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Optimal Operating Point of a Hydrogen Fueled SOFC Models Using Al-Nour Software

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Abstract: The solid oxide fuel cell (SOFC) is considered extremely suitable for electrical power plant application. Both high temperature (HT) and intermediate temperature (IT) SOFC performances are investigated using models which are built in Aspen customer modeller. Moreover, this paper introduces a new simulation software, called Al-Nour V.1.0-2012 software application. The interface of Al-Nour V.1.0-2012 software was mainly implemented based on the educational theory of User's Split Attention, that is; the entire software works with only one screen for all operations without any scrolling (user-friendly interface). This application reflects the fact that Al-Nour software does not require the user to have any previous training. The performance of HT-SOFC and IT-SOFC models is evaluated and compared using both software applications . The simulation results show that, the cell voltage value increases by raising the operating pressure, operating temperature, and hydrogen partial pressure. The electrical power output value from the SOFC is increased simultaneously by increasing the current density . Furthermore, the IT-SOFC has a higher cell voltage than the HT-SOFC.

نقطة التشغيل الأمثل لنماذج خلايا وقود الأكاسيد الصلبة باستخدام برنامج النور

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الملخص: تعتبر خلية وقود الأكاسيد الصلبة مناسبة للغاية لتطبيقات توليد الطاقة الكهربائية . لقد تم بحث اداء خلية وقود الأكاسيد الصلبة بنوعيها المرتفعة والمتوسطة درجة الحرارة باستخدام نماذج تم تصميمها في برنامج المحاكاة

المعروف (Aspen customer modeller) . بالاضافة الى ذلك ، فان هذه الورقة البحثية تقدم برنامج محاكاة جديد يسمى برنامج ا لنور (Al-Nour software) . تم تصميم واجهة الاستخدام في برنامج النور اعتمادا على عدد من النظريات التعليمية بحيث يشتغل البرنامج وبجميع جوانبه ضمن شاشة واحدة فقط . لذا فإن مستخدم برنامج النور ليس بحاجه لأي تدريب مسبق على كيفية الاستخدام . وبعد تقييم ومقارنة أداء خلية وقود الأكاسيد الصلبة بنوعيها المرتفعة والمتوسطة درجة الحرارة باستخدام كلا البرنامجين أظهرت النتائج ان مقدار جهد الخلية يزداد بارتفاع كل من ضغط الخلية ودرجة حرارتها و الضغط الجزئي للهيدروجين. وأن مقدار الطاقة الكهربائية المتحصل عليها من الخلية يزداد بالتزامن مع ازدياد كثافة التيار . كما ان جهد الخلية المتوسطة درجة الحرارة أعلى من جهد الخلية المرتفعة درجة الحرارة .

Keywords: *Fuel cells; SOFC; Modelling*

1. INTRODUCTION

Fuel cells, particularly solid oxide fuel cells, are free of ozone destructive emission **as** there is in principle no carbon monoxide or nitrogen oxide in the exhaust gas. In fact, only carbon dioxide and water steam are emitted, while traces of nitrogen oxide may be generated in residual combustion processes. These two species are greenhouse gases but the total amount is far less than with conventional plants due to the increase in efficiency [1] .

The Solid Oxide Fuel Cell (SOFC) is considered an excellent device for future plants, expected to produce clean electrical energy at high conversion rates, low emission and low noise levels. Yet SOFC technology must be improved in many ways so that both performance and reliability increase while cost remarkably decreases.

The operating temperature of high temperature solid oxide fuel cell (HT-SOFC) is between 950 and 1000°C because the YSZ solid electrolyte has low ionic conductivity at lower operating temperatures. The high operating temperature causes many serious problems, such as physical and chemical degradation of the electrode materials, and so it is desirable to develop SOFCs operating at or below 800°C. Such operating temperatures can be achieved by using an extremely thin but dense YSZ electrolyte or a more conductive electrolyte [2]. Several recent works focused on intermediate temperature solid oxide fuel cell (IT-SOFC).

