation of the chemical reactions is essential for simulating SOFCs. In SOFCs with DIR, these reactions are divided into reforming and electrochemical reactions. Reforming reactions are related to methane steam reforming (MSR) and water gas shift (WGS).

Although these reactions take place at the catalytic surface, the rate of these reactions are given per unit volume because they occur throughout the anode porous media. In several studies, the rate of MSR and WGS reactions is presented by mol.m⁻³.s⁻¹ [11, 17, 19, 21]. Since electrochemical reactions occur at the contact surface of the anode and the electrolyte, their rate is given per unit area. Eqs. (1) and (2) show the electrochemical reactions, (3) indicates the MSR, and (4) represents the WGS.

$$H_2 + 1/2 O_2 \rightarrow H_2 O \tag{1}$$

$$CO+1/2 O_2 \rightarrow CO_2 \tag{2}$$

$$CH_4 + H_2 O \leftrightarrow CO + 3H_2$$
 (3)

$$\text{CO+H}_2 \text{O} \leftrightarrow \text{CO}_2 + \text{H}_2$$
 (4)

An important aspect of these reactions for simulation is related to their rate, and the material of the catalyst is very influential on it. Since the catalyst material used in the fuel cell is nickel and is heterogeneous due to the phase of the reactants, the following equations are used to simulate t MSR and WGS rates [35]:

$$RR_{SMR} = K_{SMR}^{+} P_1 P_3 - K_{SMR}^{-} P_2 (P_4)^3 \left[\frac{mol}{m^3 s}\right]$$
(5)

$$RR_{WGS} = K_{WGS}^{+} P_2 P_3 - K_{WGS}^{-} P_4 P_5 \left[\frac{mol}{m^3 s}\right]$$
(6)

where K^{+}_{SMR} and K^{-}_{SMR} represent the rates of the forward and backward MSR reactions, and K^{+}_{WGS} and K^{-}_{WGS} are considered as the rates of the forward and backward WGS reactions. Table 1 indicates the rate coefficients of these two reactions:

Table 1. Rate Coefficient of Steam Reforming Reaction and Water Gas Shift Reaction at Different Temperatures [35]						
Temperatur	re (K) K^+	_{WGS} (mol m ⁻³ pa ⁻² s ⁻¹)	K- _{WGS} (mol m ⁻³ pa ⁻⁴ s ⁻¹)	K ⁺ _{SMR} (mol m ⁻³ pa ⁻² s ⁻¹)	K ⁻ _{SMR} (mol m ⁻³ pa ⁻² s ⁻¹)	
1073		1.5E-7	1.4 E-7	2.3E-8	1.4E-20	
1123		3.2E-7	3.5 E-7	8.0E-8	1.5E-20	
1163		3.6E-7	4.3 E-7	1.6E-7	1.5E-20	

The reaction rates of the electrochemical reactions depend on current density and are calculated using the following equations:

$$RR_{EC} = \frac{cd \times A_{AA}}{4 \times F} \tag{7}$$

where cd, A_{AA} , F, and RR_{EC} are the current density, active surface area, Faraday constant, and electrochemical reaction rate, respectively.

Since electrochemical reactions include oxidation of hydrogen and carbon monoxide, each of their rates should be calculated separately using Eqs. (8) - (11):

$$i = i_{CO} + i_{H_2}$$
 (8)

$$n_{H_2} = \frac{i_{H_2}}{i}$$
(9)

$$RR_{EC,H_2} = RR_{EC} \times n_{H_2} \tag{10}$$

$$RR_{EC,CO} = RR_{EC} \times (1 - n_{H_2}) \tag{11}$$

In this model, n_{H2} equals 0.75.

After determining all the reaction rates, heat and concentration sources should be specified by heat and concentration sources. Reforming reactions happen over the entire SOFC, but electrochemical reactions occur only on the active area of the fuel cell. Eqs. (12) - (16) are related to the heat and concentration sources in all areas, except the active area [36, 37]:

$$\frac{dC_{CH_4}}{dt} = -RR_{SMR} \tag{12}$$

$$\frac{dC_{H_2O}}{dt} = -RR_{SMR} - RR_{WGS}$$
(13)

$$\frac{dC_{CO}}{dt} = RR_{SMR} - RR_{WGS} \tag{14}$$

$$\frac{dC_{H_2}}{dt} = 3RR_{SMR} + RR_{WGS} \tag{15}$$

$$\frac{dC_{CO_2}}{dt} = RR_{WGS} \tag{16}$$

The following equations are used to determine heat and concentration sources for the active area

$$\frac{dC_{CH_4}}{dt} = -RR_{SMR} \tag{17}$$

$$\frac{dC_{H_2O}}{dt} = -RR_{SMR} - RR_{WGS} + RR_{EC,H_2}$$
(18)

$$\frac{dC_{CO}}{dt} = RR_{SMR} - RR_{WGS} - RR_{EC,CO}$$
(19)

$$\frac{dC_{H_2}}{dt} = 3RR_{SMR} + RR_{WGS} - RR_{EC,H_2}$$
(20)

$$\frac{dC_{CO_2}}{dt} = RR_{WGS} + RR_{EC,CO}$$
(21)

