

Modelling of Solid Oxide Fuel Cell - A Review

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Abstract— This paper focuses on the study of fuel cells as a renewable source of energy which is environment friendly and much more consistent in performance as compared to solar and wind energy because it is not site dependent and has higher efficiency. In this paper we compared the different type of modeling methodologies. This paper mainly focuses on detailed analysis of dynamic modeling. Dynamic modeling deals with the study of dynamic model of solid oxide fuel cell (SOFC) based on transfer function. The dynamic model gives detailed analysis of effect of temperature variation and effect of activation, Ohmic and concentration losses on the dynamic performances of SOFC.

Index Terms— Solid oxide fuel cell (SOFC), distributed generation, dynamic modelling, lumped, distributed parameter, control volume transfer function.

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1 INTRODUCTION

Energy sources available today are fast depleting and there is a need to switch to alternative sources that can assure a better future. Rigorous environmental regulations restricting emissions of green house gases, SO_x, and NO_x have left just a few options. It has generated a lot of attention towards the fuel cell as one of the alternative sources of clean energy. Fuel cells are electrochemical devices that directly convert chemical energy to electrical energy. Since it does not involve any rotary or thermal components, it does not suffer from any friction and combustion loss. Moreover, the unused fuel from the cell can be used to generate more power, contributing to its high over-

all efficiency. Among various fuel cells, the low temperature proton exchange membrane fuel cell (PEM) and the high temperature solid oxide fuel cell (SOFC) have been identified as the likely fuel cell technologies that could capture the most significant fuel cell market in the future. This paper will focus on SOFC. [3]

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2 Principle of Fuel cell

Fuel cells produce power through electrochemical reactions, in fuel cell by passing a hydrogen-rich gas over an anode, air (oxygen) over a cathode and introducing an electrolyte in-between to enable exchange of ions power is produced. On the ability of the electrolyte the effectiveness of this process is strongly dependent to create the chemical reactivity which is needed for ion transport. As a result, fuel cells are classified on the basis of electrolyte type [15]:

1. Polymer Electrolyte Fuel Cell (PEFC);
2. Alkaline Fuel Cell (AFC);
3. Phosphoric Acid Fuel Cell (PAFC);
4. Molten Carbonate Fuel Cell (MCFC);
5. Solid Oxide Fuel Cell (SOFC).

Fuel cell is an electrochemical device that converts chemical energy of hydrogen and oxygen directly into electrical energy [17]. With the help of Fig.1 we can understand the conversion of chemical energy to electrical energy. The overall reaction gives water as its by-product, so fuel cells are environmental friendly [15], [17], [18].

3 Solid oxide fuel cell

SOFC is high temperature fuel cell. Operating temperature of SOFC is 700-1000 °C. SOFC electrolytes are conventionally anionic conductors wherein oxygen anions transport through the electrolyte. In SOFCs, oxygen from air is reduced at the cathode, and hydrogen is oxidized at the anode. Usable heat, water vapour, and possibly carbon-dioxide are the products of the electrochemical reaction. A schematic of fundamental SOFC operation is given below in Figure 1