In a previous paper [3], the validated numerical models for internally reformed HT and IT SOFCs are built in Aspen customer modeller and integrated in Aspen Plus™. The simulation results show that the electrical outputs from the SOFC and gas turbine are increased simultaneously by increasing the turbine inlet temperature.

This paper presents hydrogen powered solid oxide fuel cell models. This type of installation can be very suitable to complement the intermittent generation of renewable energies, such as solar or wind generation. So the validated numerical models for HT and IT SOFCs are built in bath Aspen customer modeller and the new approach to the development of a SOFC model, which is called Al-Nour V.1.0-2012 software application. These models give a precise description of every thermal and electrochemical process taking place inside the cell.

2. FUEL CELL MODEL

The current challenge is that the commercial process simulators (Such as AspenPluseTM, HYSYS software) do not have a model of basic SOFC stack. Therefore, to enable performing SOFC system simulation using one of the simulators, one must construct an SOFC stack model that can be implemented in them. The most common approach is to develop a complete SOFC model in a programming language (such as Fortran, C^{++}, Aspen customer modeller), and then link it to a commercial process simulator as a user defined model or subroutine.

This paper introduces a new approach through a novel software application, to develop a SOFC model that has been defined as Al-Nour V.1.0-2012 software application.

2.1 Al-Nour V.1.0-2012 software application

Al-Nour 2012 software has become an alternative to the current simulators that does not need any compiler or special equipment to act other than the Microsoft IE. It has been prepared using a number of sophisticated programming languages (DHTML, Java, and JavaScript) where the interface and mechanism of the software were implemented based on a number of theories in Educational technology and psychology.

2.1.1 Usability and Interface Design

The interface was mainly implemented based on the educational theory of User's Split Attention, that is; the entire software works with only one screen for all the operations without any scrolling (user-friendly interface). This application reflects the fact that Al-Nour 2012 does not require the users to have any previous training (see Figure 1) .

2.1.2 Skill and Ability Improvement

The user-friendly interface of Al-Nour 2012 and the simplicity of how to use it motivate the users to learn complex operations with less time and enjoy more to learn difficult operations. Based on our experience of using Aspen customer modeller, it is obvious that learning through Al-Nour 2012 is easier because of the presentation style of the input and output information, which is very clear and simple to deal with. Therefore, it improves the instructors' skills and abilities because they will be able to improve and change their way of teaching with their students.

2.1.3 Interactivity

Interactivity is a mutual action between the learner, Al-Nour 2012, and the learning material (the problems the learners are going to solve). Learners will be faster to learn, and have better attitudes toward learning when using Al-Nour 2012 especially when the other techniques like audio, video and the technology of the virtual-reality are embedded.

2.2 Modelling assumptions

The assumptions and conditions of the models used in the simulation program are as follows:

- Steady state conditions with negligible frictional losses;
- Negligible changes of potential and kinetic energies in any process;
- Changes in the composition of the anode and cathode gases are only significant in the flow direction;
- Oxidant and fuel are considered ideal gases;
- Nernst potential is independent of hydrostatic pressure graduations;
- The operating temperature of the cell is equal to the temperature of the outlet cathode and anode.

In a fuel cell, gaseous reactions are converted into product species, heat and electrical power. The calculation procedure of the model can be divided into three general parts: an electrochemical reaction calculation procedure, an electrochemical performance model calculation procedure and the mass and energy balance. The electrochemical reaction model takes into account all chemical reactions in the cell. The electrochemical performance model takes into account the effect of all forms of overpotential on the stack performance. It allows for determining cell losses, cell voltage, and heat source.

The calculation program involves the following procedures.

- Give gas stream inlet conditions and other inputs such as fuel utilisation factor and fuel cell area.
- Guess an initial operating temperature.
- Calculate the current density.

- Calculate the electrochemical reaction unknowns.
- Calculate the Nernst voltage and all cell losses in order to evaluate the cell voltage.
- Solve the mass and energy balance of the gas compositions to obtain the outlet gas temperature and operating temperature of the cell.