2.1.2. Diffusion model

Diffusion plays a significant role in the simulation of SOFC. This phenomenon consists of momentum, heat, and mass diffusion, and the related parameters are dynamic viscosity, heat conductivity, and the mass diffusion coefficient.

In this study, the dynamic viscosity of the gas mixture is determined by the Wike method [38], as follows:

$$\mu_{m} = \sum_{i=1}^{n} \frac{y_{i} \mu_{i}}{\sum_{j=1}^{n} y_{j} \varphi_{ij}}$$

$$\left[\int_{1} \left(M_{i} \right)^{\frac{1}{4}} \left(\mu_{i} \right)^{\frac{1}{2}} \right]^{2}$$
(22)

$$\varphi_{ij} = \frac{\left[1 + \left(\frac{M_i}{M_j}\right) \left(\frac{M_i}{\mu_j}\right)\right]}{\left[8 + \left(1 + \frac{M_i}{M_j}\right)\right]^{\frac{1}{2}}}$$
(23)

Where y_i , μ_i , and M_i are the mole fraction, viscosity, and the molecular mass of the gas, respectively.

Further, the thermal diffusivity is determined by Eq. (24):

$$\alpha = \frac{k}{\rho C_P} \tag{24}$$

Due to the fact that the thermal conductivity of solid and fluid must be considered in porous media, the effective heat conduction coefficient is defined. This parameter is calculated by Eqs. (25) - (27) [33]:

$$(25)$$

$$(25)$$

$$(2\sqrt{1-\varepsilon}) \cdot \left(\frac{(1-\sigma)B \cdot \ln\left(\frac{1}{\sigma B}\right)}{(1-\sigma B)^2} - \frac{(B+1)}{2} - \frac{(B-1)}{(1-\sigma B)} \right)$$

$$K_{eff} = K_f \left((1-\sqrt{1-\varepsilon}) + \frac{(1-\sigma B)}{(1-\sigma B)} \right)$$

$$\sigma = \frac{K_f}{K_s} \tag{26}$$

$$B = 1.25 \left[\frac{(1-\varepsilon)}{\varepsilon} \right]^{\frac{10}{9}}$$
(27)

where k_{f} and k_{s} are the coefficients of thermal conductivity of the fluid and the porous media, respectively.

The mass diffusion mechanism in a porous area is divided into molecular and Knudsen diffusion. Molecular diffusion is more effective if the pores are much wider than the mean free path of the molecules, while Knudsen diffusion is more important if the pores are much smaller. In many porous media areas, including SOFCs, both means of diffusion are important and should be considered. Furthermore, a parameter is defined as effective diffusion, which is a combination of both mechanisms and is obtained from Eq. (28) [39].

$$D_{i,eff} = \varepsilon^{1.5} \left(\frac{D_k + D_{i,m}}{D_k \cdot D_{i,m}} \right)$$
(28)

where D_k and $D_{i,m}$ are the molecular and Knudsen diffusion coefficients that can be calculated using Eqs. (29) – (31) [40, 41].

$$D_k = \frac{2}{3} r_p \sqrt{\frac{8RT}{\pi M}}$$
(29)

$$D_{i,j} = 0.0018583 \left(\frac{1}{M_i} + \frac{1}{M_j}\right)^{\frac{1}{2}} \frac{T^{\frac{3}{2}}}{P\Omega i_j \sigma_{ij}^2}$$
(30)

$$D_{i,m} = \frac{1 - y_i}{\sum_{j \neq i}^{m} \frac{y_i}{D_{i,j}}}$$
(31)

where P represents the absolute pressure, r_p indicates the size of catalyst particles, M shows the molar mass, Ω_{ij} is considered as the collision integral, and σ_{ij} means the collision diameter.

