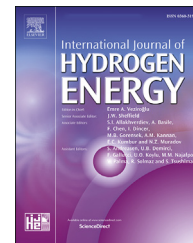


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Three-dimensional numerical simulation and experimental validation on ammonia and hydrogen fueled micro tubular solid oxide fuel cell performance

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HIGHLIGHTS

- Numerical and experimental investigation of MT-SOFC has been conducted simultaneously.
- The performance of AS-MT-SOFC is superior next to CS-MT-SOFC.
- The effect of working cell temperature is more influential than the operating pressure.
- The predicted maximum possible power density for direct ammonia fed is very close to hydrogen.
- The numerical result suggested that ammonia will be the primary fuel for SOFCs.

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ABSTRACT

The main aim of this research is to investigate the performance of ammonia-powered microtubular solid oxide fuel cells in order to use ammonia as a possible candidate for eco-friendly and sustainable power generation systems. The performance of a direct ammonia-powered cell has been elucidated and validated with the experimental results of pure hydrogen gas at Nigde Ömer Halisdemir University Prof. T. Nejat Veziroğlu Clean Energy Research Center. For both studies, the cathode electrode is supplied with atmospheric air. The performance of anode, electrolyte, and cathode-supported microtubular solid oxide fuel cells has been compared numerically. The findings confirmed that the peak possible power densities obtained numerically using direct ammonia, hydrogen and experimentally using pure hydrogen gas are 628.92 mW/cm², 622.29 mW/cm² and, 589.28 mW/cm² respectively at the same geometrical dimensions, component materials, and operating parameters. Thus, the results of this study demonstrate that simultaneous experimental and numerical studies make a great contribution to minimizing biases due to literature data during model validation. The numerical simulation also indicates that the performance of cathode supported is superior to that of anode supported cells run with hydrogen and ammonia fuel. Likewise, parametric sweep analysis asserts that the working temperature has a greater effect than operating pressure on tubular cell performance.

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Therefore, the results of this study advise that ammonia will become a carbon-free alternative fuel for solid oxide fuel cells in the coming years.

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Nomenclature

i	Current density, A/m ²
i_0	Exchange current density, A/m ²
E_{Nernst}	Nernst voltage
Ni-YSZ	Nickel- Yttria stabilized zirconia
YSZ	Yttria stabilized zirconia
LSM	Lanthanum Stabilized Manganite

Greek Symbols

η_{act}	Activation overpotential, V
η_{ohm}	Ohmic overpotential, V
η_{con}	Concentration overpotential, V
α	Transfer coefficient

Abbreviations

AS- MT-SOFC	Anode Supported Micro-Tubular Solid Oxide Fuel cell
CS-MT-SOFC	Cathode-Supported Micro-Tubular Solid Oxide Fuel cell
ES- MT-SOFC	Electrolyte Supported Micro-Tubular Solid Oxide Fuel cell
H ₂ -MT-SOFC	Hydrogen-Fueled Micro-Tubular Solid Oxide Fuel cell
MT-SOFC	Micro -Tubular Solid Oxide Fuel Cell
NH ₃ -MT-SOFC	Ammonia-Powered Micro-Tubular Solid Oxide Fuel cell
PEN	Positive Electrode- Electrolyte- Negative Electrode
SOFCs	Solid Oxide Fuel Cells
TPB	Triple-Phase Boundary

different alternative fuels at higher efficiency. It is a fact that electrochemical cells are a promising nominee to solve the scarcity of fossil fuel resources and their adverse effects on the environment.

Solid oxide fuel cell (SOFC) is a solid-state ionic fuel cell device that works mainly at a higher temperature. Besides, they provide internal fuel reforming opportunities that have prodigious contribution in reformer allied cost minimization and enabling the use of different fuels in the systems. Additionally, they enable the application of inexpensive materials as a component of the fuel cell. They can also run with contagious fuels like carbon monoxide with minimal poisoning. Fundamentally, the geometrical configuration of SOFC has been classified into three. These are planar, tubular, and monolithic types. Among them, the planar type is simple for production and stacking in addition to delivering higher electrical efficiency. Nevertheless, the sealing and thermo-mechanical allied doubts are still needed further investigations. On the other hand, a Micro-tubular solid oxide fuel cell (MT-SOFC) can solve the sealing difficulties and thermochemical aligned snags faced in planar [1–4]. As well, MT-SOFC has the capability to generate higher volumetric energy density coupled with higher thermomechanical shocking resistance, short thermo-cycling process, fast start-up, and shut-down time over the planar types. They are also manageable and applicable everywhere when there is energy in demand.

MT-SOFCs are also ceramic-based electrochemical energy converters designed as cathode supported (CS), electrolyte supported (ES), anode supported (AS), and metal-supported (MS) with concentric small tube shapes. They are operated at moderate and high temperatures using a variety of alternative fuels. They offer numerous advantages over other SOFC applications [3]. As a result, recently, the mechanical strength and electrochemical characteristics of the cells are investigated for use in APU devices for future vehicles [5]. The volumetric power density of T-SOFCs has a non-linear relationship with cell diameter [1]. As a result, the diameter of the cell is reduced as much as possible with considerable adequate strength for mechanical support.