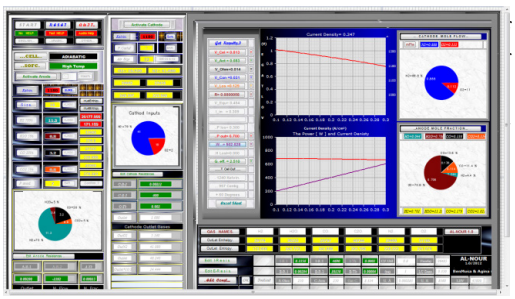

Figure (1). Al-Nour V.1.0-2012 software application

2.3 Electrochemical model

In the models, the chemical reactions are assumed to be in equilibrium, *i.e.* that they occur instantaneously and reach the equilibrium condition spontaneously at each position. For SOFC models the electrochemical reactions are as follows:

$$\tfrac{1}{2}O_2 + 2e^- \rightarrow O^{2-} \quad \text{cathode} \quad \text{..... (1)}$$

$$H_2 + O^{2-} \rightarrow H_2O + 2e^- \quad \text{anode} \quad \text{..... (2)}$$

$$H_2 + \tfrac{1}{2}O_2 \rightarrow H_2O \quad \text{overall reaction} \quad \text{..... (3)}$$

$$O + H_2O \Leftrightarrow O_2 + H_2 \quad \text{..... (4)}$$

The electrochemical and water-gas shift reactions are exothermic, their reaction rates should be calculated using the definitions of equilibrium constant and fuel utilization factor:

$$K_p = \frac{\gamma_{H_2} \times \gamma_{O_2}}{\gamma_O \times \gamma_{H_2O}} \quad \text{..... (5)}$$

$$z = u_f \left(\dot{n}_{H_2 in} + \dot{n}_{COin} \right) \quad \text{..... (6)}$$

The analysis of these two reactions is complex because their rates of reaction depend on the inlet molar rates, the fuel utilisation factor u_f, the operating temperature and operating pressure.

The equilibrium molar flow rates can be calculated using stoichiometric balance on the shift and electrochemical reactions:

$$\gamma_{H_2O} = \frac{\dot{n}_{H_2O,inlet} - y + z}{\dot{n}_{an}} \quad \text{..... (7)}$$

$$\gamma_{CO} = \frac{\dot{n}_{CO,inlet} - y}{\dot{n}_{an}} \quad \text{..... (8)}$$

$$\gamma_{H_2} = \frac{\dot{n}_{H_2,inlet} + y - z}{\dot{n}_{an}} \quad \text{..... (9)}$$

$$\gamma_{CO_2} = \frac{\dot{n}_{CO_2,inlet} + y}{\dot{n}_{an}} \quad \text{..... (10)}$$

$$\gamma_{O_2} = \frac{\left(\dot{n}_{O_2,inlet} - z/2\right)}{\left(\dot{n}_{ca} - z/2\right)} \quad \text{..... (11)}$$

$$\gamma_{N_2} = \frac{\dot{n}_{N_2}}{\left(\dot{n}_{ca} - z/2\right)} \quad \text{..... (12)}$$

2.4 Electrochemical performance model

The fuel cell is treated as a single control volume to which the steady state flow energy equation is applied with the assumption of negligible change of kinetic and potential energy. In order to determine cell performance, the overpotential must be deducted from the Nernst potential (E), which represents the ideal performance.

$$V_{cell} = E - V_{loss} \quad \text{..... (13)}$$

where

$$E = \frac{RT}{2F} \ln K + \frac{RT}{2F} \ln \left(\frac{p_{H_2} p_{O_2}^{1/2}}{p_{H_2O}} \right)$$

2.4.1 Evaluation of the overpotential HT-SOFC

The overpotential, which is a very important parameter in the analysis of fuel cell performance, is expressed by activation (V_{act}), ohmic (V_{ohm}) and concentration (V_{conc}) overpotentials. Activation

overpotential, which estimates losses due to slow electrochemical kinetics, is calculated as follows:

$$V_{act} = ai\exp\left(\frac{b}{T}\right) \quad \text{..... (14)}$$

Where $a = 2.83\times10^{-4}$ Ωcm^2 and $b = 8360$ °K are the coefficients which obtained by Solheim from experimental data from Umimura, and the temperature T. And it can be calculated according to [4].