2.2. Lattice Boltzmann method (LBM)

By defining distribution functions, the LBM is a mesoscale method is suitable to simulation of diffusion in complex geometries and physical phenomena and is more accurate than conventional CFD methods. In this method, the Navier-Stokes is replaced by Eq. (32), the Boltzmann relation equation, which can be used to obtain Navier-Stokes equations [42].

$$\tilde{f}_{\nu k}(x,t+\Delta t) = f_{\nu k}(\vec{x},t) - \frac{\Delta t}{\tau_{\nu}} \left[f_{\nu k}(\vec{x},t) - f_{\nu k}^{eq}(\vec{x},t) \right] + \Delta t \tilde{F}_{k}$$

where c, f_{vk} , f_{vk}^{eq} , τ_{v} , and $\tilde{F_{k}}$ represent the velocity, distribution function, equilibrium distribution function, relaxation time, and force, respectively.

$$f_{vk}(\vec{x} + c_k \Delta t, t + \Delta t) = \tilde{f}_{vk}(x, t + \Delta t)$$
⁽³³⁾

$$f_{vk}^{eq} = W_k \rho \left[1 + \frac{\vec{c}_k \vec{u}}{c_s^2} + \frac{1}{2} \frac{(\vec{c}_k \vec{u})^2}{c_s^4} - \frac{1}{2} \frac{\vec{u} \vec{u}}{c_s^2} \right]$$
(34)

$$\tau_v = \frac{v}{c_s^2 \Delta t} + 0.5 \tag{35}$$

where w_k is the weighting factor.

Eqs. (32) and (33) can be used to determine the porous area and Eq. (34) is replaced by Eq. (36) [32]:

$$f_{vk}^{eq} = W_k \rho \left[1 + \frac{\vec{c}_k \vec{u}}{c_s^2} + \frac{1}{2} \frac{(\vec{c}_k \vec{u})^2}{\varepsilon c_s^4} - \frac{1}{2} \frac{\vec{u} \vec{u}}{\varepsilon c_s^2} \right]$$
(36)

 \tilde{F}_{k} is obtained by Eq. (37):

$$F_{k} = W_{k} \rho \left(1 - \frac{1}{2\tau_{v}} \right) \left[\frac{\vec{c}_{k} \cdot \vec{F}}{c_{s}^{2}} + \frac{(\vec{u}\vec{F} \cdot \vec{c}_{k} \vec{c}_{k})}{\varepsilon c_{s}^{4}} - \frac{\vec{u} \cdot \vec{F}}{\varepsilon c_{s}^{2}} \right]$$
(37)

where \vec{F} is the total body force and includes an external force, the inertia caused by porous media, and (20)

the viscous diffusion $.\vec{F}$ is calculated by Eq. (38) [43]:

$$\vec{F} = -\frac{\varepsilon \upsilon}{K_p} \vec{u} - \frac{1.75}{\sqrt{150\varepsilon K_p}} |\vec{u}| \vec{u}$$
(38)

 K_p is the permeability and is calculated as follows [34]:

$$K = Da L^2$$
(39)

where Da and L are the Darcy number and the characteristic length, respectively.

The presented distribution function and the equilibrium distribution function are used to solve for the flow field, although another distribution function should be applied to solve for the temperature and concentration field. Eq. (40) is the distribution function for the temperature field, while the Eq. (41) is related to the concentration field: (40)

$$f_{ik}(\vec{x} + \vec{c}_{k}\Delta t, t + \Delta t) = f_{ik}(\vec{x}, t) + \frac{\Delta t}{\tau_{t}} \Big[f_{ik}^{eq}(\vec{x}, t) - f_{ik}(\vec{x}, t) \Big] + \Delta t S_{t}$$
(41)

$$f_{lk}(\vec{x} + \vec{c}_k \Delta t, t + \Delta t) = f_{lk}(\vec{x}, t) + \frac{\Delta t}{\tau_t} \Big[f_{lk}^{eq}(\vec{x}, t) - f_{lk}(\vec{x}, t) \Big] + \Delta t S_l$$

 S_t and S_1 are related to the heat and mass sources, respectively. As mentioned in the chemical model, the heat and mass sources were obtained by calculating the reaction rates. τ_t and τ_1 are the relaxation times and acquired by Eqs. (42, 43):

$$\tau_t = \frac{\alpha}{c_s^2 \Delta t} + 0.5 \tag{42}$$

$$\tau_l = \frac{D}{c_s^2 \Delta t} + 0.5 \tag{43}$$

where α and D are the effective thermal diffusivity and effective mass diffusion coefficient, respectively. The model chosen for this method in this research is two-dimensional with nine motion directions and is known as D2Q9. It is determined by the following speed vectors and weighting factors :

$$\vec{c}_{k} = \begin{cases} (0,0) & k = 0\\ (0,\pm 1), (\pm 1,0) & k = 1-4\\ (\pm 1,0) & k = 5-8 \end{cases}$$
(44)

$$w_{*} = \begin{cases} \frac{4}{9} & k = 0\\ \frac{1}{9} & k = 1 - 4\\ \frac{1}{36} & k = 5 - 8 \end{cases}$$
(45)

