Investigation on performance of SOFC in hydrocarbon fuel

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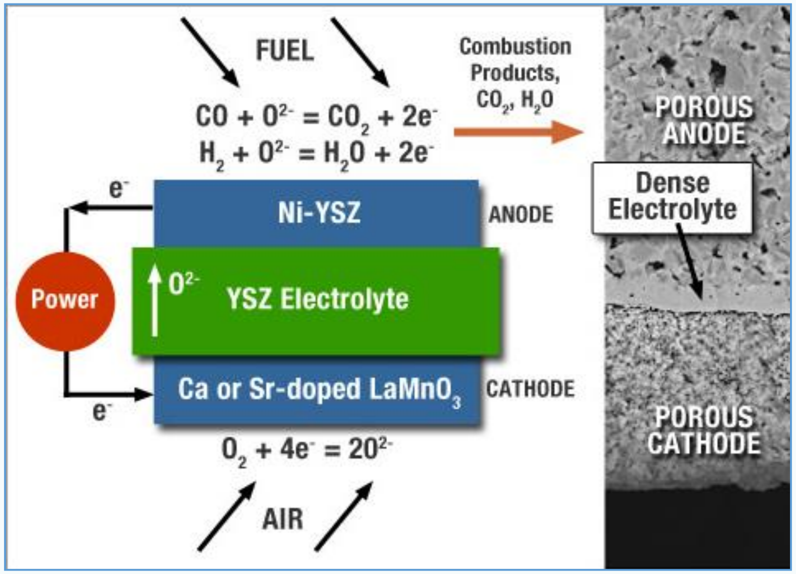
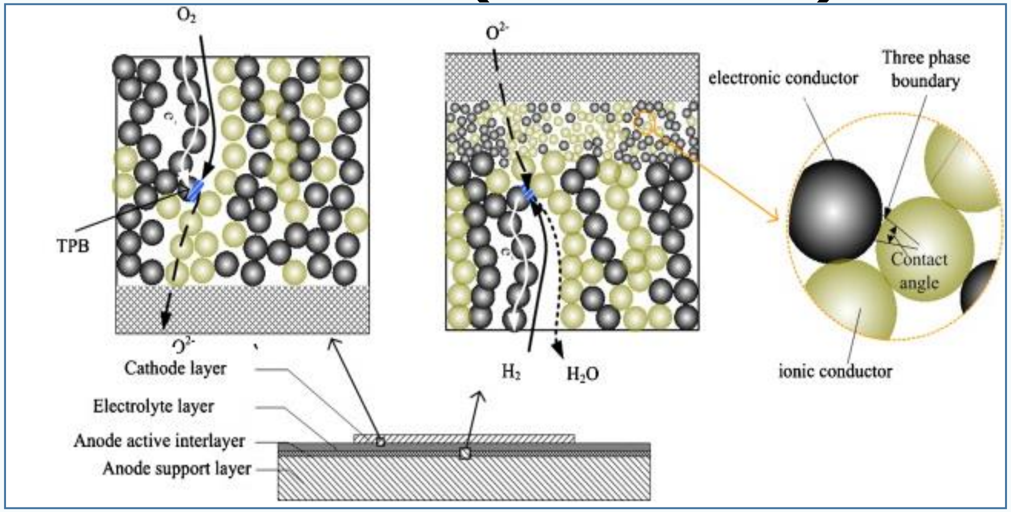
Solid Oxide Fuel Cell (SOFC)





- **At the anode:**

  $H_2 + 2O_2^- \rightarrow 2H_2O + 4e^-$.