They are developed and manufactured with sub-millimeter to millimeter diameter to enhance the volumetric power density, thermal shock resistance, and start-up time. They are mainly fabricated using customary extrusion and coating practices. However, according to the report of numerous studies, MT-SOFC has been developed with a huge discrepancy in tube diameter, cell length, and positive electrode-electrolyte-negative electrode (PEN) thickness. The thickness of the anode predominantly varies from 200 to 300 μm but it is also reported from 130 μm to 2 mm. As well,

Introduction

Presently, the bulk energy demands of our world are intrinsically gratified through fossil fuels combustion using conventional power generating devices. Further, the demand for comprehensive energy is swiftly snowballing from time to time connected with people's economic and life quality enhancement. Nonetheless, the ignition of fossil fuels is the major cause of environmental alteration due to toxic, acid, and greenhouse gas emissions. Therefore, searching for eco-friendly renewable energy sources coupled with efficient and affordable technologies is an immediate solution for contemporary energy demand and environmental obliteration. In line with this, fuel cell technology is fascinating more thoughtfulness as green energy generating devices use

the inner diameter of the tubular cell is centered about 2 mm but it diverges from 0.8 mm to 2.2 mm. The cell length also diverged from a few millimeters to 160 mm [6]. These wide discrepancies of MT-SOFC geometric parameters may be allied with the abilities of fabrication and the absence of comprehensive understating on the relationship between the cell performance and geometries.

Different numerical and experimental characterization of SOFC performance has been conducted and published for the scientific community that can browse elsewhere [7–21]. Among them, Ni [22] has developed a 2D thermo-electrochemical model of NH_3 -SOFC to examine the electrochemical reactions, thermal decomposition of ammonia, fuel flow rate, mass, and heat transfer. The results show that higher power output can be obtained when the inlet temperature of NH_3 -SOFC is increased, but the gradient near the SOFC inlet is significantly higher. Furthermore, their work realized that the performance of the NH_3 -SOFC decreased slightly when the intake velocity was increased from 1 m/s to 10 m/s. However, the temperature field was not greatly affected. This finding differs from different simulations that revealed that a reduction inflow rate could lead to a drop in temperature change [23]. Kishimoto et al. [24], have also studied the propagation of temperature, mass, flow, and electrochemical quantities within the cell using a 2D numerical model of NH_3 -SOFC. Their results show that SOFCs powered by direct ammonia and pre-decomposed ammonia have comparable performance. Further, Tan [25] investigated a 3D numerical simulation of SOFC using internally cracked ammonia as fuel to examine its performance. The results of the study show that the current distribution is poor due to the poor gas distribution in the air electrode. Hajimolana et al. [11], developed a dynamic model of NH_3 -T-SOFCs to study the electrochemical performance and its decomposition rate. Ammonia was found to perform almost identically to hydrogen fuel. Hence, ammonia is a suitable fuel candidate to replace hydrogen.

Zhang et al. [16], conducted a gas chromatographic study on NH_3 -AS-SOFC using a thin YSZ electrolyte. The experimental results confirmed that ammonia was completely decomposed into free hydrogen and nitrogen under the action of Ni catalyst before reaching the TPB. The results of different studies have also shown that the extraction of hydrogen from ammonia is not an ideal solution for fuel cells to operate at low temperatures. However, SOFC with a direct supply of ammonia and related chemicals is a more efficient and economical solution compared to other cells [26]. Further, Leung et al. [27], have reviewed various works on NH_3 -SOFCs for power generation. Their review proves that ammonia is both economically and technically feasible. Farhad and Hamdullahpur [28] have also studied a liquid ammonia-supplied AS-SOFC and 100 W have achieved using 0.8 L of ammonia at 0.73 V and 800 °C.

Wojcik et al. [20], have performed experimental work on NH_3 -T-SOFC using YSZ electrolyte at 800 °C and they were the first to share their experience. Their studies confirmed that the performance of an ammonia-powered cell using Pt electrodes without any catalyst is virtually the same as that of a hydrogen-powered one. Alongside, Fournier et al. [29], have investigated the performance of direct ammonia fuel cells and

obtained maximum power densities of 10 mW/cm² and 75 mW/cm² using 1 mm and 0.4 mm thick electrolytes, congruently. Dekker and Rietveld [30] also investigated the use of ammonia as a sustainable fuel for SOFCs using NiO-YSZ/YSZ/LSM-based PENs to study cell voltage as a function of current, temperature, and ammonia flow. The results of the study showed that ammonia improved cell efficiency by 13% compared to dry hydrogen. S.S. Shy et al. [31], have examined the power performance and electrochemical impedance of the pressurized NH_3 -AS-SOFC at different pressures and temperatures. Their results show that the power density of NH_3 -SOFC increases linearly with increasing operating temperature and pressure. Boersma and Sammes [32] also conducted an experimental study on the ammonia cracking performance of Ni between 500 and 800 °C. Studies have shown that Ni has very good performance compared to Ag and Pt, with 90% ammonia conversion at 800 °C. Consistent with this, Goodman and Choudhary [33] have realized that electrodes prepared from Ni can produce 5–10 times higher power density compared to Ag and Pt.

