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## Study of natural gas powered solid oxide fuel cell simulation and modeling

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# Study of natural gas powered solid oxide fuel cell simulation and modeling

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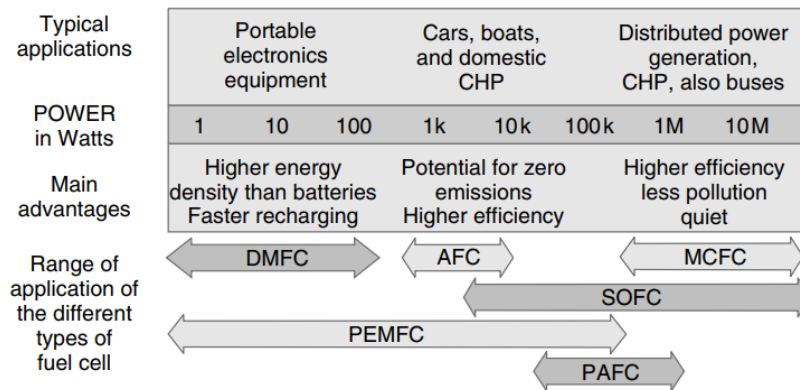
**Abstract:** Solid oxide fuel cell (SOFC) system has been proposed to address the issue of waste gas emission due to gas flaring in oil and gas industry. System has unique advantage of consuming the waste gases and generating electricity as by product. To analyze and quantify the proposed benefits, a robust cell performance model is highly desirable. A detailed understanding of SOFC component including electrode, electrolyte, interconnect, fuel processing and electrochemical reactions are first step in accurate determination of characteristic performance of the system. For this purpose, a review of modeling philosophies of SOFC system was undertaken in this study. Specifically, SOFC simulation and modeling using commercial software such as Aspen Plus, Aspen Hysys was focused in detail. SOFC models available in literature are either mathematical model or numerical models and ever evolving and improving. SOFC simulation rely on split approach due to absence of built-in module. Authors have developed an Aspen Hysys simulation model using split approach and discussed briefly here. Split approach approximates the SOFC phenomena, thereby inducing error. To overcome this deficiency, authors are developing a MATLAB based user model that can be integrated using 'user unit operation' available in Hysys. Details of the MATLAB program approach is included.

## 1. Introduction

Fuel cell is an old and proven technology that has been known to the mankind since 1938. Sir William Robert Grove is commonly referred as father of the fuel cell as he firstly demonstrated the concept using water electrolysis and reverse electrolysis that produces the electricity (1). Fuel cell technology has significantly grown ever since and offers promising pathways for inexpensive, safe and clean energy today with application from domestic electricity supplies to automobile to space to air travel and communication. Loosely based on type of electrolyte material used, fuel cell is categorized in different categories namely polymer electrolyte membrane fuel cell (PEM / solid electrolyte), Alkaline fuel cell (AFC / liquid electrolyte), direct methanol fuel cell (DMFC / solid electrolyte), molten carbonate fuel cell (MCFC / liquid electrolyte), Phosphoric acid fuel cell (PAFC / liquid electrolyte), Solid-Oxide Fuel Cell (SOFC / solid electrolyte) and have wide range of application, operating and usage. Among these, a PEM fuel cell is most common and acceptable type of the fuel cell. It consists of proton-conducting polymer electrolyte and precious metals such as platinum containing electrodes. A PEMFC has advantage of low temperature (<100 °C) and reliable operation. But even at a low concentration of carbon monoxide (CO) in ppm, can severely poisons anodes and reduce cell performance. Therefore, requirement of an ultra-pure hydrogen feed is prohibiting its wider application and technology maturity.

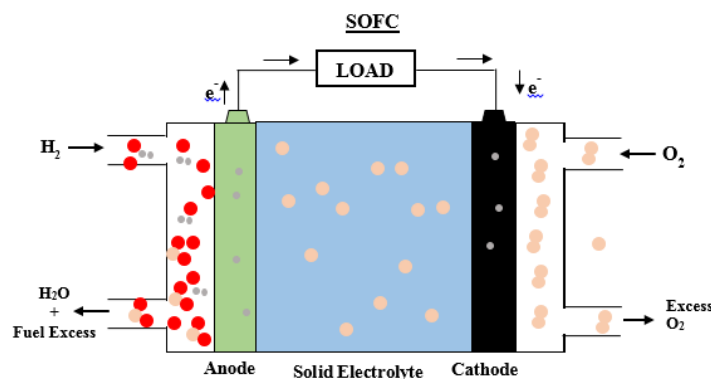


In contrast to PEMFC, a SOFC is quite tolerant to impurities including CO. SOFC utilizes a ceramic based solid electrolyte to transport oxygen-ions between electrodes. SOFC systems employ solid electrode and electrolytes and operation range 500-1000 °C (2). Because the solid materials, it involves only gas and solid only (binary phase). This makes it simpler system than all other type of fuel cells as. Due to its extended operating temperature range, SOFCs are preferable option for various CHP systems beginning sub kilowatt to multi-MW. A summary of the application of various fuel cells is given by Larmini and Dicks [2]. Overall impact of fuel cells becomes significantly more visible and important on CHP systems of any size and scale applications.



**Figure 1.** Applications and main advantages of fuel cells of different types, and in different applications [2]

As can be inferred from above figure 1, SOFC has a wider application advantage due to its high efficiency and high temperature of operation. A typical SOFC working principle is shown in Figure 2. The fuel is supplied at anode, while oxidant enters at cathode. Reduction of oxygen and oxidation of fuel takes place. The negative oxygen ion is transferred from cathode to anode. Water is formed as by product electron is released. The electron then passes through an external load to produce electricity.