Ohmic overpotential, which estimates losses associated with ionic and electronic resistance throughout the fuel cell, can be calculated according to [5].

$$V_{ohm} = iR_t \quad \text{..... (15)}$$

Please note that, fuel cell DC current (I) can be derived by the stoichiometric balance on the anode semireaction, assuming that all cells have the same behaviour. This current can be calculated in IR-SOFC by the mole number of the cell reactions, $\dot{n}_{H_2}$, $\dot{n}_{CO}$ and $\dot{n}_{CH_4}$, and the Faraday number. But in case of the external reforming ER-SOFC, there is no methane $\dot{n}_{CH_4}$ in the cell.

$$I = 2\left(\dot{n}_{H_2} + \dot{n}_O\right)F \quad \text{.....(16)}$$

The resistance of all materials used in the SOFC components can be calculated as follows:

$$R_t = \frac{a\delta\exp\left(\frac{b}{T}\right)}{A} \quad \text{..... (17)}$$

Where a and b are constants that are specific to the materials. δ is the equivalent thickness of the diffusion layer, and A is the active area. Some experimental data extracted from [7] are presented in Table 1.

Concentration overpotential, which estimates losses due to mass transport limitations, becomes significant when amounts of current are drawn from the cell, it can be calculated according to [5].

$$V_{conc} = -\frac{\overline{R}T}{n_eF}\ln\left(1-\frac{i}{i_L}\right) \quad \text{..... (18)}$$

2.4.2 Evaluation of the overpotential in IT-SOFC

The model of the IT-SOFC stack used in this paper is based on an existing IT-SOFC model [2]. In this model the cell utilises an electrolyte with a thickness of 25 μm, a 50-μm thick cathode, and a 250-μm thick anode. The cells are assumed to be stacked between bipolar interconnect plates. In contrast to HT-SOFC, which uses a ceramic interconnect, the IT-SOFC uses a lower operating temperature that allows the use of metal alloys. All cell losses are lumped together in one equivalent resistance. The cell resistance is assumed to have the following temperature dependence [4]:

$$R_{tot} = \mathrm{A}\exp\left(\frac{\Delta\mathrm{E}}{\mathrm{K}\times T}\right) \quad \text{..... (19)}$$

Where T represents the cell operating temperature and $\mathbf{K}$ is the Boltzmann constant. The activation energy ($\Delta\mathrm{E} = 1.01\times10^{-19}\,\mathrm{J}$) and the pre-exponential factor ($\mathrm{A} = 2.98\times10^{-4}$) were chosen to fit the experimental data reported by [4].

Figure 2 gives a schematic view of the SOFC. Incoming flows into the control volume are the anode and cathode inlet gasses, while the outgoing are the anode and cathode outlet flows. Electrical power is transported over the boundaries and heat can also be extracted (see Figure 2).

The First Law of Thermodynamics applied to the fuel cell stack in steady state conditions, then gives

$$\dot{Q} + \dot{W} = h_{a-in}(T_{a-in})\dot{n}_a + h_{c-in}(T_{c-in})\dot{n}_a - h_{a-out}(T_{a-out})\dot{n}_{a-out} - h_{c-out}(T_{c-out})\dot{n}_{c-out} \quad \text{.... (20)}$$

$\dot{W}$ is the electrical power, the indexes a and c stands respectively for the anode and cathode gases. $\dot{Q}$ is the heat transfer rate between the fuel cell stack and the surroundings. If the cell is adiabatic this heat transfer rate becomes zero ($\dot{Q} = 0$) and, assuming that anode and cathode gasses leave at the same temperature, (T_{out}), the energy balance simplifies to:

$$\dot{W} = h_{a-in}(T_{a-in})\dot{n}_a + h_{c-in}(T_{c-in})\dot{n}_a - h_{a-out}(T_{out})\dot{n}_{a-out} - h_{c-out}(T_{out})\dot{n}_{c-out} \quad \text{..... (21)}$$

The electrical power produced by the fuel cell is calculated by:

$$\dot{W} = V_{cell} I \quad \text{..... (22)}$$

The operating temperature of the cell (T) is equal to the outlet temperature of the cathode and anode. This approach is utilized by Kimijima et al [2005].

$$T = T_{out} \quad \text{..... (23)}$$

The value of T_{out} can be determined by solving the equations (21) and (22) simultaneously. The operating temperature of the cell is simply determined from the above equation (23), when the value of T_{out} is known.