Zhang et al. [34], have fabricated AS-T-SOFC by extrusion method with 15 μm YSZ electrolyte and tested it with direct ammonia. The results confirmed a peak power density of 200 mW/cm² at 800 °C with no NO_x emissions, which is almost identical to the AS-T-SOFC supplied by hydrogen (202 mW/cm²). Ma et al. [35], also conducted an experimental study on liquid ammonia-fed AS-SOFC prepared by dry pressing method with 30 μm YSZ electrolyte. The results confirmed a power density of 299 and 526 mW/cm² at 750 °C and 850 °C, respectively. Kong et al. [36], have been studied MT-SOFC stability using operating temperatures and ambient pressure. Their outcomes confirmed that the probability of anode catastrophe has been observed at ambient pressures and working temperatures. Moreover, the thickness of the air electrode is as small as possible than the maximum thickness of the cathode to ensure the stability of the MT-SOFC.

According to the finding of Sin et al. [5], the ceria-based MT-SOFC that runs with humidified hydrogen gives a maximum power density of 1.3 W/cm² at 550 °C. The study also indicates that the ohmic polarization of the cell is 0.2, 0.6, and 1 V at cell temperatures of 550, 500, and 450 °C respectively. Timurkutluk et al. [37], have been produced AS-MT-SOFC via extrusion method and tested by pure hydrogen to characterize the cell's performance at an operating temperature of 800 °C. The influence of anode functional coating thickness on the tubular cell performance was also investigated. The plausible maximum power density achieved in their study is 500 W/m² at a single coating of anode functional layer. Likewise, Soydan et al. [4], have been also produced AS-MT-SOFC and characterized it in terms of performance, production, and cost analysis. The PEN materials used in this study were NiO-YSZ of the anode, YSZ of electrolyte, and LSM-YSZ of the cathode functional layer. The test has been performed using hydrogen gas at a temperature of 700, 750 and 800 °C. Their result disclosed that the highest and lowest power density found is 251 W/m² and 190 W/m² at 800 °C and 700 °C respectively.

Furthermore, diverse fuels have been researched as possible energy sources for fuel cells [1,2,11,38–49]. Allied with this, some studies have been performed on pre-decomposed and direct ammonia-powered fuel cells, but

many of them have focused on flat designs. Likewise, several numerical modeling and experimental works have been done to examine the characteristics of MT-SOFC running with hydrogen and hydrocarbon fuels. This is because Micro-tubular cells have higher volume power density, mechanical stability, high resistance to thermal shock, higher active surface area, and no sealing problems compared to the planar type. However, in previous studies, numerical simulations and experimental studies were performed separately. As a result, published experimental data has been used for model validation which may lead to hasty conclusions. This shows that there is a lack of literature consisting of numerical modeling and experimental work performed simultaneously using similar geometry and operating parameters. For that reason, the central goal of the present article is to create a 3D numerical model of AS-MT-SOFC using COMSOL Multiphysics software based on the Batteries and Fuel Cells module described in the software. Simultaneously, the model performance has been characterized experimentally to validate the developed theoretical model and to examine the performance of ammonia as a possible direct fuel for MT-SOFC. This is because most studies are monolithic, i.e. numerical and experimental researches are not conducted simultaneously. Consequently, most of the theoretical model is validated and elucidated by the work of others that may deviate due to different PEN material and geometrical dimensions. Moreover, experimental results are not clearly listed in tables in the reported literature but are reported in the form of figures and graphs, which are prone to errors during digitization. A numerical study was also performed to compare the performance of AS, ES, and CS-MT-SOFC using ammonia and hydrogen to examine which supported tubular cells have better performance, which was not explicitly reported in the literature. Thus, this study plays a favorable role in filling the contemporary gaps in the discipline.

Numerical modelling and experimental characterization of MT-SOFC

A three-dimensional AS-MT-SOFC model has been developed using commercially available COMSOL Multiphysics software. The model is composed of anode, electrolyte, and cathode from inside to outside portion of the tubular cell. Therefore, the fuel goes through the inner anode tube and the air enters into the outer side of the cathode compartment. Numerical simulation analysis was also performed using this software. The material used for numerical simulations and experimental work is porous nickel oxide-yttria stabilized zirconia ceramic (NiO-YSZ), often used as an anode component in SOFCs. This is because nickel has a triple role; as a catalyst, electrode, and current collector. The anode thickness consists of anode functional coating and anode support thickness. The model has also a cathode layer of $\text{La}_{0.8}\text{Sr}_{0.2}\text{MnO}_3$ (LSM) and dense yttria-stabilized zirconia (YSZ) electrolyte that has been sandwiched between the electrodes.

For this experimental characterization, AS-MT-SOFCs manufactured at Niğde Ömer Halisdemir University Prof. T. Nejat Veziroğlu Clean Energy Research Center were tested under pure hydrogen. The anode support micro-tube was

produced via the extrusion method. After pre-sintering at 1100°C , an anode functional layer was added via dip coating. Both anode layers were then co-sintered at a temperature of 1150°C . Similarly, the electrolyte layer was coated on the anode functional layer by dip-coating technique. The anode-supported electrolyte structure was then co-sintered at 1400°C . Cathode functional and current collecting layers were coated in the given order similarly. The cells were prepared for the performance tests after co-sintering of both cathode layers at 1050°C . The details of the micro-tubular cell fabrication and testing can be found elsewhere [35]. The numerical developed model and the fabricated cell used for experimental work are schematically presented in Fig. 1(a) and (b) respectively. The geometrical dimensions, numerical and fitting parameters are also displayed in Table 1 and Table 2 congruently.