**Figure 2.** Working principle of a SOFC fuel cell system

A summary of the reactions occurring in the cell given below [2]:

Overall reaction in the cell;



Anodic electrochemical reaction;



Cathodic electrochemical reaction;



Due to significantly higher temperature of operation and tolerance, any hydrocarbon fuels can in principle be used with minimum treatment or without rigorous external fuel oxidation and processing that produces hydrogen fuel. This feature of fuel processing elimination makes SOFCs technology attractive. This in turn allow various hydrocarbon fuel choices for fuelling a SOFC system. Notable fuel choices include, hydrogen, associated and non-associated natural gas, methanol, ethanol, biomass and liquid hydrocarbon mixtures such as gasoline, kerosene. Liso et al. [3] using methane, ethanol, methanol, gasoline as fuel option demonstrated the flexibility of a SOFCs performance. As summarized by Weber et al., important SOFC components that helps in understanding of processes includes type and nature of anode and cathode materials, electrolyte, metallic interconnect and sealing, materials [4-5]. A brief overview and review of recent progress is pre-requisite to understand and enable subsequent modeling of phenomena occurring inside the cell.

## 2. Key SOFC Component and Advancement

A details analysis and understanding of advancement in the major aspects of SOFC system is required to be able to understand the transport and reaction processes.

### 2.1. Anodic material

SOFC anode typically consist of composite ceramic based material. The requisite characteristic of an anodic material is highly porous material that support ionic transport of ions and electronics. The material should support and facilitate the movement of electron ion phases. Zirconia cermet is a default choice of anodic material and it consist of ceramic and nickel metallic component. There are two main reason why Ni is used as metallic phase in anode. Firstly, it possesses excellent stability and have high electronic conductivity. Secondly, it is highly stable in chemically active environment.

Electrons are released at anode-electrolyte interface boundary travels through the conducting phase. The oxygen ions get transported through the pores of the ceramic phase. Metallic phase material is crafted from catalytic active source and therefore support the heterogeneous reaction of the system. Performance of an electrode directly depend on the composition and structure of the phase. Hence a fine control mechanism is needed to produce a metallic phase of desired activity for electrodes [6]. Ionic phase, metallic phase and gas phase form a network of three-phase boundary. The control of this three-phase bouncy is essential to achieve desired anode characteristics and overall cell electrochemical performance. Anode SOFC material essential meet five characteristics features [7]. Firstly, it should provide active sites for catalytic activity. Secondly, it should have good electronic conductivity. Thirdly, thermal stability should be such as way that its thermal expansion properties are similar to hydrocarbon fuel and other components present in the system. Fourthly, it should have good mechanical stability and have high transport efficiency to / from the three-phase boundary. None of the currently used anode materials fulfil all these requirements. Due to its critical nature, search for an ideal anode material is going at a high pace. Together with cathode, anode is the most preferred aspect and area of current research.

Zirconia stabilized by Nickel / yttria (Ni / YSZ) is currently preferred anode material. Performance degradation with time, coking propensity of Ni for hydrocarbons, low tolerance to sulfur and other acidic compounds and volume uncertainty and instability are some of the major issues with this anode material (8). A number different anode materials involving different metallic phases are being proposed and

tested (9-11). For direct hydrocarbon operated systems, Ceria based anode material such as yttria (YSZ) or ceria doped samaria (YDC and SDC), are alternative choices for. As these materials possesses coking suppression abilities, they allow utilization of gaseous hydrocarbons including methane rich fuels with low steam requirement for fuel. Another alternative material with good characteristic features is Perovskite ceramics. A Perovskite ceramic can be described by a generic formula of  $ABO_3$ . The alphabet 'A' represents large cations such as Pb, La, Ca and Sr, alphabet B are small cations such as Co, Ti, Zr, Cr, Fe and Ni, As reported by Tao et al, Perovskite ceramics anode are tolerant to carbon deposition as well as poisoning by sulfur compounds (12). Nickel free Perovskite ceramics has comparable electrochemical performance (13, 14).

### 2.2. Cathodic materials

In the SOFC cell, cathode provides the site for reduction of the oxidant. The reduction releases ions that passes through the electrolyte to anode. Finding a suitable cathode material has been a challenge due to the nature of the requirements. Due to excellent corrosion and oxidation resistance characteristics, noble metals such as Ag, Ru, Rh, Au, Pd, and Pt were preferred choice of materials since the early stages of SOFC development. Due their prohibitive cost, these materials have been losing the application and are being replaced by alternate materials [15-18].

A cathode material should facilitate transportation of oxidant /  $O_2$  / air from the cathode entry channel for reduction at three-phase boundary of cathode and electrolyte. Materials such as strontium-doped lanthanum manganite (LSM) exhibits high catalytic efficiency for the dissociation of oxygen molecules and therefore used a material of choice.

Cathode material typically consist of perovskite materials such as strontium cobalt oxide ( $SrCoO_3$ ) or strontium-doped lanthanum manganite (LSM), which exhibits catalytic efficiency for the dissociation of oxygen molecules. Electrochemical performance of a cathode material depends on aspects such as materials composition, materials doping process, process condition of sintering, material density, surface morphology, and resistivity [19-23]. As search for an ideal cathode material goes on, above factors should be taken into account to develop a new material.

### 2.3. Electrolyte materials

In a SOFC system, anode and the cathode layers are separated by a solid layer of electrolyte material. The electrolyte typically consists of a ceramic material that restrict the gas transport, while supporting the ion movement. Any gas transport would lead to thermal oxidation of the fuel resulting in release of heat and loss of fuel. This fuel would have contributed to the electrochemical process and produced electrical energy. Therefore, a desirable electrolyte material should possess excellent ionic conductivity to facilitate movement of oxygen ions from one end of the electrolyte to the other end. As oxidants enters from cathode side, oxygen ions are produced at the interphase of cathode and electrolyte. While fuel enters at the anode side, and these ions are consumed at the interface of anode and electrolyte. As electrons will be produced at the anode and electrolyte boundary by the oxidation of the fuel, the electrolyte material should not possess any electronic conductivity. Even with a low electronic conductivity, electrons will diffuse through the electrolyte layer to the cathode side and might not pass through the external load causing loss of potential.