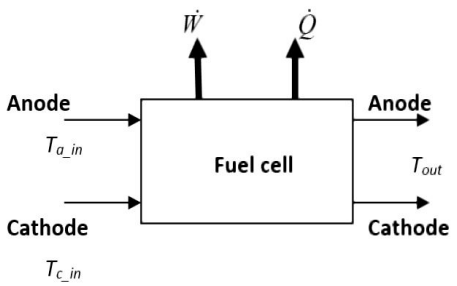

Figure (2). Schematic of thermodynamic analysis of SOFC stack.

Table (1). Calculation-based parameters for SOFC

Parameter	Value
Limiting current density (i_L)	350 mAcm^{-2}
Electrolyte Ohmic resistance constant	a = 0.00294 and b = 10350
Electrolyte thickness	δ = 0.004 cm
Interconnect Ohmic resistance constant	a = 0.1256 and b = 4690
Interconnect thickness	δ = 0.01 cm
Cathode Ohmic resistance constant	a = 0.00811 and b = 600
Cathode thickness	δ = 0.200 cm
Anode Ohmic resistance constant	a = 0.00298 and b = -1392
Anode thickness	δ = 0.015 cm

3. RESULTS AND DISCUSSION

The activation overpotential at different operating temperatures is shown in Figure 3 . The results show that the activation overpotential increases with increasing current density, but decreases with increasing operating temperature. Please note that Figure 3a is presented by Aspen customer modeller while Figure 3b is presented by Al-Nour 2012 software.

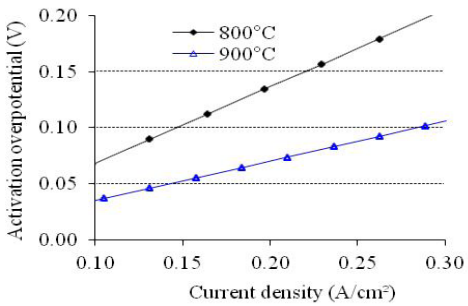

Figure (3a). Effect of operating temperature on activation overpotential of HT-SOFC (by Aspen customer modeller)

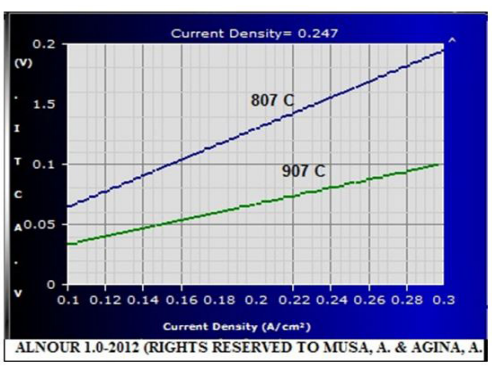

Figure (3b). Effect of operating temperature on the activation overpotential of HT-SOFC (by Al-Nour 2012 software).

The Ohmic overpotential at different operating temperatures is shown in Figure 4 . The Ohmic overpotential could be reduced by lowering the cell thickness or by increasing the operating temperature.