In this work, a single AS-MT-SOFC is modeled numerically using finite element-based COMSOL Multiphysics software. As a well, to develop a reliable simulation model, coupled multiphysics variables are parameterized and evaluated to solve the partial differential equations. Further, the fundamental assumption considered during the numerical modeling is that pure ammonia is supplied into the anode whereas the atmospheric air is feeding into the side of the cathode under a steady state. Laminar flow is presumed in all conduits and reactants are considered as ideal and incompressible gases that operated under a constant temperature of 800°C . The model performance is characterized in terms of Butler–Volmer, incompressible Navier Stokes, and Brinkman equations. The basic control model equations as a function of the computational domain are shown in summary form in Table 3.

Results and discussion

The main aim of this research is to carry out numerical and experimental investigation on the performance of ammonia-powered micro tube solid oxide fuel cells (NH_3 -MT-SOFC) in order to use ammonia as a possible candidate for eco-friendly and sustainable power generation systems. The performance of NH_3 -MT-SOFC has been investigated numerically and compared with the experimental and numerical results of H_2 -MT-SOFC. The model is verified with the experimental results, and the fitting correlation between the numerical simulation results and the experimental results is presented in the form of figures. The electrochemical performance of the model and the test is elucidated and characterized as a function of power density and polarization curves. The model is developed and simulated using COMSOL 5.6, a commercial multiphysics software that employs the finite element method to discretize the partial differential equations. The analysis was performed using the built-in parametric direct solver using MUMPS, a linear system solver designed for multiprocessing architectures. Since the cell voltage is the input, a parametric solver in COMSOL is used to generate polarization and power density curves for a specific set of operating conditions.

Numerical simulations and experimental characterizations of MT-SOFCs have been systematically investigated using the same geometrical orientations and dimensions. The

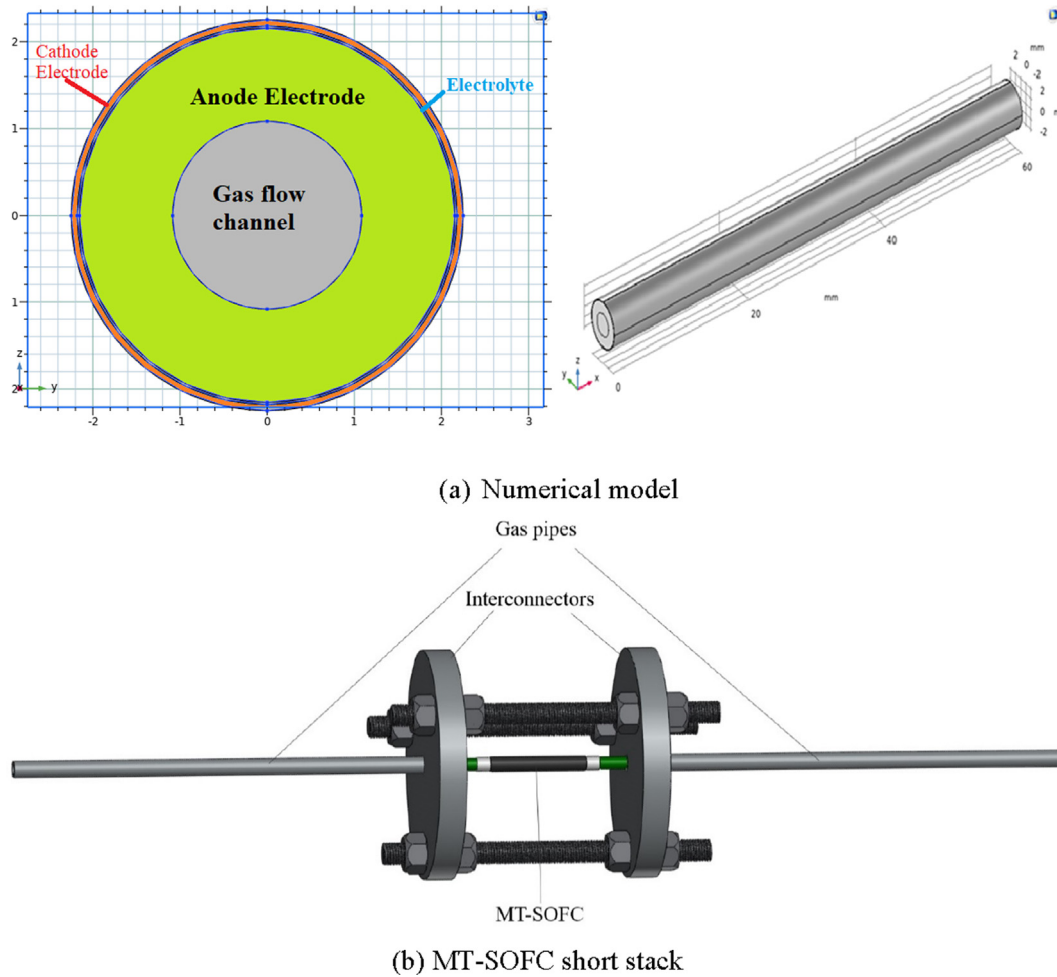


Fig. 1 – Micro-tubular solid oxide fuel cell schematically drawing.