An electrolyte material should be stable in oxidizing environment existing at the cathode – electrolyte interphase and reducing environmental existing at the anode – electrolyte interphase. YSZ is currently choice of electrolyte material as it possesses excellent stability in both oxidation and reduction environments present in the system [24-29]. The search for an ideal electrolyte is ongoing and a lot of research studies are being undertaken. Thin film electrolyte (~10  $\mu m$ ) are preferred electrolyte choice of research studies as thickness reduces the ohmic losses.

### 2.4. Metallic interconnect material

There are two main functions of a SOFC interconnect. Firstly, it provides an electrical contact between the anodes of one individual cell and cathode of the neighboring cell. Secondly, it acts as a physical barrier for the protection of the cathode / anode material of one individual cell from the reduction /

oxidation of the neighboring fuel / air channel (30). Therefore, stability of interconnect materials in oxidizing and reducing environments is pre-requisite and must be fulfilled. Additionally, it provides structural support to the stack material. Cost contribution of interconnects can be significantly in a stack overall cost and depends on system's operating conditions. Sophisticated refractory alloy or ceramic based materials such as lanthanum chromate are preferred materials for interconnect [31, 32].

### 2.5. Sealing material

Method of sealing of the ceramic components is a major issue for SOFCs as it directly affects the requisite gas tightness of the system. This issue is particularly critical for planar SOFCs and can severely limit the performance. A sealing should possess high thermal and mechanical stability under oxidizing and reducing environment at the typical operating conditions of the system. Thermal and mechanical stability is particularly critical for the SOFC stacks as any considerable thermal expansion difference between the glass and cell components can lead to high residual stress as well as might leads to crack at the sealing interface. This in turn also compromises the cell integrity and electrochemical performance. Sealing material typically consist of glass and glass ceramic. These are preferred choice for a planar SOFCs as it exhibits desired characterize features.

Developing reliable sealing glass has achieved low success due the electrochemical reaction involved ta the interphases. The interfacial reaction among sealing material and fuel, oxidants other components of SOFCs causes performance degradation of stacks. The interaction of glass-ceramics with Fe-Cr alloy interconnect is the main concern area among the various possible interaction and reactions, is of a great concern. As demonstrated by Zhang et al., Nb<sub>2</sub>O<sub>5</sub> addition in a borosilicate sealing system improves as it enhances the thermal and mechanical stability by decreasing the interaction among the glass and Fe-Cr metallic interconnect in cells [33]. In ceramic stacks, glass ceramics have been used as sealing materials, but the migration of silica component leads to issues with anode and cathode reactions and performance.

### 2.6. SOFC poisoning by impurities

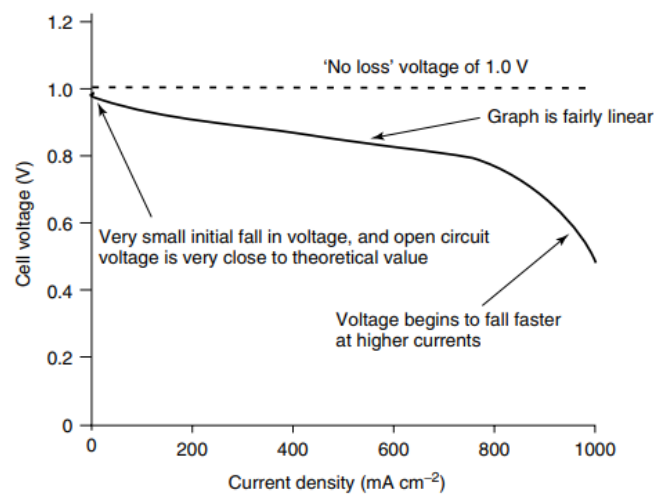
High temperature SOFC is tolerant to fuel impurities to carbon monoxide, which is a strong poison for low to moderate temperature operating fuel cells. But SOFC cells are susceptible to sulfur and chloride compounds. Fuel impurities such as H<sub>2</sub>S, CH<sub>3</sub>SH, COS, Cl<sup>-2</sup> and iloxane shows poisoning effects on commonly used anode material of Ni-YSZ cermet, thereby having detrimental effect on cell performance [34]. Especially, currently used anode materials have limited tolerance to sulfur compounds that are normally present in many hydrocarbons' fuels including natural gas. The sulfur poisoning of anode leads performance reduction in conjunction carbon deposition that leads to anode deactivation [12]. One of the reasons for interest in Perovskite ceramics material for anode is its better sulfur tolerance than Ni-YSZ anodes.

## 3. SOFC Performance

In a typical SOFC system, electrons through the external circuit with an external load due to the potential difference between anode and cathode. However, electrochemical processes occurring inside the system are not simple. These processes are mostly complicated and complex as it involves several intermediates and phases. The charge transfer electrochemistry at the interphase of electrode - electrolyte have been focus of many research, review and studies. The cell operation involves various electrochemical irreversibilities that leads to several potential losses that decrease the net voltage output of the cell. Total resistance of electrodes in the cell comes from the factors such as resistance from internal flow, polarization resistance from concentration gradient, resistance from contact and polarization resistance due to activation. Among these most critical is internal resistance and refers to the resistance offered by the electrode for electron transport. It depends on the electrode material's electronic / metallic phase conductivity and electrode micro - structure and thickness. Contact resistance arises due to imperfect contact of electrodes with electrolyte structure. As resistive losses causing overpotential losses of the cell depends on the local current density, it can be minimized by choice of electrode material as well as

by management and control of the micro-structural characteristic's properties at the time of the fabrication [35].