- **At the cathode:**

  $O_2 + 4e^- \rightarrow 2O_2^-$

- **The overall cell reaction:**

  $O_2 + 2H_2 \rightarrow 2H_2O$

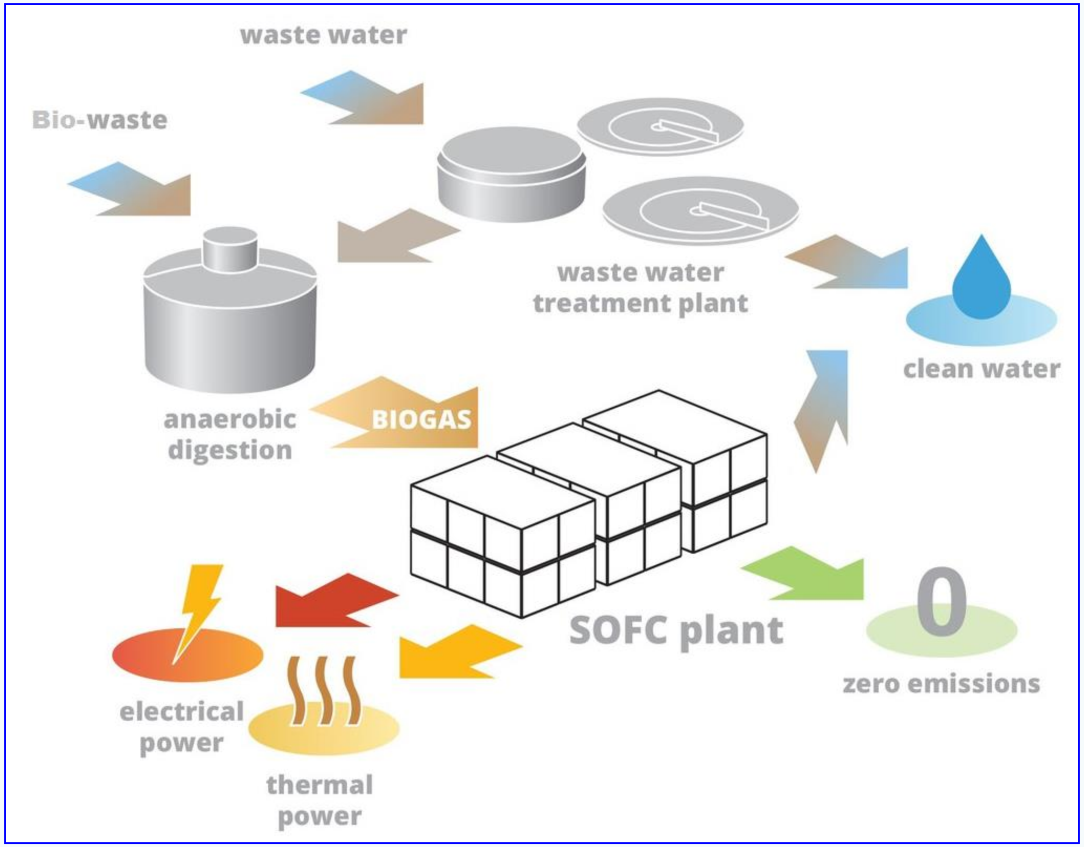
Roles of Electrolyte:

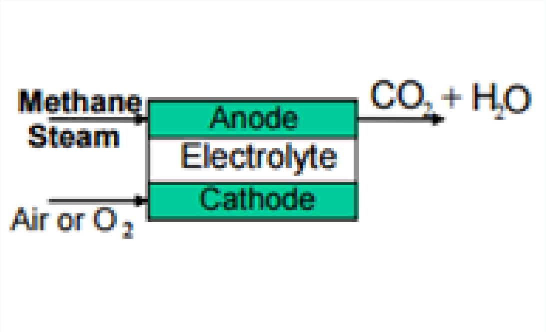
- Oxygen ion conduction
- Physically seperates the fuel from oxidant

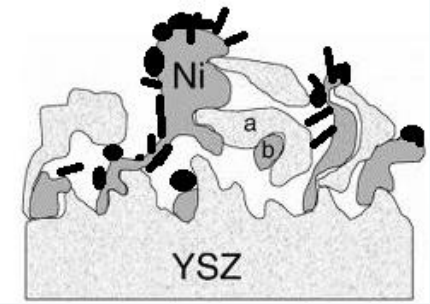
Roles of Electrode:

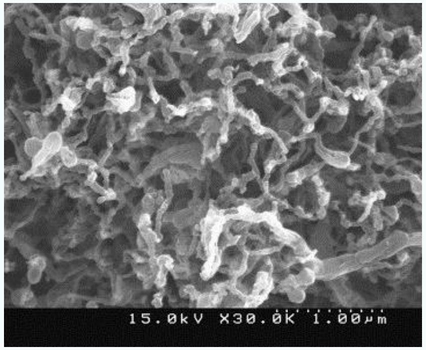
- Hosts triple phase boundary to support electrochemical reactions
- Provides path for O^{2-} ions/electrons
- Provides channels for gas diffusion
- Gives mechanical support to system

Hydrocarbon Compatible SOFC









- ➢Most promising clean energy source
- ➢Expansion of potential fuel range
- ➢Eliminates fuel preprocessing
- ➢Increases overall system efficiency
- ➢Bottle Neck: Carburization of SOFC anodes

Genesis of Present work

- State of art anode cermet is prone to carburization in hydrocarbon fuel
- An optimum feed/ operating conditions have to be established to minimize carbon deposition.
- In the typical SOFC anode, carbon deposition is an unsteady state progress
- Analysis of unsteady variation of porosity and catalytic activity of SOFC anode would be helpful in establishing the durability of SOFC in given fuel feed conditions

Objectives

- ➢ To simulate the performance of SOFC with the reformed feed (CH_4+Steam) using COMSOL
- ➢ To predict the performance degradation over the long duration (3000 h)

Physics Involved

- **Secondary current Distribution:** Determines current profile. Accounts for the effect of the electrode kinetics and losses due to resistance

- **Transport of Concentrated Species:** Determines species flux across electrode. Involves flow of species across the porous electrodes via diffusion and transport of oxide ion

- **Free and Porous Media Flow:** Determines flow profile. Accounts for flow in channel and porous media

Reactions Involved

Methane-steam reforming reaction rate:

$$R_r = a(k_{f,r} p_{CH_4} p_{H_2O} - k_{b,r} p_{CO} p_{H_2}^3)$$

CO water-gas shift reaction rate:

$$R_s = a(k_{f,s} p_{CO}\, p_{H_2O} - k_{b,s} p_{CO_2} p_{H_2})$$

Methane cracking reaction rate:

$$R_C = a\left(\left(\frac{1}{3600 M_C}\right)\left(\frac{k_{f,C}\left(p_{CH_4} - \frac{p_{H_2}^2}{K_{p,C}}\right)}{\left(1 + k_H \sqrt{p_{H_2}}\right)^2}\right)\right)$$

Boudouard reaction rate:

$$R_B = a\left(\left(\frac{1}{3600 M_C}\right)\left(\frac{k_{f,B} K_{CO}\left(p_{CO} - \frac{1}{K_B}\frac{p_{CO_2}}{p_{CO}}\right)}{\left(1 + K_{CO} p_{CO} + \frac{1}{K_{CO_2} K_{CO}}\frac{p_{CO2}}{p_{CO}}\right)^2}\right)\right)$$

Mathematical models for Parameter study

Porosity variation rate:

$$\frac{d\varepsilon}{dt} = -\frac{\varepsilon r_C M_C}{\rho_C}$$

Where $r_C = (R_C + R_B)$

Catalyst activity variation rate:

$$\frac{da}{dt} = -k_a r_C^2 c_C a$$

.