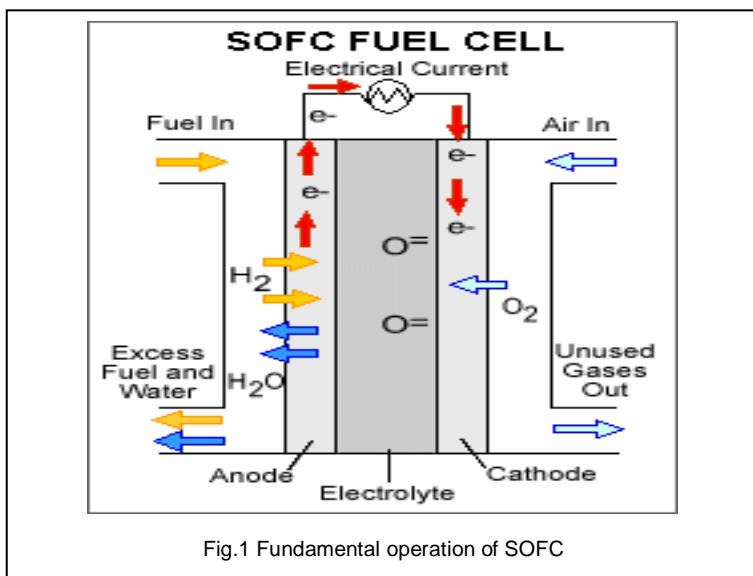


Fig.1 Fundamental operation of SOFC

SOFC is conventionally comprised of an anode cermet made of nickel supported upon yttria-stabilized zirconium (Ni-YSZ), an electrolyte that is formed from YSZ, a cathode made of strontium-doped lanthanum magnate (LSM), and a metallic or ceramic interconnect which is used for electrically interconnecting cells to form a stack, as well as providing the gas flow channels for the reactants.

In order to facilitate the application of SOFCs, in conjunction with reduced Research and development costs, there is a need for accurate performance models to aid scientists and engineers in component and process design. Some of the modelling types are described below-

4 SOFC Modelling Types

- 1) Dynamic modelling
- 2) Distributed modelling
- 3) Lumped modelling
- 4) Thermal modelling
- 5) Electrical modelling
- 6) Thermoelectric modelling

4.1 Dynamic Modelling

In Dynamic models we used to inspect responses of fuel cells under a range of operating conditions.

A study on modelling and simulation of fuel cell which includes partial pressures of respective species (hydrogen, oxygen and water) and different losses (Ohmic, activation and concentration loss) are measured under constant fuel flow and constant utilization mode and responses are drawn for different temperatures, in this dynamic model.

The studied model includes the effect of activation, Ohmic and concentration losses on the dynamic performances of SOFC. In dynamic modelling we check the performance of the model for constant utilization mode and constant fuel flow mode of operations. The effect of altering operating temperature on the performance of SOFC is also analyzed for two modes of operation in the present work.

4.2 Distributed modelling

The distributed modelling is done based on a CV approach. The flow rate and partial pressure at each CV are different in distributed modelling. The modelling considers the reactants and product composition as well as the physical shape (geometry) of the cell. The hydrogen as fuel enters into the anode channel, and air goes to the cathode channel. The fuel diffuses into the anode TPB through the porous anode, where it reacts with the incoming oxygen ions to produce water. In the same manner, oxygen diffuses into the cathode TPB through the porous cathode. The oxygen ions which are generated in the TPB of the cathode travel through the solid oxide electrolyte to the anode TPB to react with the fuel. The unutilized air and hydrogen are exhausted to the balance of the plant facilities. The fuel and air enters each CV at different concentrations from the cathode channel and the anode channel, respectively. Hence, the partial pressure measured at each CV is different and is a function of time and space. This partial pressure governs the dynamics of the fuel cell.[9, 20, 23, 24]

4.3 Lumped modelling

The lumped model approach, at the exit point of the fuel cell, we use the partial pressure of the species. In the lumped model, the partial pressure of the species is represented by an equivalent RC circuit. A lumped model uses the fundamental electrochemical equations and equivalent electrical components. The model developed is for a single cell. This approach can be easily extended to model "a fuel cell stack." The lumped model is of reduced complexity and is amenable to real-time applications. In lumped model the fuel cell is considered as a single lumped system, which reduces the complexity and computation time. In lumped model the species enter the cell through one end and leaves through the other end. The mass conservation is applied at one end of the fuel cell. [9, 24, 25]

4.4 Transient modelling

This model is based on the electrochemical and thermal modelling, secretarial for the voltage losses and temperature dynamics. The single cell is discretized using a finite volume method where all the governing equations are solved for each finite volume. The temperature, the current density, and the gas concentration distribution along the axial direction of the cell are presented. The dynamic behaviour of electrical characteristics and temperature under the variable load is simulated and analyzed. For easy implementation in the VTB platform, the nonlinear governing equations are discretized in resistive companion form. The developed model is validated and design optimization of the cell under variable operating conditions and geometric condition.

The virtual test bed (VTB), software developed at the University of South Carolina, provides an effective computational environment to simulate the dynamic performance of the SOFC stack.