2.3. Electrochemical simulation

Since numerical model results are validated using an I-V curve, it is necessary to obtain this curve by calculating the SOFC voltage for different currents. This is calculated by using Eq. (46) [44, 45] in which E is obtained from the Eq. (47):

$$V = E - \eta_{act,a} - \eta_{act,c} - \eta_{conc,a} - \eta_{conc,c} - \eta_{ohm}$$
(46)

$$E = E^{0} - \frac{RT}{nF} \ln \left(\frac{P_{H_{2}} P_{o_{2}}}{P_{H_{2}o}}^{\frac{1}{2}} \right)$$
(47)

where R equals the gas constant, T is considered as temperature (K), and P_{H2} , $P_{o2,,}$ and P_{H20} are the partial pressures of hydrogen, oxygen, and steam on the anode and cathode TPB [46].

 E^0 is the reversible potential and isobtained by using the following equation, Eq. (48):

$$E^{0} = 1.253 - 2.4516 \times 10^{-4} T$$
 (48)

2.3.1. Activation overpotential

Activation overpotential is related to the electrode kinetics in the reaction area, and is due to the necessity of activation for the transportation of electrical charge. This overpotential can be calculated using the Butler-Volmer Eq. (49) [45]:

$$J = J_0 \left[\exp\left(\frac{\alpha z F \eta_{act}}{RT}\right) - \exp\left(-\frac{(1-\alpha)z F \eta_{act}}{RT}\right) \right]$$
(49)

 J_{o} represents the exchange current density. z is the number of electrons involved in the reaction and equals 2. α as the transfer coefficient and is assumed to be 0.5 [45, 47, 48].

The exchange current density for the anode and cathode is obtained using Eqs. (50) and (51) [44]:

$$J_{0,a} = K_a \frac{72X \left[D_p - \left(D_g + D_p \right) \varepsilon \right] \varepsilon}{D_p^2 D_g^2 \left(1 - \sqrt{1 - X^2} \right)} \left(\frac{P_{H_2o}}{P_{ref}} \right) \left(\frac{P_{H_2}}{P_{ref}} \right) \exp \left(\frac{E_{act,a}}{RT} \right)$$
(51)

$$J_{0,c} = K_c \frac{72X \left[D_p - \left(D_g + D_p \right) \varepsilon \right] \varepsilon}{D_p^2 D_g^2 \left(1 - \sqrt{1 - X^2} \right)} \left(\frac{P_{o_2}}{P_{ref}} \right) \exp\left(\frac{E_{act,c}}{RT} \right)$$

where P_{H2O} , P_{H2} , and P_{O2} are the partial pressure of gas species on the anode and cathode TPB, k_a and k_c are the constants of the exchange current densities of the anode and cathode, X represents the ratio of the length of the grain contact neck to grain size, ε shows the electrode porosity, D_p indicates the cavity size, and D_g is regarded as the particle size on the anode or cathode. $E_{act,a}$ and $E_{act,c}$ are the anode and cathode activation energy, respectively. By using the Butler-Volmer equation, the activation loss for the anode and cathode is obtained by using Eqs. (52) and (53) [45]:

$$\eta_{act,a} = \frac{2RT}{zF} \times \sinh^{-1} \left(\frac{J}{2J_{0,a}}\right)$$
(52)

$$\eta_{act,c} = \frac{2RT}{zF} \times \sinh^{-1} \left(\frac{J}{2J_{0,c}} \right)$$
(53)

2.3.2. Concentration overpotential

This overpotential is related to electrode resistance against mass transfer of reactants and products in the reaction area. As the reactants are consumed during the reaction, their concentration at the reaction site decreases. According to Fick's model, the overpotential is obtained by Eqs. (54) and (55) [49]:

$$\eta_{conc,a} = \frac{RT}{2F} \ln \left[\frac{y_{H_2}^l \cdot y_{H_2o}}{y_{H_2o}^l \cdot y_{H_2}} \right]$$
(54)

$$\eta_{conc,c} = \frac{RT}{2F} \ln \left[\frac{y_{o_2}^{l}}{y_{o_2}} \right]$$
(55)

where y and y¹ represent the species concentration on the electrode surface and the electrode electrolyte interface, respectively [50].