Permeability:

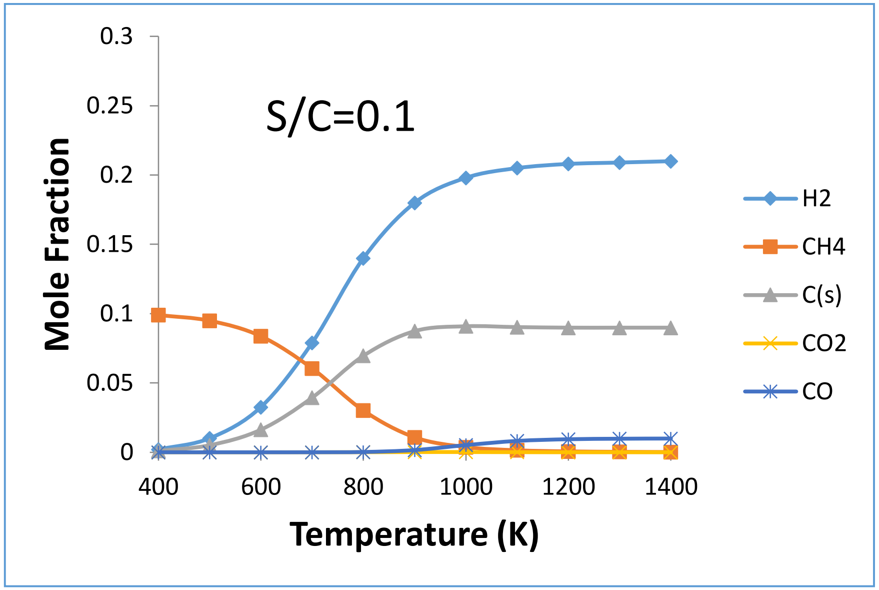
$$\kappa = \kappa_0 \left(\frac{\varepsilon}{\varepsilon_0}\right)^{3.55}$$

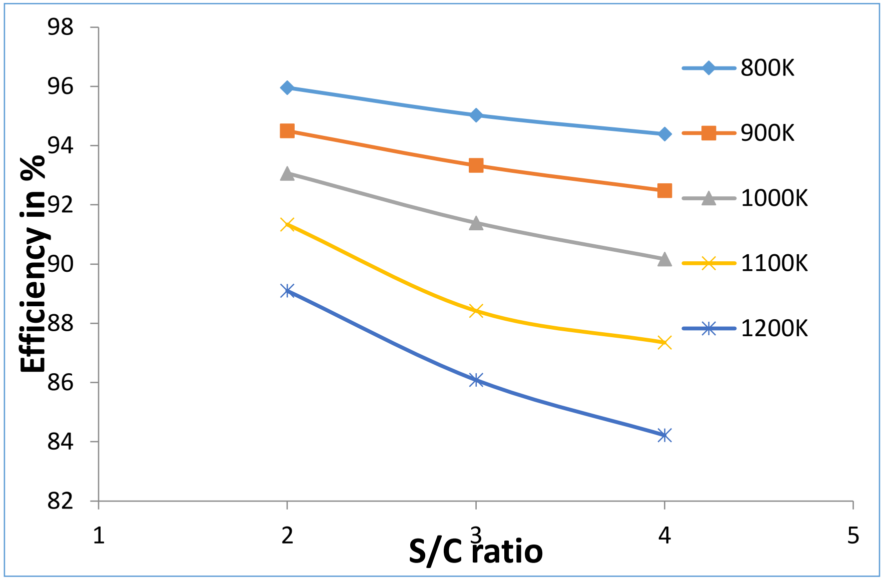
Anode Exchange current densities :

$$i_{0,H_2} = 2.1 \times 10^{11} \frac{RT}{F} \left(\frac{p_{H_2O}}{1.78 \times 10^9 p_{H_2}}\right)^{0.266} \exp\left(\frac{-1.2 \times 10^5}{RT}\right)$$

$$i_{0,CO} = 0.84 \times 10^{11} \frac{RT}{F} \left(\frac{p_{CO_2}}{1.63 \times 10^9 p_{CO}}\right)^{0.266} \exp\left(\frac{-1.2 \times 10^5}{RT}\right)$$