4.5 Thermal modelling

The heat loss is absorbed by the solid part, which is released from chemical reaction and electrical resistance, and it is further transferred to the fuel and air steam. The air entering from the air feed tube is preheated by the air in reaction. The following assumptions are made for the thermal model.--

1. Within the solid part of each cell, heat release and absorption arising from reforming, shifting, electrochemical reactions and electrical resistance occur.
2. By convection heat transfer, heat transfer between solid part and gas steams occurs. Here radiation heat transfer between solid part and gas steams is not considered. It is not considered because the radiation exchange between the gas and solid was found to be negligible compared to the convective transport.
3. We neglected the axial conduction heat transfer between nodes also.
4. At each element the cell voltage is equivalent.

4.6 Electrical modelling

The expression of output voltage of stack is written below-

$$V_{stack} = NE_o - V_{act} - V_{con} - V_{ohm}$$

From the above equation, it can be observed the voltage loss in

the fuel cell is caused by the activation polarization (V_{act}), the ohmic polarization (V_{ohm}) and the mass transportation loss or concentration polarization (V_{con}) which is caused by electrochemical reactions. The voltage-current characteristic of SOFC can be divided into three regions [10, 26, 27, 29];-

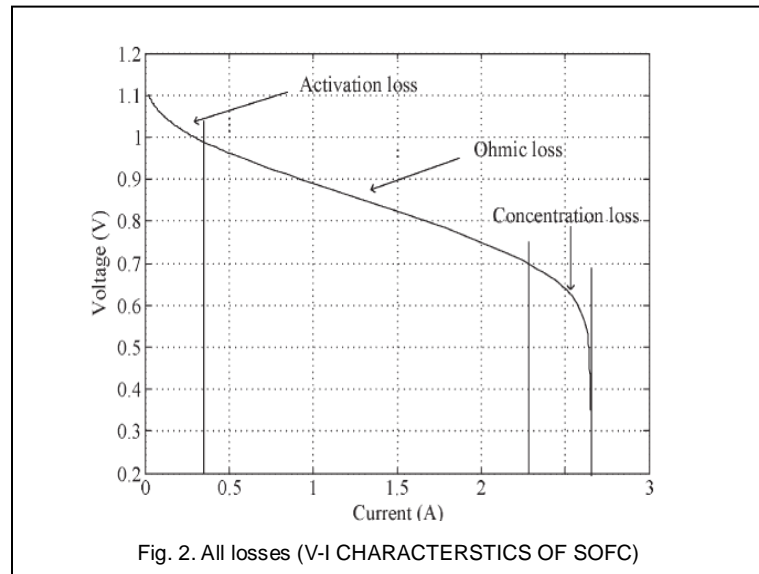


Fig. 2. All losses (V-I CHARACTERISTICS OF SOFC)

- 1st - the voltage change has logarithmic relation with the current.
- 2nd- In the medium current density region, the voltage changes approximately linearly with the change in current
- 3rd- The third part of the V-I curve of a fuel cell is related to the concentration loss for high current operation.

S.NO.	Modelling type	Methods
1)	Dynamic modelling	In this modelling SOFC is analysed under two basic modes named as – under constant fuel flow mode and under constant fuel utilisation mode.
2)	Distributed modelling	In this modelling controlled volume approach is considered and flow rate and partial pressures are different at each CV.
3)	Lumped modelling	In this modelling partial pressure is considered only at exit point. This model is less complex and applicable to real time application.
4)	Transient modelling	In this modelling electrochemical and thermal aspect is considered. Voltage losses and temperature variation effect is also calculated.
5)	Thermal modelling	In this modelling we mainly focus on heat loss due to chemical reactions and heat loss due to electrical resistance.
6)	Electrical modelling	In this modelling various type of losses of fuel cell is calculated and fuel cell voltage is obtained using NERNST equation.

5 Detailed analysis of dynamic modeling

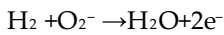
In dynamic modelling we start the modelling from the source of generation of energy accompanied by different losses of energy and finally we study the dynamics that affects generation of energy and all various losses.