The performance prediction of SOFC is quite difficult due to complex charge transfer phenomenon involved. A voltage vs current performance of a typical SOFC system with operating temperature of approx. 800 °C is shown in figure 3 (2). As can be inferred from the graph, when higher current density is withdrawn from the cell, its overpotential performance drops from the possible highest voltage. Highest voltage that can be drawn from a SOFC under reversible condition is the open circuit voltage (OCV) or 'no – loss' voltage. Therefore, actual cell voltage will always be less than the OCV voltage as fraction of OCV will be used for driving charge transfer reaction that takes place at the interface of electrodes and electrolyte. The cell potential has a fairly linear relationship at small to moderate current densities but becomes non-linear at higher current densities of the cell. Initially, when current is drawn from the cell, the drop-in voltage is relatively small due to less overpotential required for charge transfer. OCV is the highest voltage that cell can produce, and it is equal to the theoretical OCV value.



**Figure 3.** Variation of voltage of a SOFC operating at 800 °C [2]

#### 4. SOFC Cell Modeling

The electrochemical phenomena that occurs in SOFCs is quite complex and some of the phenomena are not understood and clear enough. Therefore, most models of electrochemical phenomenon occurring inside the SOFC system are usually simplified representations of the actual physical and chemical processes. Hence accuracy of these model predictions requires model validation from experimental data over a full range of operations. SOFCs performance its behavior prediction using numerical simulation involving models of the various complex electrochemical processes and their interactions is therefore a relative recent trend in fuel cell research [36]. Theories, philosophies and approach behind modeling of fuel cell is best summarized by Eikerling [37]. This article presents the highlight of the achievement and bottlenecks like developing multiscale and multi-parameter, electrode structure vs functions, model implementation etc. Therefore, a comprehensive model of a SOFC can be developed by incorporating contribution from aspects such as electrochemistry, heterogeneous chemistry, heat and mass transport and unit cells and stacks.

##### 4.1. SOFC Electrochemistry

Activation overpotential (potential needed to drive the charge transfer at electrodes interface), ohmic overpotential (potential needed to overcome the ionic resistance of the electrolyte material), concentration overpotential (potential needed to overcome transport limitation with in porous electrode structure), charge transfer are main resistance factors that needs to be accounted in electrochemistry. Additionally, charge transfer chemistry (reaction pathways, reaction kinetics and mechanism, and rate

limiting steps) of the active electrochemical species and Nernst equation modification and solution are integral to the cell electrochemistry.

In a SOFC, electrochemically active species of H<sub>2</sub> and CO are involved in charge transfer process. Among the two, H<sub>2</sub> oxidation kinetics usually dominates over CO oxidation. Butler - Volmer equation for hydrogen oxidation, equation (7) and oxygen reduction, equation (8) are as follows;

$$i = i_0 \left[ \exp\left(\frac{(1+\beta_a)F\eta_a}{RT}\right) \exp\left(-\frac{\beta_c F\eta_a}{RT}\right) \right] \quad (7)$$

and

$$i = i_0 \left[ \exp\left(\frac{\beta_a F\eta_c}{RT}\right) - \exp\left(-\frac{\beta_c F\eta_c}{RT}\right) \right] \quad (8)$$

The cell operating potential, results from the collected differences in the electric potential among both phases in the cell [35]. The operating cell potential depends on the overpotential losses and can be written as a function of local current density,  $I$  as in equation (9);

$$E_{cell} = E_{rev} - \eta_a(i) - |\eta_c(i)| - \eta_{ohm}(i) - \eta_{conc}(i) \quad (9)$$

Where  $\eta_a$  and  $\eta_c$  are the activation losses at the anode and cathode side respectively,  $\eta_{ohm}$  is the Ohmic overpotential, and  $\eta_{conc}$  is the concentration overpotential. For the case of hydrogen oxidation  $E_{rev}$  is given by Nernst equation in equation (10);

$$E_{rev} = E^0 + \frac{RT}{2F} \ln\left(\frac{P_{H_2,a} P_{O_2,c}^{1/2}}{P_{H_2O,a}}\right) \quad (10)$$

Where,  $E^0$  is the electro-motric force (EMF) at standard pressure.

Nernst potential ( $E_{rev}$ ) is commonly referred as open circuit voltage (OCV). This is the maximum possible potential that can be derived from a cell operating reversibly. Therefore, the Nernst potential is also known as the reversible potential. Therefore, actual potential will always be lower than the Nernst potential during the operation of the cell due to the irreversibilities.

Equation (7), equation (8), equation (9) that are non-linear and coupled with equation (10) can be solved by two different approaches to find the performance of the system. Firstly, it can either be solved for the local current density,  $i$ , by fixing the operating cell potential,  $E_{cell}$ . Secondly, these equations can be solved for cell potential by fixing the average current density. An iterative solution approach will be required.

#### 4.2. SOFC Heterogeneous Chemistry

As Ni-YSZ is predominantly common material of anode, reaction mechanism of CH<sub>4</sub> on Ni is of utmost interest. Even though perovskite materials have exhibited improved characteristic performance but their use as anode material in commercial installation is still not there. For methane or any other hydrocarbon fuel, catalytic reactions will occur inside the anode structure leading to a complex chemical composition of the reactants at the interphase. Intermediate products such CO, CO<sub>2</sub> and H<sub>2</sub>O, which are formed at the interphase also actively takes part in the catalytic chemistry, thereby affecting the kinetics of fuel oxidation. Therefore, understanding of the catalytic kinetics is critical for precise cell performance prediction and consumption of fuel. A review and summary of various heterogeneous mechanism of CH<sub>4</sub> over Ni is given by Zhu et al. [38].