Table 1 – Geometrical parameters.

Dimensions	ES-T-SOFC	AS-T-SOFC	CS-T-SOFC
	Size	Size	Size
Electrolyte Thickness	2 mm	160 μm	160 μm
Anode Thickness	20 μm	2.14 mm	160 μm
Cathode Thickness	20 μm	160 μm	2.14 mm
Inside Diameter	2.2 mm		
Cell Length	60 mm		

electrochemical cell performance was tested with pure hydrogen and atmospheric air coupled with a mass flow controller made by VESTEL. The tubular cells are heated with an electric furnace controlled by a thermocouple system, and the resulting electrical power output is measured by a potentiostat meter. The test is carried out at a working temperature of 800 °C under atmospheric pressure, which is the same as the theoretical modeling temperatures. The anode side is feeding with pure hydrogen at a flow rate of 0.8SLM and the cathode chamber is feeding with normal air at a flow rate of 1.6SLM. Similarly, an equivalent flow rate has been defined for numerical model analysis. Flow rate is a critical parameter that determines the performance of the fuel cell. Results show

Table 2 – Operating and fitting parameters used in modeling.

Parameters	Value
Initial cell polarization	0.05[V]
Inlet composition (Anode)	Pure ammonia gas
Inlet composition (Cathode)	Air (21% O ₂ , 79% N ₂)
Inlet Temperature	1073[K]
Pressure	1[atm]
Equilibrium voltage (Anode)	0[V]
Equilibrium voltage (Cathode)	1.1[V]
Reference diffusivity	3.16e-8m ² /s
Porosity	0.4
Electrolyte conductivity of SOFC	$3.34 \cdot 10^4 \exp\left(\frac{10300}{T}\right)$ [50]
Cathode exchange current density	1.2[A/m ²]
Anode exchange current density	6.2[A/m ²]

that the output power increases at higher fuel flow rates. This is usually due to a decrease in the concentration overpotential as additional hydrogen gas is supplied to the active reaction site. This effect can be seen more clearly in the high current density region where the concentration overpotential is effective. Accordingly, the open-circuit voltage accomplished

Table 3 – Governing equations.

Nernst voltage (E_{Nernst})	$E_{\text{Nernst}} = \frac{-\Delta G}{nF} - \frac{RT}{nF} \ln \left(\frac{\text{PH}_2\text{O}}{\text{PH}_2 * \text{P}\sqrt{\text{O}_2}} \right)$
Cell voltage (V_{cell})	$V_{\text{cell}} = E_{\text{Nernst}} - \eta_{\text{ohmic}} + \eta_{\text{act}} + \eta_{\text{con}} + \eta_{\text{conta}}$ Where, $\eta_{\text{ohmic}} + \eta_{\text{act}} + \eta_{\text{con}} + \eta_{\text{conta}}$ are the ohmic, activation, and concentration polarizations at cathode and anode electrodes
Bulmer-Volmer Equation	$i = i_{0,j} \left[\exp \left(\frac{n\alpha F \eta_{\text{act},j}}{RT} \right) - \exp \left(- \frac{(1-\alpha)nFj}{RT} \right) \right], j = a, c$ Where α is the charge transfer coefficient and $i_{0,j}$ is the exchange current density at the anode ($j = a$) and cathode ($j = c$).
Continuity Equation	$\frac{\partial(\epsilon_{\text{eff}} \rho)}{\partial t} + \frac{\partial(\epsilon_{\text{eff}} \rho u_i)}{\partial x_i} = S_m$
Momentum Equation	$\frac{\partial(\rho_{\text{eff}} u_i)}{\partial t} + \frac{\partial(\rho_{\text{eff}} u_j u_i)}{\partial x_j} = - \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left(\mu_{\text{eff}} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right) + S_{di}$
Energy Equation	$\frac{\partial(\rho C_p T)}{\partial t} + u_i \frac{\partial(\epsilon \rho C_p T)}{\partial x_i} = \frac{\partial}{\partial x_j} \left(k_{\text{eff}} \left(\frac{\partial T}{\partial x_j} + \frac{\partial T}{\partial x_i} \right) \right) + S_T$
Chemical species	$\frac{\partial(\rho C^k)}{\partial t} + \frac{\partial}{\partial x_i} (\gamma \rho u_i C^k) = \frac{\partial}{\partial x_i} \left[\rho D_{\text{eff}}^k \left(\frac{\partial C^k}{\partial x_j} + \frac{\partial C^k}{\partial x_i} \right) \right]$

in this experimental investigation is 1.02 V. This work can explain the drop in open-circuit voltage due to internal current leakage caused by electronic conduction through the electrolyte. Yet, the peak power density that has been obtained experimentally at 0.5 V is 589.28 mW/cm². At the same operating voltage, the maximum power accomplished numerically using pure hydrogen and ammonia as a primary fuel is 622.29 mW/cm² and 628.92 mW/cm², concurrently. The results of the work indicate that the maximum power variation between the numerical and experimental study of H₂-MT-SOFC is negligible. This suggests that simultaneous work on numerical simulations and experimental studies has a beneficial effect on reducing bias during model validation.