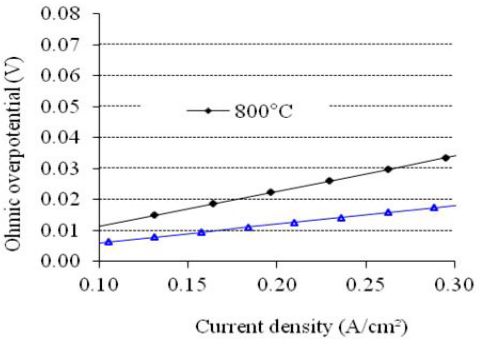

Figure (4a). Effect of operating temperature on the Ohmic overpotential of HT-SOFC (by Aspen customer modeller)

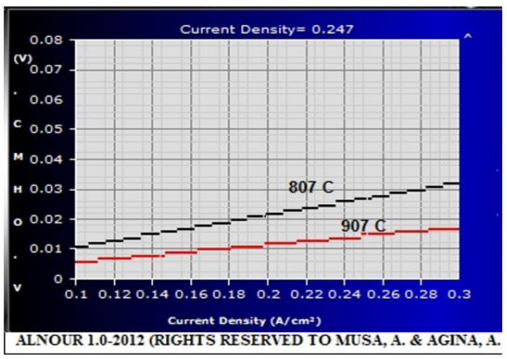

Figure (4b). Effect of operating temperature on Ohmic overpotential of HT-SOFC (by Al-Nour 2012 software)

The effect of the operating temperature on the concentration overpotential is given in Figure 5. The results show that the concentration overpotential increases with increasing current density and operating temperature. It can be seen that there is a significant increase in concentration overpotential when the operating of HT-SOFC approaches the limiting current density.

The performance of a fuel cell stack is usually described by plotting the well-known polarization curve, which relates the cell voltage to its current density. This plot is affected by all the typical overpotential losses (activation, concentration and ohmic) of the fuel cell under investigation and can be used to analyse their values. The polarization curve of the HT-SOFC used in the stack is presented in Figures 6 and 7.

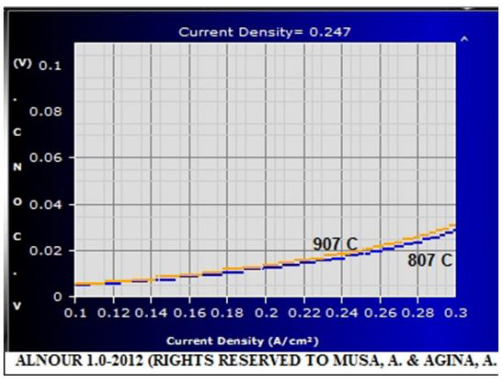

Figure (5). Effect of operating temperature on concentration overpotential of HT-SOFC

Figure.6 shows the performance of the HT-SOFC as a function of operating temperature in form of the cell voltage versus current density. As shown in the literature, Chan (2002), the results indicate that the higher the operating temperature, the lower will be the Nernst potential. As more current is drawn from the SOFC, however, a higher cell voltage can be maintained under higher temperature operation at the same current density.

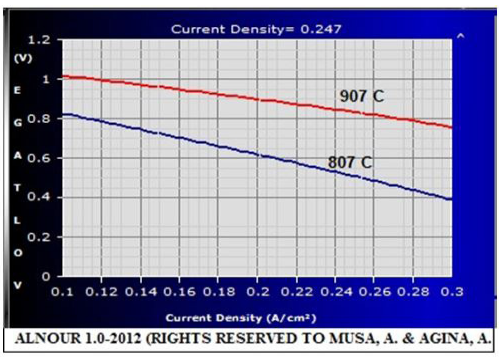

Figure (6). Effect of operating temperature on cell voltage of SOFC

Figure 7 shows the performance of the HT-SOFC

as a function of operating pressure. According to the Nernst equation, the cell voltage value increases by raising the operating pressure, hydrogen and oxygen partial pressure or by lowering the anode water mole fraction.

By increasing cell operating pressure, it is possible to get the best performance even if a higher cost must be taken into account, due to the energy and investment for compressors. Many other authors (Chan 2002; Kimijima 2005; Calise 2006) have proposed similar results.

Figure (7). Polarization curve of HT-SOFC at constant operating temperature T=907 °C

Figure 8 shows the relationship between the current density and the electrical output from the SOFC. The power or the electrical output from the SOFC is increased simultaneously by increasing the current density (eq.22).