#### 4.3. SOFC Heat and Mass Transport

Since SOFC electrode are porous with multi - flow channels, modified form of the general heat and mass conservation equation are needed. The Dusty Gas Model (DGM) can be used to model multi component species transport in porous media. Xu et al., has described the detail equations to calculate DGM diffusion coefficients to calculate the heat and mass transport of the cell [39]. Amiri et al. [40] has developed a mathematical model for entire SOFC transport phenomena. Developed mathematical



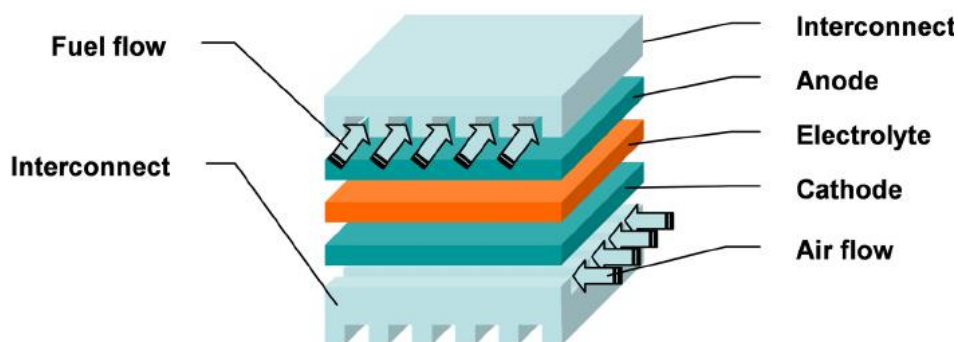
model was for a tubular micro-solid oxide fuel cell and accounted for mass, momentum, heat, and electric charge transfer. The model also included reversible and irreversible heat generation and detailed electrochemical reactions. Experimental data on electrochemical performance and temperature distribution was used to validate the simulation results. Negligible local heating within the electrodes and negligible temperature gradients along the cell's active length are main finding of the study [41].

#### 4.4. SOFC Unit Cells and Stack

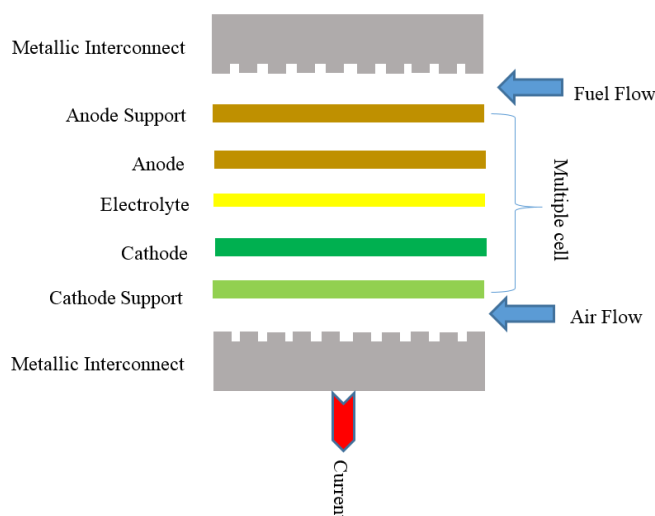
In lieu of the complex electrochemical interaction and kinetics, SOFC models are usually simplified representations of the actual physics and chemistry, and accuracy of the model predictions needs to be validated using experimental data. Therefore, numerical simulation of SOFC characteristics employing detailed models of physical and chemistry processes and their interactions is relative new focus of SOFC research.

A complete SOFC system typically includes of a SOFC stack (with variable number of SOFC cells), fuel pre-reformer, fuel ejector, after burner, pre-heater and cogeneration unit. This is done in order to maximize the benefit of high temperature SOFC operation, thereby recovering heat. Above arrangement allow the combined heat hybrid system to reach efficiency up to 80% [42]. All these components are integral and important and have to be considered for the prediction of the cell efficiency and performance of a single or stack of SOFC power generation system [43].

It is desirable to have a SOFC system model comprising of fuel cell stack with its auxiliary components that can predict the cell performance under different conditions and process parameters. Amiri et al. have done outstanding work in this aspect. They have first developed a rigorous SOFC module 43 for a stand-alone SOFC cell. This was then extended to simulate an entire SOFC fuel cell stack system with auxiliary units [44-45]. This work was a good effort to model the stack as it considered factors such as flow maldistribution in the stack manifold, balance of plant (BoP) components and interaction between the stack and the BoP. They have reported another study involving a short stack composed of six micro-tubular fuel cells. This study was mainly focused on stack's electrochemical performance under different electrical connection configurations such as parallel, series and mixed / parallel-series at intermediate temperatures (46). Negligible performance differences were found among different arrangements. A parallel-series configuration was found to best suitable for stack assembly. As can be inferred from above listed studies, fuel cell stack modeling is a work in progress and different aspect and factors needs to be investigated. Zhang et al. [47] have used Aspen Plus A SOFC system may include fuel pre-processors, heat exchangers, turbines, bottoming cycles, etc., all of which can be very effectively modeled in process simulation software. The focus of the study was on optimization of the fuel cell stack and the balance of plant with respect to efficiency and economics to come up with an improved design of a fuel cell system. Therefore, new studies are needed to look for internal SOFC phenomena such as anode blinding by carbon deposition, recycling of depleted fuel, heat and thermal management etc. and analyses at compartment, channel and cell scales. Figure 4 and figure 5 represent schematic of the SOFC stack for counter flow configuration and a single cell for co-current configuration [39].



**Figure 4.** A 3-D schematic presentation of counter flow SOFC stack



**Figure 5.** A planer SOFC with co-configuration flow

When natural gas or other hydrocarbons such as diesel, kerosene etc. are used as primary fuel, the fuel is pre-reformed to a certain extent (often completely) prior to feeding to the fuel cell stack. Nevertheless, the anode of the cell also provides ample opportunity for the fuel to undergo reforming. The reforming reactions produce synthesis gas,  $H_2$  and  $CO$ , undergoing charge transfer reactions at the electrode and electrolyte interfaces. The reaction products ( $H_2O$ ,  $CO$  and  $CO_2$ ) further replenish the reforming chemistry within the cell. However, the reaction products also dilute the fuel thereby decreasing the Nerst potential as well as the current density of the cell. Generally, the reactants and the products have opposite fluxes within the porous anode. Additionally, Knudson diffusion limitation within the porous electrodes can lead to steep gradients of the species concentration profiles at the electrode-channel interfaces, thereby affecting the chemical kinetics [36].