2.3.3. Ohmic overpotential

Because the conductivity of electrodes and connectors is much higher than that of the electrolyte, they can be ignored. Thus, ohmic overpotential can be calculated by the cell ohmic resistance, Eq. (56) [45] in which L is the electrode thickness measured in micrometer:

$$\eta_{ohm} = 2.99 \times 10^{-11} JL \exp\left(\frac{10300}{T}\right)$$
 (56)

2.4. Geometry and boundary condition

The Solution domain is shown in Fig. 2a. It includes the SOFC, fuel inlet, and product outlet. The SOFC is located at the end of the fuel path, and the entire system is housed in a furnace at 800°C. The LBM model is used to simulate all three parts. Of these three parts, the SOFC media is porous, and it's governing equations are different from the two other parts (Eqs. (34), (36)). On the other hand, the electrochemical and reforming reactions occur only in the fuel cell.

The boundary condition for inlet flow are $u = u_{inlet}$, $C=C_{inlet}$, v = 0, and T = 373 K, and at the outlet, the gradients of velocity, concentration, and temperature are set to be zero. On the walls, the values of concentration and velocity are zero, and the temperature is equal to the furnace temperature. In LBM, the macroscopic boundary conditions have to be applied in the form of the distribution function. A shematic of a D2Q9 LBM model is presented in Fig. 2b. The outside distribution functions are known due to the streaming process, and the inside distribution function function (dotted lines) are unknown. Because of the noslip condition of the flow field at the wall of pipes, the uknown distribution functions are determined by using a bounceback scheme, as follows:

North:
$$f_4 = f_2$$
, $f_7 = f_5$, $f_8 = f_6$ (57)

South: $f_2 = f_4$, $f_5 = f_7$, $f_6 = f_8$ (58)

East:
$$f_3 = f_1$$
, $f_6 = f_8$, $f_7 = f_5$ (59)

West:
$$f_1 = f_3$$
, $f_5 = f_7$, $f_8 = f_6$ (60)



Fig. 2. (a) Solution domain (b). Known and unknown distribution functions of domain boundaries.

3. Experimental Setup

As demonstrated in Fig. 3, the experimental equipment consists of two separate ways to supply fuel to the anode side and air to the cathode side. The upper part is dedicated to the fuel for the anode side and the lower part to the air for the cathode side. There are two separate pipes for each section, the pipe smaller in diameter is the fuel-air inlet, and the larger pipe is the outlet of the reaction products.

SMART2 (WonATech Co., Ltd.) and autolab (302N) were applied to control gas flow and measure the I-V curve, respectively. Linear sweep voltammetry was used to study and evaluate the electrochemical performance of the SOFC.

Alumina was used for the fuel and air supply pipes and silver wires for voltage and current measurements due to high oven temperatures and redox conditions, as well as conformity with the SOFC structure. The sensors were used for measuring, and the accuracy was 0.2% for the current and voltage measurement and 2 Kelvins for the temperature. The scan rate of voltammetry was 1A s⁻¹.



Fig. 3. Experimental setup used for electrochemical measurements.

The anode, electrolyte, and cathode were made of nickel-YSZ cermet, dense YSZ, and Strontiumdoped Lanthanum Manganite (LSM), respectively. Silver paste and silver mesh were used as a current collector on the anode and cathode side of the fuel cell. The properties of a solid oxide fuel cell and test conditions are seen in Table 2.

parameter	Value
Test conditions of SOFC	
Furnace Temperature	800 °C
Operating Pressure	1 Atm
Minimum Current Density	1000 A/m^2
Maximum Current Density	7000 A/m^2
Methane Flow	40 cm ³ /min
Steam Flow	60 cm ³ /min
SOFC Properties	
Anode Thickness	400 µm
Cathode Thickness	25 µm
Electrolyte Thickness	15 µm
Diameter	2.5 cm
Active Area.	1 cm^2
Porosity	0.35
Heat Conductivity	5.4 W/(m.K)

Table 2. Test Condition and SOFC Parameters

Activation of the anodewas performed with hydrogen. In the first step, hydrogen was purged at a molar ratio of 5% for 2 hours. The activation continued with pure hydrogen.

4. Results and discussion

Using methane as a fuel can cause carbon deposition and the fast degradation of the SOFC. The most important factor in carbon production is the S/C ratio. In the present study, the distribution of reactant concentrations, temperature distribution, and the rate of reforming reactions was studied since they greatly effect on SOFC performance and its degradation. In this regard, the effect of the Reynolds number on the inlet fuel flow, current density, porosity, and steam to carbon ratio of the inlet flow were investigated. In mentioned parameters, the results of the different values of the parameters were compared with the base state, which is based on the conditions presented in Table 3.