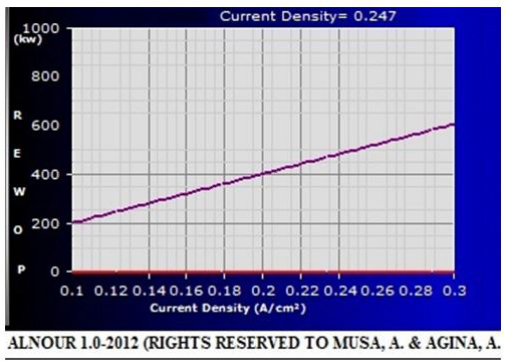

Figure (8). Electrical power produced by the cells as a function of current density

The HT-SOFC and the IT-SOFC models are simulated in order to evaluate and compare their performances. The simulation results show that the IT-SOFC has a higher cell voltage and power than the HT-SOFC (see Figure 9) , because of lower losses of a metal alloys, which is utilized as the electrolyte in the IT-SOFC model.

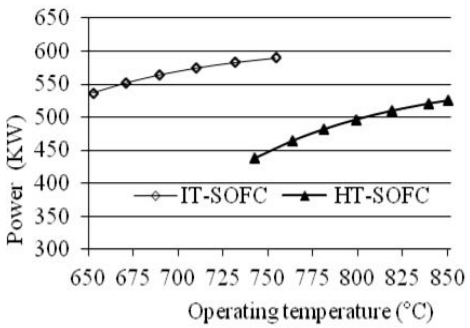

Figure (9). The SOFC models power as a function of operating temperature at current density= 0.250 A/cm³ (by Aspen customer modeller)

4. CONCLUSION

The high efficiency and lower pollutant emission feature of fuel cells compared to other technologies make them an attractive technology for energy generation. In this work a new approach to the development of a SOFC model, called Al-Nour 2012 software (version 1.0), is presented. This software has risen as an alternative that does not need any compiler or special equipment to act than the Microsoft IE. It has been prepared using a number of sophisticated programming languages (DHTML, Java, and JavaScript) where the interface and mechanism of the software were implemented based on a number of theories in Educational technology and psychology.

The simulation results show that the activation, the concentration and the Ohmic overpotential increase with increasing current density, but the activation, and the Ohmic overpotential decrease with increasing operating temperature. Moreover, the cell voltage value increases by raising the

operating temperature and operating pressure, but the high operating temperature causes many serious problems.

In addition, the HT-SOFC and the IT-SOFC models are simulated in order to evaluate and compare their performances. The results indicate that the IT-SOFC has a higher cell voltage and power than the HT-SOFC.

5. NOMENCLATURE

A_{cell}	active cell area (m^2)
E	Nernst potential (V)
F	faraday's constant (96487 kC $kmol^{-1}$)
g	molar Gibbs free energy (kJ $kmol^{-1}$)
h	specific enthalpy (kJ $kmol^{-1}$)
i	current density (A cm^{-2})
i_L	limiting current density (A cm^{-2})
p	partial pressure (Pa)
n	molar flow (mol s^{-1})
n_e	number of electrons participating in the reaction (Mole$^-$ mol^{-1})
$\dot{Q}_{cv}$	heat transfer rate in a control volume (kW)
$\dot{Q}$	heat (kW)
R_t	ohmic resistance of HT-SOFC material ($\Omega\ m^2$)
$\overline{R}$	universal gas constant (8.314 kJ $kmol^{-1}K^{-1}$)
R_{tot}	cell resistance of IT-SOFC satck-($\Omega\ cm^{-2}$)
T_{cell}	cell temperature (°C)
u_f	total fuel utilization
V_{cell}	cell voltage (V)
V_{act}	activation overpotential (V)
V_{ohm}	ohmic overpotential (V)
V_{conc}	concentration overpotential (V)
$\dot{W}_{cv}$	work transfer rate in a control volume (kW)
γ	mole fraction

Subscripts and Superscripts

0	at standard temperature and pressure
i	Initial
p	Product
R	reaction or reactants

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