5.1 Dynamic modelling in electrodes

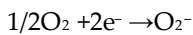
5.1.1 Source of energy

SOFC converts chemical energy of fuel and oxidant to electrical energy through reactions [38]:

Anode:



Cathode:



The reaction releases electrons as well as builds up difference of potential energy between anode and cathode. This Difference is known as open circuit voltage (OCV) or electromotive force (EMF). The OCV has been well studied, both theoretically and experimentally. OCV is affected by partial pressures and temperature and modelled by the Nernst equation.

$$E = E_o + \frac{RT}{2F} \ln \left(\frac{P_{\text{H}_2} P_{\text{O}_2}^{0.5}}{P_{\text{H}_2\text{O}}} \right)$$

When anode and cathode are connected through an external circuit, the released electrons flow from anode to cathode and thus sustain continuous reactions. The electron flow is called current. Once the external circuit is closed, the voltage of fuel cell drops because of losses including activation losses, ohmic losses, and concentration losses, as elaborated below.

5.1.2 Activation losses

Every electrochemical reaction needs some activation energy to generate sufficient amount of electrons. For a reaction to take place it must overcome the energy barrier which is mainly due to charge transfer resistance between electrodes and electrolyte. Activation losses are usually described by the Butler-Volmer equation-

$$i = i_o \left\{ \exp \left(\beta \frac{nF \eta_{act}}{RT} \right) - \exp \left[- (1 - \beta) \frac{nF \eta_{act}}{RT} \right] \right\}$$

If only static response is considered, the operational voltage of fuel cell can also be modelled by-

$$V = E - i R_{in} - A \ln \left(\frac{i}{i_0} \right) - B \ln \left(1 - \frac{i}{i_l} \right)$$

Where R_{in} is the internal resistance, i_l is the limiting current density at which the fuel is used up at a rate equal to its maximum supply speed.

5.1.3 Concentration losses

The electrical chemical reaction occurs at the triple phase boundary (TPB) which is the interface between the electrode and the electrolyte. Fuel gas must pass through the porous electrode before reaching the reaction site. The mass transport in porous media appears largely through diffusion, and it is determined by concentration gradient. Therefore the actual fuel concentration and flux at reaction site is lower than that in the fuel channel due to concentration losses. Namely, the partial pressure of the reactant on the reaction site is lower than that in the supply site of the reactant. Both static and dynamic properties of fuel cells are affected by this. If there is a sudden increased demand in the current, it will take time to build a concentration gradient to have required reactants to arrive at the reaction site. As a result, the operational voltage drops right away after a higher current demand. Therefore, the transport process along the flow channels and along the electrodes confines the load following ability of the fuel cells.

5.1.4 Ohmic losses

The operational voltage is also reduced by the internal resistance. Qiet al. [52] modelled the Ohmic losses dynamically by considering the effect of double layer capacitance and inherent resistance. The effect was simulated by an equivalent RC circuit which is a substitute of the equivalent circuit proposed in Larminie and Dicks [38]. The dynamics of the equivalent circuit was described by ordinary differential equations (ODE).

In addition to the losses as discussed so far, there are also transport losses in the flow channels, i.e. the losses by the gas transport from the admission of flow channels to the interface between the flow channel and the electrodes through which the reactant diffuses. This is discussed in the next section.

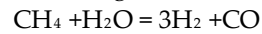
5.2 Dynamic modelling in flow channel

In SOFC it is necessary to deliver fuel and oxidant to reaction site to maintain the electrochemical reaction. Reactants are supplied through the flow channels. Fuel concentration in the fuel flow channel is determined by mass transport. With reforming/shifting reaction the transport phenomena in the fuel flow channel get more complex, for syngas fuel. We can describe flow in the channel by the mass conservation and momentum conservation.

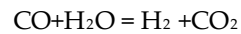
[19], Iora et al. [25], and Jiang et al. [28] built models with consideration of fluid dynamics of fuel flows in the fuel channel. Cheddie and Munroe [12], Kopasakis et al. [37], and Xie and Xue [48] also investigated the effects of flow dynamics on cell voltage following the similar modelling approach.

Often, the fuel of SOFC is Syngas, which is a mixture of CH₄, H₂, CO, H₂O, and CO₂. While H₂ and CO can directly participate in the electrochemical reaction, through reforming/shifting reaction with catalyst aid in anode CH₄ and H₂O can be converted to H₂ and CO.