Table 3. Values of Base-state Parameters

Parameter	Value
Current Density	6000 A/m ²
Porosity	0.35
Reynolds Number of Inlet Fuel Flow	10
Steam to Carbon Ratio	1.5
Furnace Temperature	800 °C

The values for the base state parameters are derived from the information presented in Table 2, and the current density value of 0.7 V.

4.1. Validation

For using developed model to evaluate of different parameters effect, the validity of the model should be verified. Therefore, the results obtained from the model should be compared with laboratory results. Thus, a fuel cell was prepared with the specifications presented in Table 2 and was analyzed by using the experimental setup. In this experiment, the methane fuel flow was a 40ccm and 60ccm steam, and the inlet temperature was 100 ° C. As shown in Fig. 4, the experimental results were compared with the numerical results, and the model was shown to have an acceptable accuracy, with the highest error being 2% at 5000 A/m² current density and a minimum error of 0.1% at 6000 A/m².



Fig. 4. Validation of numerical result by experimental data.

4.2. Base state

Due to the heat and mass sources caused by the reactions in the fuel cell, temperature and mass gradients are much higher in the area where the fuel cell is located than in other areas. In this regard, and with the aim of showing better changes, the results obtained for this area have been presented and examined. On the other hand, considering the dimensions of the fuel cell and the importance of temperature and reactant concentrations on MSR reaction rate , variation in temperature and concentration of gases are shown in three areas with magnification in each figure. These three zones are the center of the active and inactive area and the border between them.

Fig. 5 demonstrates the changes in the concentration of the gases and distribution of temperature in the base state. Since electrochemical reactions occur only in part of the fuel cell active area, the SOFC is divided into two areas, active and inactive. Due to the difference between heat and concentration sources in these two areas, the temperature and concentration of gases are different. In this regard, the rate and gradient of temperature, and gas concentrations at the centers of the two regions and the boundary between them were different (Figs. 5-13).

Fig. 5a shows the changes in methane concentration. Due to the concentration resulting from the reforming process, the lowest methane concentration is in the active area of the SOFC, with the lowest concentration at its center reaching 0.065 kg/m³. However, the concentration of steam (Fig. 5b) increases despite consumption during the reforming reaction, with the highest concentration of steam at the center of the cell being 0.48 kg /m³, which is related to its production during the electrochemical process. Figs. 5c and 5d show the changes in the concentration of carbon monoxide and hydrogen. These gases are consumed by electrochemical reactions and produced by reforming reactions, and the concentration of the two gases at the inlet is zero. Electrochemical reactions take place at the active area and in the center of the fuel cell, and therefore the consumption of hydrogen and carbon monoxide is higher in this area. As a result, the concentration of these two reactants at the end of the fuel cell is higher, so that the concentration of hydrogen reaches 0.14 kg/ m3 and the concentration of carbon monoxide reaches 0.06 kg/m3. while it reaches the highest in the upper and lower parts, with a concentration of hydrogen of about 0.14 kg/m³, and a concentration of carbon monoxide of 0.06 kg/m³. Changes in carbon dioxide concentration are shown in Fig. 5e, as carbon dioxide is produced through the electrochemical reaction of carbon monoxide. The highest concentration of carbon dioxide is 0.22 kg/m³ at the cell center, The temperature changes are shown in Fig. 5f, the highest temperature being 1100 k at the core of the SOFC, due to the heat produced by electrochemical reactions.



Fig. 5. Concentration and temperature distribution for the base condition.

4.3. Current density

Current density plays a main role in the heat and concentration sources. Thus, it is considered as one of the most important parameters affecting the distribution of concentration and temperature. In this regard, simulations were performed for two current densities, 2000 A/m² and 4000 A/m², except in the basic state in which the current density was 6000 A/m². The results of distributing concentrations and temperatures are