To predict an accurate performance of a single SOFC or stack, the SOFC model equation needs to be incorporated with models of transport of chemical species in anode and cathode, fluid flow in fuel and air channels, kinetics in anode, heat and mass transport in fuel / air channels and electrode as well as heat transport in entire solid structure of the cell. For this purpose, three-dimensional model, two-dimensional model, one-dimensional model and three-dimensional models of SOFC stack performance are available in literature.

## 5. Results and Discussion

Background review of the phenomenon happening in SOFC system is presented above. This section describes and summarize the result of SOFC system modeling and simulation. This section is divided in three section and each section focus on experimental data on SOFC performance with simulation data validation, SOFC system simulation using split approach and SOFC simulation using MATLAB model, respectively.

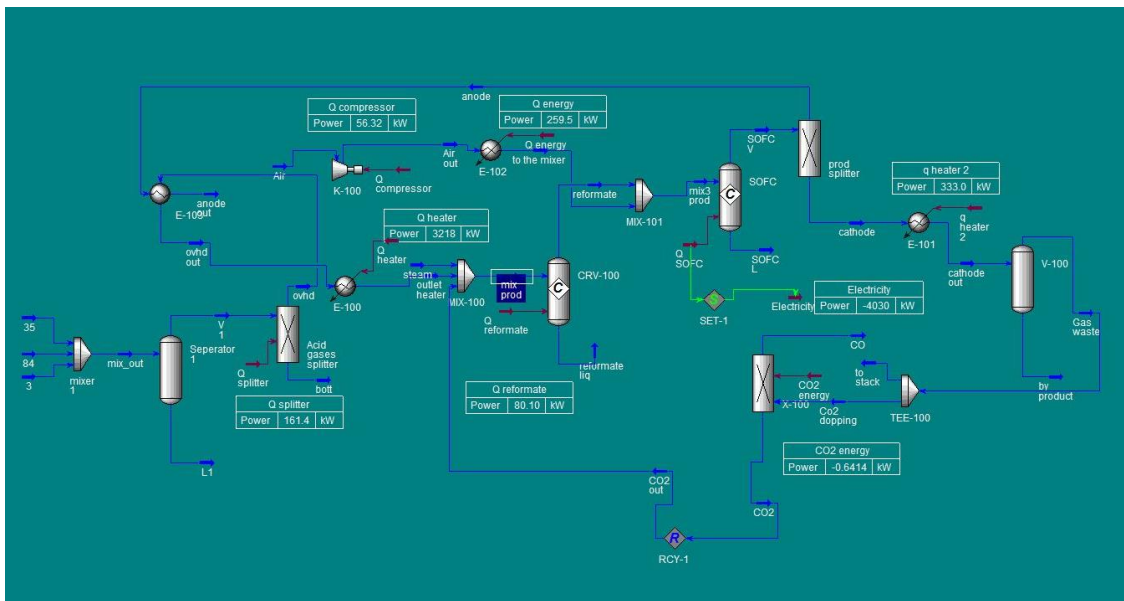
### 5.1. SOFC Simulation and Modeling

A SOFC system model for a standalone SOFC cell and for an integrated system comprising of fuel cell stack with its auxiliary components needed to model and predict the performance and validation. This task would have been easy by employing one of the commercial process simulations and flowsheeting software such as Promax, Aspen Hysys, Aspen Plus, Pro II, Unisym, CHEMCAD etc. software. However, no in-built SOFC module exists within any of these commercial flowsheet simulation software. Therefore, efforts are being done to come up with a rigorous SOFC model that can be integrated to the standard software.

In literature, many studies have been reported on Simulation of small to medium sized SOFC systems using commercial software. Almost all studies have utilized Aspen Plus software due to inherent

advantage such as better solid modeling, stability and accuracy of the results [47-52]. SOFC simulation modeling is a work in progress and provides important bridging to numerical, mathematical and experimental pathways have been employed. The advantage of a simulation modeling is that user can create different case studies and scenarios and achieve a high optimization for the cell.

The authors have used academic version of the Aspen Hysys software (v10) to simulate and model performance of a SOFC fuel cell system that employs waste natural gas as fuel. The details of this simulation model and performance is given here [53]. The study used a split modeling approach to come up with the SOFC fuel performance. Hysys V10 is the version of the software and Peng Robinson property package was employed. A snapshot of the simulation model is shown in figure 6. This simulation was conducted using the simulation parameters listed in table 1. The amount of electricity output for the model was 20197.3 KW. Option of energy integration was explored, and it was found that power generation after energy integration was approximately 18.5% more at 23888.3 KW.