Reforming:



Shift:



In addition to axial flow transport, H₂ and CO in the fuel flow channel diffuse into anode and the reaction products in the anode such as H₂O and CO₂ diffuse back to the fuel flow channel. Due to the swap density of the fuel flow changes and therefore the flow momentum also changes. Hence flow velocity along the axial direction of the flow channel is no longer a constant. The reforming reaction is endothermic, and it occurs on the surface of anode, with the aid of anode catalyst and heat from the cell. The shifting reaction occurs in the main flow body. It is slightly exothermic and therefore also heats up the fuel flow [53].

Qi et al. [53] built a model according to detailed dynamics of SOFC, in which he consider the reacting fuel flow as well as mass transport in porous anode, energy transport between the solid cell and gas phase fuel, heat transfer between the solid cell and fuel, and fluid dynamics of the reacting fuel flow in fuel channel. The model was presented as state space equations.

5.3 Modeling of temperature dynamics

In the Nernst equation we noticed that temperature has a direct effect on the voltage. Energy conservation law governs the dynamics of the SOFC temperature as described by Eqs. (4) and (5).

$$\rho C_p \left(\frac{\partial T}{\partial t} + v \nabla T \right) = k \nabla^2 + \ddot{q}$$

$$\rho C_p \left(\frac{\partial T}{\partial t} \right) = k \nabla^2 + \ddot{q}$$

The current passing through the internal resistance produces heat and the electrochemical reaction itself is an exothermal reaction. Thus, the overall SOFC cell can be seen as an exothermal device. So the temperature of SOFC cell is higher than its environment. If the insulation of the SOFC is not proper, considering the heat exchange between the cell and its surroundings becomes equally important. Inside SOFC, all the three modes of heat transfer exist i.e. conduction, convection, and radiation and heat exchanges strongly depend on the geometry. Achenbach [1] modelled the temperature of a planar

SOFC stack in three dimensions. The objective was to study temperature distribution of a planar SOFC. In addition to the heat produced by the SOFC cell, the model considered convective heat exchange between the cell and the fuel gas. Ota et al. [49] modelled the temperature dynamics of a tubular SOFC in one dimension, where conduction, convection and radiation were all considered. Qi et al. [53] modelled the temperature dynamics for a tubular SOFC. The main objective was to study the mechanism that is governing the temperature dynamics. Heat generated from electrochemical reactions, heat produced from the internal resistance, conduction, convection, and radiation, heat exchanged due to gas flow, and heat due to fuel reforming/shifting reaction etc. were all considered in their model [53].

SOFC operates at a high temperature so the heat transfer through radiation should not be neglected. This has inspired several researchers [42, 25, 53] to consider the radiation heat transfer between solid components. However, most researchers neglected the radiation heat absorbed by fuel and air flow. Since methane (CH₄), steam (H₂O), and carbon monoxide (CO) composition in fuel flow is high, the radiation heat that is absorbed by the fuel flow should be considered [44].

6 Validation of dynamic models

Conducting practical experiments in order to test the dynamic responses of SOFC is still considered to be difficult due to difficulty in setting up the experiment, such as where to place thermocouple to measure the electrode temperature without interfering its dynamics. The fuel cell dynamic response has a repetitive nature is also a problem. Existing literatures about the dynamic experiment of SOFC are sparse. Most of the dynamic models developed so far have not been validated through experiment data [7].

Although direct experiment validation is difficult, researchers have attempted to validate models through other indirect methods. For example, by comparing the Nyquist plot of the model with the experimental electrochemical impedance spectroscopy (EIS) tests; Qi et al. [52] validated part of dynamic models that they developed. By comparing the simulated results at different external load with the experimental V-I curve, many researchers attempted to validate models. However, the comparison of the steady state simulation results with experiment V-I curve should not be overstated [43]. Because there are many parameters in SOFC models, many different combinations may produce same V-I curve [43].

Another method used for validation is to compare simulated dynamic responses from different independently developed models available in the literature, as Sedghisigarchi and Feliachi [45] and Qi et al. [53] did. Even though validating SOFC dynamic models as a whole is difficult, a good amount of study has been done on model describing each single mechanism and some of them have been validated such as the model

of open circuit voltage (OCV), heat conduction, heat convection, and mass diffusion.

7 Analysis and discussion

We can summarize the dynamics of SOFC into five main sources. They are as below: dynamics due to electrochemical reaction, due to diffusion within electrodes, due to internal impedance, due to mass transfer in fuel channels, and due to heat transfer.