shown in Figs. 6 and 7, and the results of the rate of the reforming process are illustrated in Fig. 14a. Based on the obtained results, by varying the current density and changing concentration and thermal sources, the balance between the concentrations changes as the current density increases from 2000 A/m² to 6000 A/m², leading to an increase in the rate of electrochemical reactions. This results in increasing hydrogen and carbon monoxide consumption and heat production, as well as, changing the hydrogen concentration from 0.0575 kg/m³ to 0.0425 kg/m³, the carbon monoxide from 0.1225 kg/m³ to 0.105 kg/m³ at the center of the cell, and the temperature from 1080 k to 1100 k. On the other hand, as the temperature increases and the concentration of hydrogen and carbon monoxide decreases, the reforming reaction rate increases from 10.7 mol.m⁻³.s⁻¹ to 12.4 mol.m⁻³.s⁻¹ at the center of the cell, leading to a decrease in methane concentration from 0.1 kg/m³ to 0.065 kg/m³. An increase at the rate of electrochemical reactions leads to an increase in steam and carbon dioxide production, which results in increasing the concentration of steam from 0.31 kg/m³ to 0.48 kg/m³ and in carbon dioxide from 0.12 kg/m³ to 0.22 kg/m³ at the center of the SOFC.



Fig. 6. Concentration and temperature distribution for current density = 2000 A/m².



4.4. Steam to carbon ratio

Steam is necessary for the MSR process and producing hydrogen from methane. The amount of steam is determined by the S/C parameter, which represents the ratio of the steam to carbon moles. This parameter affects the performance of SOFCs since a low S/C ratio can lead to carbon deposition, and a high ratio causes fast degeneration of SOFCs. Thus, the effect of varying this parameter was investigated in the present study, and the required calculations were performed for the 3 different values of S/C. The results for the base state in which S/C equals 1.5 are shown in Fig. 5, and the results for the other values (1, 2) are presented in Figs. 8 and 9. Since an increase in S/C leads to a reduction in the concentration of methane at the inlet due to the constant pressure and flow, it decreased the concentration of methane in the cell core from 0.105 kg/m³ to 0.045 kg/m³. Accordingly, the decrease in methane concentration in the core of the cell reduced the MSR rate, (Fig. 14b), from 14.5 mol.m⁻³.s⁻¹ to 10.8 mol.m⁻³.s⁻¹ at the cell core. By decreasing the MSR rate, carbon monoxide concentrations decreases from 0.145 kg/m³ to 0.0725 kg/m³ and hydrogen concentration from 0.05 kg/m^3 to 0.0325 kg/m^3 at the SOFC core.



Fig. 8. Concentration and temperature distribution for S/C = 1.



Fig. 9. Concentration and temperature distribution for S/C = 2.

4.5. Porosity

The porosity in the anode is very important for the penetration of reactants into the active area of the cell and to engage in electrochemical reactions. Since the porosity is 0.35 for the basic state and is in the range of 0.3-0.4 in different studies, simulations for 0.3 and 0.4 porosity were performed. The results are shown in Figs. 10, 11, and 14c.

Reducing the porosity by diminishing the diffusion leads to a decrease in the concentration of methane in the fuel cell, but on the other hand, it leads to a decrease in water outflow and heat transfer outside the fuel cell. This results in an increase in the concentration of water and temperature in the fuel cell. So that, methane concentration decreased from 0.07 kg/m³ to 0.06 kg/m³, steam concentrations ranged from 0.47 kg/m³ to 0.50 kg/m³, the temperature increase from 1090k to 1110k. However, the changes in concentrations of hydrogen and carbon monoxide were negligible because their sources of consumption and production are in the cell.

An increase in temperature and water concentration enhanced the MSR reaction rate (Fig. 14.c) at the cell center because of increasing temperature, but this change was slightly (from 12.4 mol.m⁻³.s⁻¹ to 12.8 mol.m⁻³.s⁻¹) due to the decrease in methane concentration and its negative impact.



Fig. 10. Concentration and temperature distribution for $\varepsilon = 0.3$.



Fig. 11. Concentration and temperature distribution for $\varepsilon = 0.4$.

4.6. Reynolds number of the Inlet flow

A parameter that greatly affects the concentration distribution of reactants is the Reynolds number. As the flow rate increases, the concentration of methane as the main reactant in the MSR reaction increases. Since the Reynolds number is 10 for the the base state, the calculations in the simulation were performed for two Reynolds numbers, 5 and 15, and the results for the concentration distribution are shown in Figs. 12 and 13.

Since the Reynolds number depends on pipe diameter, flow rate, and kinematic viscosity of the fluid, an increase of Reynolds number is done by adding the input speed due to the constant dimensions and conditions of the incoming fuel. As the input velocity increases, the fluid diffusion into the porous medium increases, and as a result, the gas concentration difference in the fuel cell and fuel channel decreases. By increasing the Reynolds number from 5 to 15, methane concentration changed from 0.03 kg/m³ to 0.09 kg/m³ and Steam concentration reached 0.48 kg/m³ from 0.49 kg/m³. Increasing methane concentration resulted in increasing the reforming reaction rate from 8.3 mol.m⁻³.s⁻¹ to 14.5mol.m⁻³.s⁻¹ (Fig. 14d).Asthereaction rate increased, the concentration of carbon monoxide rose from 0.065 kg/m³ to 0.11 kg/m³ and hydrogen concentration from 0.025 kg/m³ to 0.045 kg/m³.