As illustrated in Fig. 2, the experimental and the numerical polarization curves of H₂-MT-SOFC are aligned together. However, when compared with direct ammonia fueled NH₃-MT-SOFC; there is a minor difference as illustrated in the figure. This is the fact that ammonia carries more hydrogen molecules. Ammonia has also overwhelmed doubts about hydrogen fuel production, transport, and storage. A similar pattern was also observed in the power density curves, which indicated that the peak power density for ammonia was slightly higher than that obtained with hydrogen. The foreseen reason this numerical modeling provides a maximum power density is because of having two basic layers i.e the anode support and anode functional layers. The anode functional coating plays a favorable role in activating the electrochemical reaction and smoothing the contact between the electrode and the electrolyte, thereby reducing the overpotential loss. Again, keep in mind that an appropriate functional layer of the anode has an immeasurable contribution to the mechanical strength of the tubular cell.

In addition to experimental validation of the model with pure hydrogen, the performance of the model was compared with the work of others reported in the literature. The purpose is to explore the variation during model validation using reported experimental data and simultaneously developed numerical models and experimental work. Related to this, Mohamed et al. [51], have been produced T-SOFC using phase inversion-based co-extrusion methods and characterized the

electrochemical performance of the fabricated hollow fiber cell using hydrogen and methane gas at 700–800 °C. Thus, the present model was also validated with the work of Mohamed et al. [51], who used similar PEN materials and working temperature. As can be seen from the figure, the performance of Mohamed et al. [51], experimental work is slightly higher than the experimental work of this study. The source of variation may be raised with the geometrical parameter difference and the methods of tubular cell production.

Tubular cells made with an anode support structure benefit from a thin electrolyte. This significantly reduces the ohmic loss due to the thickness of the electrolyte, resulting in relatively lower operating temperature and higher performance. The source of ohmic polarization is because of the resistance of ions and electrons to flow through the electrolyte and electrodes respectively. However, the main ohmic loss is the electrolyte, which can be reduced by minimizing the spatial separation between the electrolyte and the electrodes. Likewise, another key issue to reduce losses is to improve the ionic conductivity of the electrolyte. Lowering temperature significantly reduces the degradation of the cell, thereby prolonging the service life yet the performance of the cell is plummeting. In addition, the design has a thin cathode layer, which provides opportunities for custom cathode material formulations to improve performance or provide chemical resistance for a variety of applications. The disadvantage of increasing the thickness of the support is that it leads to mass transport glitches.

Unlike anode supported, electrolyte-supported cells have dense electrolyte, thinner anode, and cathode electrodes. The dense electrolyte allows for improved sealing at the cell's periphery thereby the efficiency losses due to leakage of reactant is declining. Diffusion resistance is greatly reduced by using a thin anode electrode. This combined with improved sealing allows for high single-pass fuel utilization which is not achieved in anode supported cells. Furthermore, because this design has thinner cathode and anode layers, it allows for the optimization of both materials for various applications. Therefore, it can contribute an imperative role to developing improved performance or chemically resistant

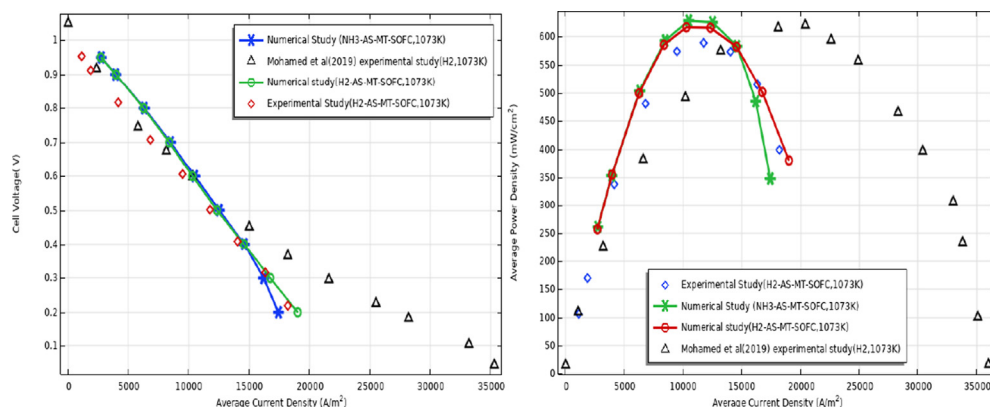


Fig. 2 – Performance comparison between the numerical and experimental study of ammonia and hydrogen-fueled AS-MT-SOFC.

anode and cathode formulations. However, the critical issues for ES are that thick electrolytes increase ohmic losses thereby the power density is reducing. As a result, it requires a higher operating temperature to achieve equivalent performance yet most materials are not suitable for higher working temperatures.