**Figure 6.** Aspen Hysys simulation model of integrated SOFC fuel cell system

**Table 1.** Basic parameters for SOFC simulation model

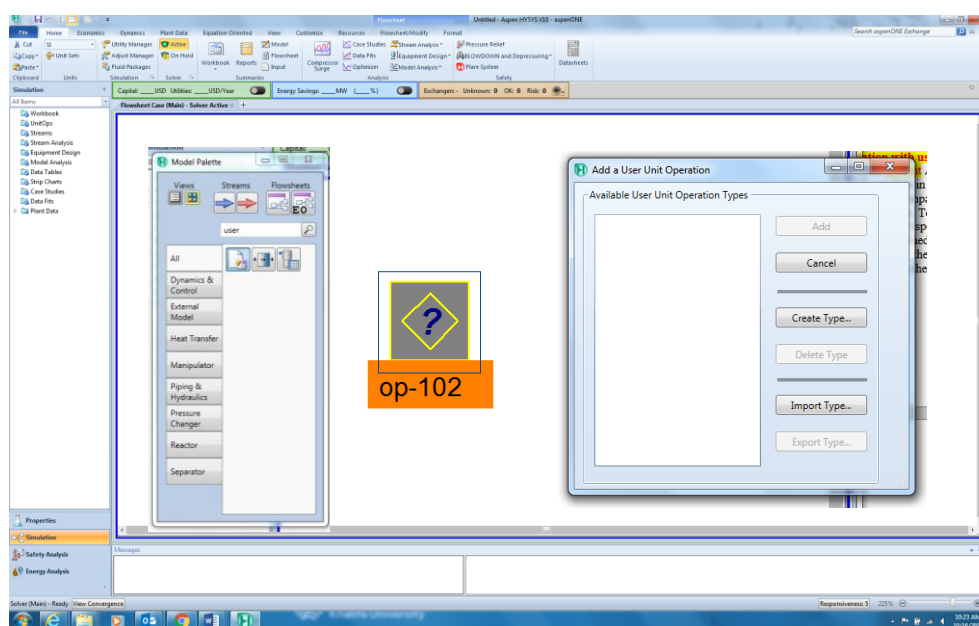
Parameters	Values
Type	A Single SOFC cell
Fluid Package	Peng Robinson
Base parameter	CH <sub>4</sub>
Feed	Waste gas (Consisting of methane and other impurities)
Composition	Methane upto 85%
Parameter of interest	Energy / Electricity
Unit	SI
Software version	V10
Nature	Steady state and Dynamic simulation

Subsequently this model was fine-tuned and analysed further. Case studies involving parameters such as fuel and oxidant's flowrate, pressure and temperature, fuel purity, presence of impurities and fuel flexibility. The performance of the model is then compared and validated with the experimental data of a standard SOFC cell. A fair agreement has been obtained with scope for further improvement (53). For this reason, this model is still not the final simulation model as improvement in performance will be undertaken.

### 5.2. SOFC Simulation with MATLAB SOFC model

The limitation of the present Aspen Hysys simulation model was primarily the absence of a built in SOFC unit operation / module in the design object pellet database of the program, which lead to

approximate representation of the SOFC processes to their nearest available unit operations. This impacted the simulation model as electrode were modeled as reactor and electrolytes as splitter and other available unit operations. To overcome this shortcoming, authors are proposing to come up with their own complete SOFC model using MATLAB that can be imported in Aspen Hysys simulation database. To import this model in Aspen Hysys simulation, ‘user unit operation’ option available in the Aspen Hysys design pellet will be used. Figure 7 shows the availability and information needed for the incorporation of a user defined unit operations. The ‘user unit operation’ can be defined by developing a code with a programming language such as Fortran 90 / 77 or MATLAB. Author choose MATLAB option as it’s more applied and stable.



**Figure 7.** Availability of user unit operation in Aspen Hysys v10

Therefore, in the current study, author is coming up with a ‘user defined SOFC model’ by coding of the SOFC electrochemistry, heat and mass transport. For this purpose, above described model (equation (7) to (10)) will be solved in a MATLAB by an iterative program. Schematic of the approach that is being followed to come up with a MATLAB program for ‘user unit operation’ is given in Figure 8. The model works top to bottom approach in either of the two mode namely, voltage or current determination. Basic SOFC details needs to be entered first as well as information about stack cell numbers. Once the feed condition and specifications are defined, the routine will be able to do an iteration to solve and find out the unknown parameters such voltage or current, flowrate of exit streams, energy and heat flow. Troubleshooting and testing of the model is underway and a MATLAB model is not yet available. Once a final MATLAB model is completed, it will be imported in Aspen Hysys simulation to obtain accurate SOFC performance through ‘user unit operation’.

A summary of the parameters that is being employed for the MATLAB model / code is given table 2. The final simulation model employing the ‘user unit operation’ using the MATLAB program is currently being pursued by the authors and final result of the new model will be publish later. Afterwards, benefits can be quantifying and at next stage of future studies, economic feasibility analysis can be conducted.

**Table 2.** Details of the parameters for MATLAB program model

Parameters	Values
a. Programing tool	
Type	Iterative program
Tool	MATLAB / Simulink program code
MATLAB Version	R2018b (9.5.0.944444)

Parameters	Values
b. SOFC Cell details	
Type	A single SOFC cell
Anode material	Ni - YSZ
Cathode material	GDC/LSCF
Electrolyte	YSZ
Capacity	1 kW
V-I characteristic	As per the reference
c. Assumption for kinetics / reaction mechanism	
Base reaction species	CH <sub>4</sub>
Reaction extent	100