7.1 Electrochemical dynamics

Catalysts smooth the progress of electrochemical reaction. The electrochemical reaction is more rapid than the rate at which the reactants can be delivered to the TPB at the anode side. The electrochemical reaction is the limiting step at the cathode side. A great attempt has been devoted toward increasing the length of TPB because in turn this has increased the oxygen reduction rate at the cathode. This results in increase in the reaction rate at the cathode to a suitable level. At both anode and cathode the dynamics due to the electrochemical reactions can be deserted in comparison with other slower dynamics in SOFC.

7.2 Diffusion dynamics in electrodes

Even though diffusion is the major resistance to the fuel delivery in electrodes, the path of diffusion (or the thickness of porous electrodes) is short. Therefore the dynamics led by diffusion are not significant, and in the time scale of milliseconds [52]. This has been confirmed by EIS tests. The realistic effect of porous electrodes on the diffusion is that reactant concentrations at the TPB are lesser than that at flow channels. So the voltage is lesser than what can be expected from the concentration of the supplied reactants in flow channels.

7.3 Internal impedance dynamics

Because of the internal Ohmic resistance in electrodes and interconnectors, ionic resistance of the electrolyte, and the double layer capacitance between electrodes and the electrolyte, the operational voltage of SOFC is reduced from its source. An equivalent RC circuit is formed by the resistance and the capacitance form. Time scale of this dynamics is also in the range of milliseconds and overlapped with the dynamics of diffusion [52].

7.4 Mass transfer dynamics in flow channels

In the flow channels, the dynamics introduced by mass transport strongly depend on the stack geometry. For a choked stack for example, the time scale of the mass transport dynamics in the stack could be in the scale of several seconds [50]. For a regular tubular design, the space time of the flow channel is less than one-tenth of a second. The mass transfer dynamics is therefore also in this time scale [53, 50, 7]. In planar SOFC, the flow rate is usually lower for the purpose of higher fuel utilization rate.

So the dynamic time scale is usually in the range of seconds and considered to be high.

7.5 Temperature dynamics

The cell temperature dynamics are in the time scale of hundreds of seconds, due to relatively large heat capacitance and large mass of solid phase of the SOFC cell and other solid phase components such as the air guidance tube. Depending on the geometry, the temperature dynamic time constant can range from 5 to 10 s [49] to 500 to 1000 s [21]. The tubular SOFC design of Siemens Power Generation has the temperature dynamic time constant of around 200 s [45, 25, 2, 47, 12, and 6]. The temperature dynamics play the dominated role in SOFC dynamic responses affecting almost all other dynamics.

6. 8 Summary of dynamic effects

Great hard work has been put on the study of the load following property of SOFC. The reaction rate at TPB normally changes immediately after the external load changes. The concentration at TPB therefore also changes almost instantly and the concentration gradient in the porous electrode follows the change. The new concentration gradient drives reactant flowing along the electrode to reach a new balance. This process takes place in the time scale of milliseconds [52]. The new diffusion rate breaks the balance of the fuel channel. Both mass transport and reforming/shifting reaction are affected until reaching a new balance. The time scale of this process is in the range of seconds [53, 50]. On the other hand, the current change also results in heat change due to the internal resistance. The changed reaction rate leads to different reaction heat flux. The steady state of the cell temperature is therefore broken. It needs hundreds of seconds to reach a new steady state [21, 49, 45, 25, 2, 47, 12, 50, 6]. This process affects the entire heat transfer and is slow; therefore it is the dominant dynamics of the fuel cells.

9 Conclusions

From above we can conclude that among all modelling dynamic modelling is mostly prefer because it covers all points which is necessary for an ideal model. It covers all the type of losses of fuel cell and also the effect of temperature and partial pressures of the fuel supplied. Dynamic modelling is most useful because in this all aspects of electrochemical, thermal and electrical are considered and all the losses which affect fuel cell voltage are also calculated to obtain accurate output voltage.

10 Acknowledgments

The authors wish to thank Dr. K. Sudhakar who has ably guided the research work and provided his valuable support as and when required. Also the authors would like to express their heartfelt gratitude towards Dr. A. Rehman, Chairman, Energy Centre without whose guidance it would have been

impossible to complete this research work.

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