Concerning the aforementioned, the effect of AS, ES, and CS-MT-SOFC fed directly with ammonia was investigated and the performance comparison of ES, AS and CS-NH₃-MT-SOFC has been plotted in Fig. 3. The study was carried out by changing the types of support, while the thickness of the other components and the operating parameters remained unchanged. Simulation results confirm that the performance of the MT-SOFC is significantly improved when cathodic support is used compared to the other supports because it has a smaller cathodic ohmic polarization. The other associated reasons are the increase in the reduction electrochemical reaction zone, which is one of the critical criteria for fuel cell design. And also, a thicker cathode electrode is attributed to the electrolyte's sharp drop in the ohmic overpotential. Compared with AS, CS has less effect on the curvilinear power density drop at higher current densities, while AS has a significant effect on the curvilinear power density drop. This

suggests that the cathode support is more dominant than the anode support during fuel cell modeling.

Finally, the effect of electrolyte support on MT-SOFC working directly with ammonia was also investigated as a function of voltage-current and power-current curves. Numerical results show that the performance of MT-SOFC using ES decreases significantly due to the increase in electrolyte thickness. The large drop in power density is due to the larger ohmic losses caused by the thicker electrolyte layer. CS-MT-SOFC outperforms AS and ES-cell under the same cell voltage and working environment. However, it is more sensitive to operating temperature, which in turn requires a cooling system. The finding also confirmed that the performance of the anode-supported tubular cell has higher performance than those supported by an electrolyte as illustrated in Fig. 3. This suggests that the type of support has a significant effect on the electrochemical performance of the fuel cell.

Effects of operating parameters

A parameter sweep analysis has been performed to investigate the influence of operational pressure and temperature on NH₃-MT-SOFC performance. The influence of working

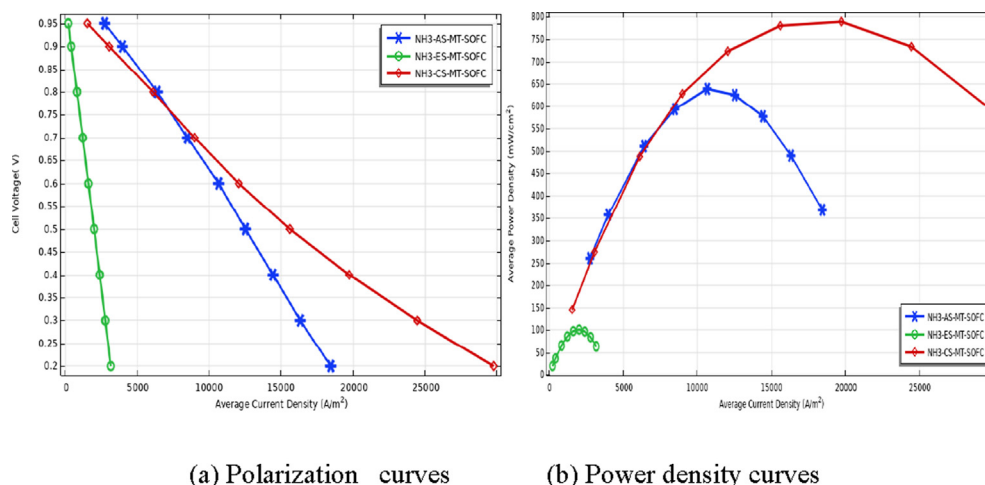


Fig. 3 – Performance comparison of ES, AS, and CS- NH₃-MT-SOFC under similar working conditions.

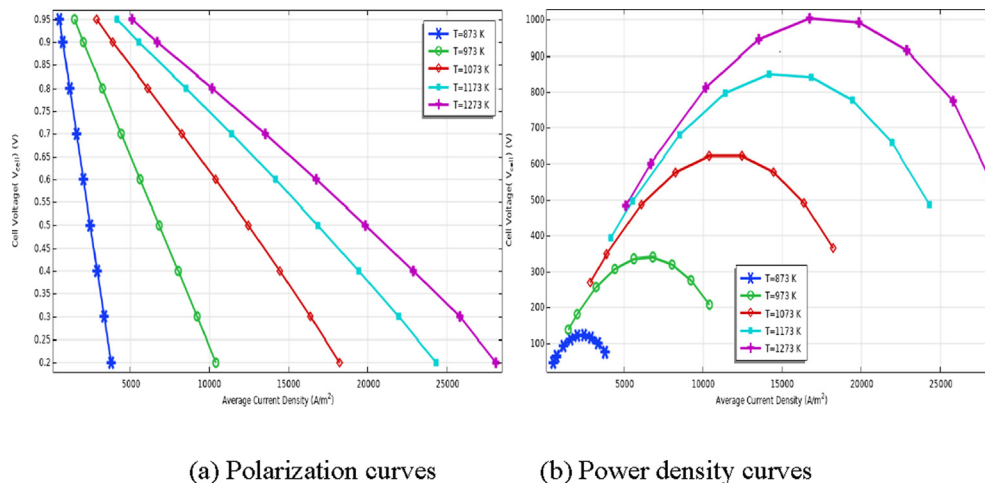


Fig. 4 – The effect of cell working temperatures on NH_3 -MT-SOFC performance.