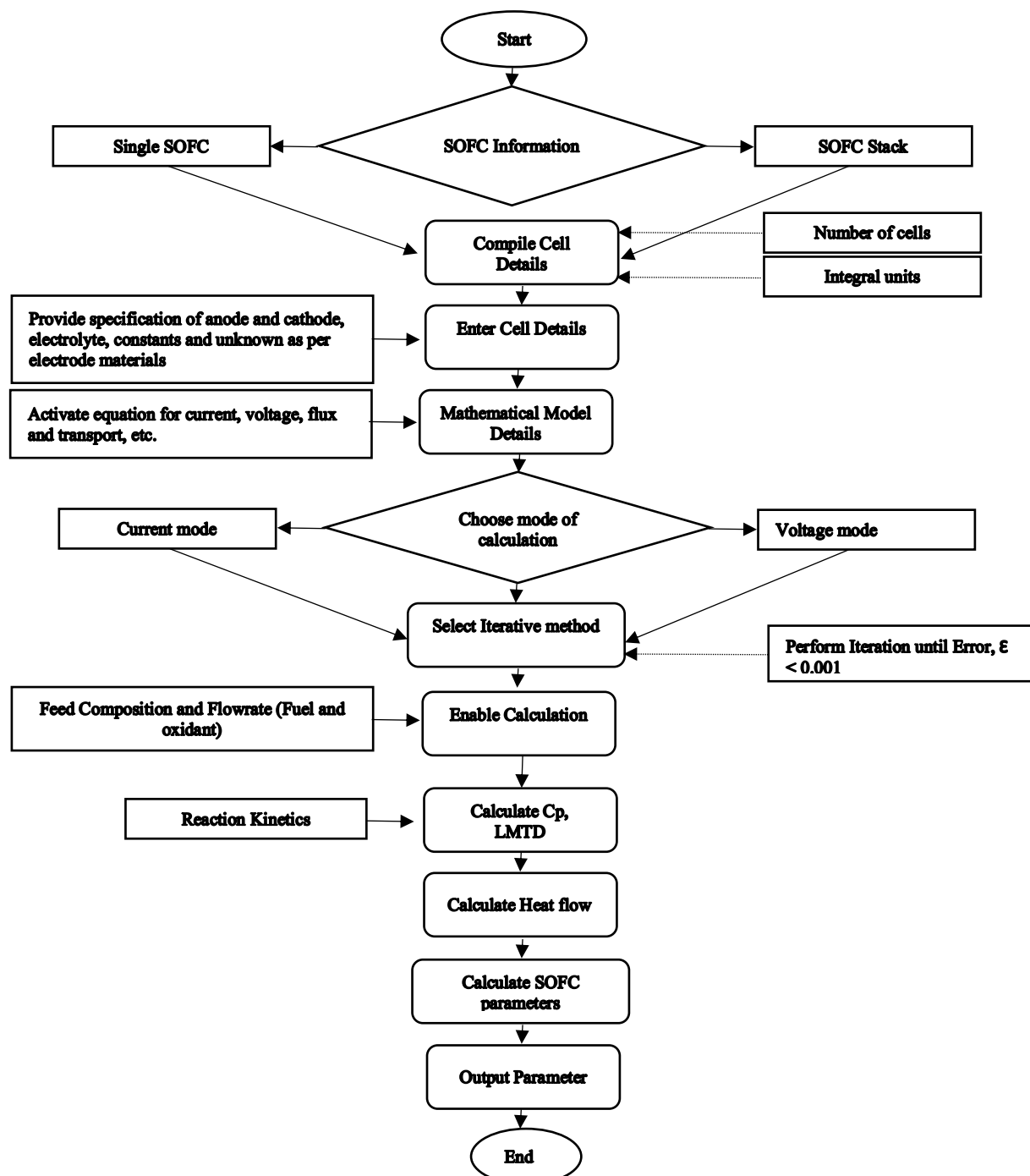


Figure 8. Schematic of the MATLAB program for SOFC performance modeling

### 5.3. SOFC reaction pathways for MATLAB model

In literature, MATLAB model has been reported for all type of fuel cells including SOFC cell and stacks. But studies are limited to using the hydrogen fuel employing Autothermal reformer or internal reforming that converts the hydrocarbon to hydrogen fuel. Two of the important studies are highlighted here. Boccaletti et al. were the first one to develop a MATLAB based simulation models for a PEMFC and SOFC (54). The study mainly focuses on the advantages and disadvantages of the SOFC cell over PEMFC. Georgis et al. [55] have developed a MATLAB model for a single SOFC system and subsequently extended to the design and operation of energy integrated solid oxide fuel cell (SOFC) systems for in situ hydrogen production and power generation. This study was based on the hydrogen as fuel. In the current study, authors have used the alternative fuel pathways i.e. directly fueled by natural gas. Therefore, reaction kinetic of both studies are altogether different. Authors work will be complimentary to the published work as Georgis et al, study involves the first pathways of fueling the SOFC, while authors have opted for the second pathway of the fueling of SOFC.

### 5.4. SOFC simulation validation and comparison methodology

To validate and compare the results of the current research, authors are using the open sources available data. There are a number of publications with experimental data of the SOFC cells and their performance and modeling. The research group of Amiri et al. (4, 5) have done extensive publication on SOFC and therefore has been selected by the authors to be the reference experimental data.

This experimental data is then compared with the split approach SOFC simulation and have been found to have a good agreement (53). Scope for further improvement of the simulation via user developed MATLAB model has been found. Now new SOFC simulation using the user. In each of the three cases, performance of the SOFC cell is obtained, i.e. experimental, split based SOFC simulation and user unit operation based SOFC. In particular, cell characteristic performance is obtained by varying the current density of the cell and corresponding voltage measurement. For statistical purpose, the simulation data is taking up to 4 decimal point only. Afterwards, the data will be plotted on a single standard x-y plot using current and potential for each of the three approaches. Percentage difference between from the experimental data will be calculated and any possible disagreement will be analyzed accordingly. Other experimental SOFC data available in open literature will also be used for further validation.

## 6. Conclusion

Due to energy conversion with high efficiency, solid oxide fuel cells are gaining increasing acceptability as a choice of energy conversion technology with range of industrial and domestic applications. Despite recent advancement in all aspect of SOFC, there is still missing link or incomplete information about exact physio-chemical processes occurring inside the cell.

Therefore, a complete robust SOFC model with universal acceptability is still not developed, either for a single cell or a stack. An accurate SOFC model should incorporate details of transport in electrodes, coupled interactions of heat and mass transport, thermo-catalytic chemistry and electrochemistry. In comparison to H<sub>2</sub> fueled SOFC, natural gas and hydrocarbon fueled SOFC leads to thermo-catalytic chemistry in the anode that affects the electrochemistry due to formation of complex composition of the gas at three phase interfaces. Therefore, development of reliable models and computational tools for the simulation of the SOFC characteristic is complex task.

In this research, authors have reviewed SOFC aspects to come up with an enhanced SOFC simulation and model, which in turn will boost SOFC performance optimization and applications. Technical review of SOFC kinetics pathways that is ore of any SOFC model has been achieved. Accordingly, a MATLAB model of SOFC has been proposed to address the technical gap in the previous SOFC modeling studies. The structure and execution approach of the proposed MATLAB model is included. The details of the integration of this MATLAB model in Aspen Hysys simulation using 'user unit operation' is presented. Result of MATLAB model incorporated SOFC performance will be done in future publication.

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