Fig. 12. Concentration and temperature distribution for Re = 5.



Fig. 13. Concentration and temperature distribution for Re = 15.



Fig. 14. Methane steam reforming reaction rate along the cell length.

5. Conclusion

This research has been applied to a precise modeling approach to evaluate key parameters in methane steam reforming. Since the cost of testing SOFCs is high and the details obtained from experimental results are insufficient for analysis, a numerical model using LBM was used to simulate SOFC performance and the effect of the parameters on the concentration and temperature distributions, and reaction rates of the reforming. Based on the results, the temperature and concentration of the reactants in the two regions are different, due to the heat and concentration sources of the electrochemical reactions. The difference between reactants concentration of these two areas is high, and the temperature of the active area is higher than in the inactive area. Even by changing the parameters, the temperature in the active area is always higher, and the rate of the MSR reaction in this area is always more than in other areas. Among the various cases simulated, the lowest concentrations of methane, carbon monoxide, and hydrogen, and the highest concentration of carbon dioxide occur at a Reynolds number of 5, which is due to the reduction in rates of mass transfers of reactants and the reaction products. In this case, the MSR reaction rate at the center of the cell is 8.3 mol.m⁻³.s⁻¹. The highest concentrations of methane and carbon monoxide happened when S/C equals 1. In the case, the high concentration of methane at the inlet results in increasing methane concentration in the SOFC, as well

as a high rate of reforming reaction, 14.5 mol.m⁻³.s⁻¹, at the center of the cell, leading to high levels of carbon monoxide concentration. In addition, when the Reynolds number is equal to 15, the reaction rate is about 14.5 mol.m⁻³.s⁻¹ in the center of SOFC because of high concentrations of the steam and methane and current density of 2000 A/m² produced the highest concentration of hydrogen and the lowest concentrations of the steam and carbon dioxide, and the lowest temperature at the center of the cell, which was related to the low electrochemical reaction rate. In this case, the reforming reaction rate was low, 8.7 mol.m⁻³.s⁻¹, due to low temperature of active area.

Nomenclature		Greek symbols
discrete lattice velocity	α	transfer coefficient
molar concentration (mol m ⁻³)		porosity
grain size(µm)	η	overpotential (V)
overall effective diffusion coefficient of species (m ² s ⁻¹)	ρ	density (kg m ⁻³)
		characteristic length parameter for interaction (Å)
diffusion coefficient between species i and species j (m ² s ⁻¹)		relaxation time
	ω	weighting factor
mass diffusion coefficient for species i in the mixture		collision integral
$(m^2 s^{-1})$		
Knudsen diffusion (m ² s ⁻¹)		Subscript
pore size (µm)	а	anode
reversible potential(V)	AA	active area
activation energy of anode (J mol-1)	act	activation
activation energy of cathode (J mol ⁻¹)	с	cathode
Faraday constant (9.6485 * 10 ⁴ C. mol ⁻¹)	conc	concentration
distribution function	ohm	ohmic
external force		
local equilibrium distribution function		Superscript
exchange current density (A/m ²)	eq	equilibrium
lattice model direction	Ι	interface
velocity coefficient of forward reaction		
velocity coefficient of backward reaction		Abbreviations
coefficients for exchange current density of the anode	cd	current density (A/m ²)
coefficients for exchange current density of the cathode	LBM	Lattice Boltzmann method
effective thermal conductivity (W $m^{-1} K^{-1}$)	MSR	methane steam reforming
fluid media heat conductivity coefficient (W $m^{-1} K^{-1}$)	RR	rate of reaction
porous media heat conductivity coefficient (W m ⁻¹ K ⁻¹)	SOFC	solid oxide fuel cell
	WGS	water gas shift reaction
thickness of electrolyte (µm)		
molecular weight (kg mol ⁻¹)		Chemical
Pressure (bar)	CH_4	Methane
universal gas constant (8.3145 J mol ⁻¹ K ⁻¹)	СО	carbon monoxide
catalyst particle size(µm)	CO_2	carbon dioxide
absolute temperature(K)	H_2	Hydrogen
molar fraction of species i	H_2O	Water

Number of electrons involved in the reaction

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