pressure is changed from 1 to 10 atm whereas the operating temperature is varied from 600 to 1000 °C. The analysis indicates that the higher operating temperature allows fuel cells to produce more electrical power compared to lower operating temperatures with the same fuel and airflow rate. The maximum electrical power density is found to be 1000 mW/cm^2 at a cell operating temperature of 1000 °C, which is higher by far from the lower operating temperature tubular cells. The anticipated reason for this phenomenon is that the diffusion of reactive gases through the porous electrode and the diffusion of ionized gases through the electrolyte increase as the temperature of the electrochemical reaction increases. The fuel cell performance increases with temperature as properties such as activation energy, diffusivity, and ionic conductivity increase at higher temperatures, yet the current leakage through the electrolyte becomes more prominent in turn reducing the open-circuit voltages. This is because the operating temperature has the greatest impact on the kinetics of the reaction and the ionic conductivity of the electrolyte. In addition to this, a higher working temperature provides an opportunity to occur complete decomposition of ammonia. Likewise, the resistance of PEN components is decreasing, but

the performance of the cathode is strongly affected by temperature.

The polarization curve is expressed as a function of cell voltage and average current density, while the power density curve is mainly expressed in terms of average current density as displayed in Fig. 4. This finding also suggests that ammonia-fueled tubular cells require higher temperatures than the corresponding hydrogen supply. According to the Arrhenius equation, the operating temperature is directly related to the conductivity of the electrolyte. As a result, as the working temperature increases, the conversion of ammonia to free hydrogen also increases, thereby enhancing cell current production. The performance of the cell is also improved due to the increased gas diffusion coefficient at high temperatures. The hydrogen molecules reach faster at the reaction zone when the diffusivity of the reactant increases. Therefore, the reduction in mass transfer losses improves the performance of the fuel cells. Likewise, the resistive polarization of the electrolyte is decreasing, thereby improving the performance of the tubular cell.

Numerical simulations show that the resistive polarization of the cell is decreasing as the operating pressure increases.

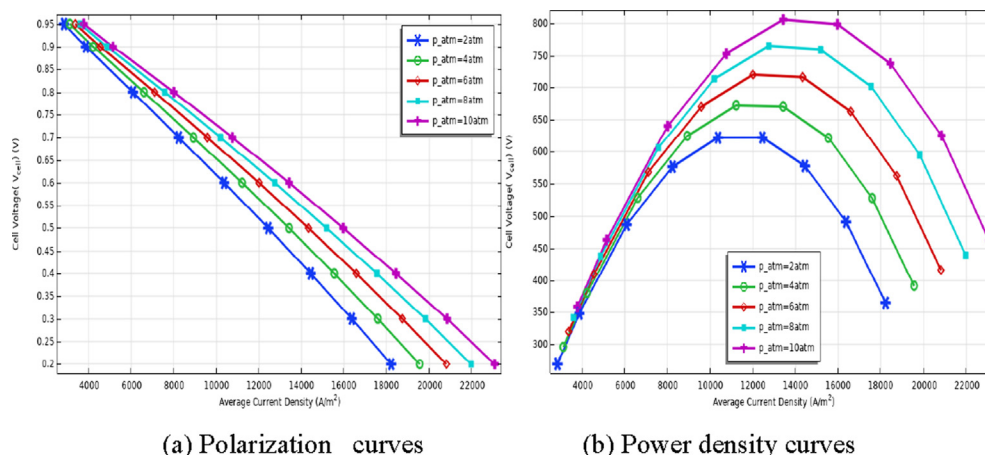


Fig. 5 – The influence of working pressures on NH_3 -MT-SOFC performance.

Related to this, at the same time, the diffusion through the porous electrode and the electrode surface coverage of the reactant species is increased. As well, the open-circuit voltage rises slightly as pressure rises. Consequently, the efficiency and power density increase with pressure. Nevertheless, the effect of pressure on cell performance is not as strong as that of operating temperature. Concerning this, when the working pressure changes from the design value to 10 atm, the power density changes from 628.92 to 800 mW/cm² with an increment of 27.2%. Yet, there is a 59% change in power density when the temperature is changed from 800 to 1000 °C. The current-voltage curve plotted in Fig. 5 shows that the cell produces a considerable amount of power.

Conclusions

In this study, numerical and experimental investigation of MT-SOFC has been conducted simultaneously. Pure hydrogen was used for the experimental work, and ammonia was directly fed into the anode for numerical simulation. The performance of NH₃-MT-SOFC has been elucidated and validated using hydrogen gas. For both studies, the cathode electrode is supplied with atmospheric air. The performance of AS, ES, and CS-MT-SOFC has been compared numerically. Accordingly, the finding of the study has drawn the following conclusions.

- Simultaneous work of experimental and numerical has been played a proportions role in reducing the deviation during model validation using literature data.
- The parametric sweep analysis indicates that the effect of working cell temperature is more influential than the operating pressure.
- The performance of AS-MT-SOFC is superior next to CS-MT-SOFC.
- The maximum possible power densities obtained numerically using direct ammonia and hydrogen are 628.92 mW/cm² and 622.28 mW/cm² respectively.
- The experimental (589.28 mW/cm²) and numerical results are nearly equivalent because of the same geometrical dimensions, PEN material, and operating parameters.
- The numerical result suggested that ammonia will be the primary fuel for SOFC in the coming soon.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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