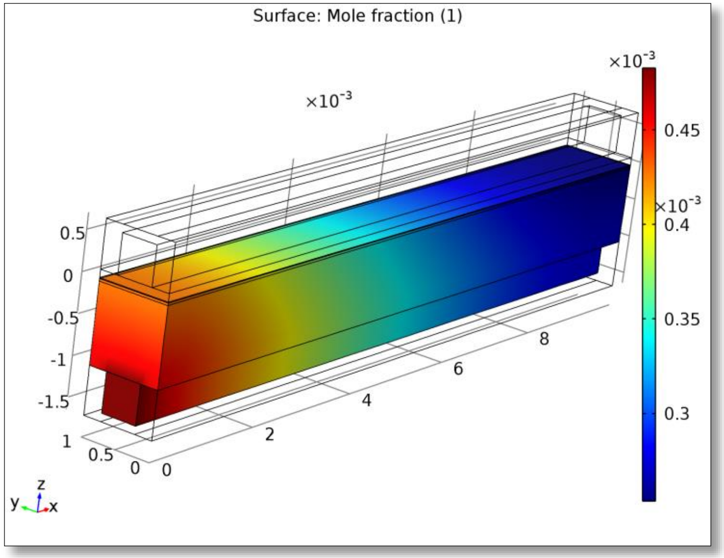
Effect of Steam



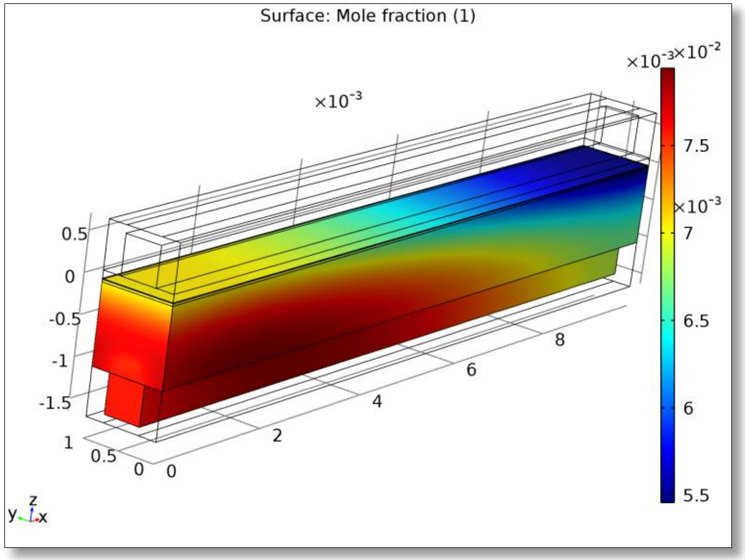


- Complete utilization of methane after >1023 K
- Efficiency decreases with increasing S/C
- η decreases steeply with increasing temperature

Fuel Utilization



Hydrogen mole fraction in anode

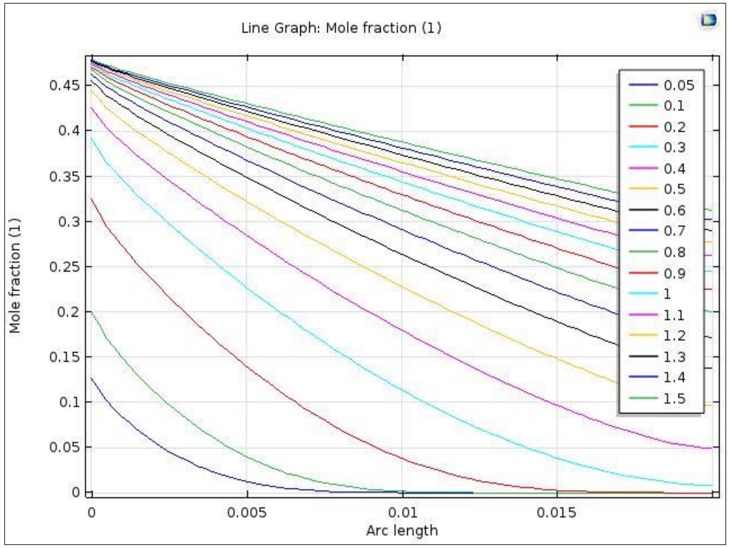


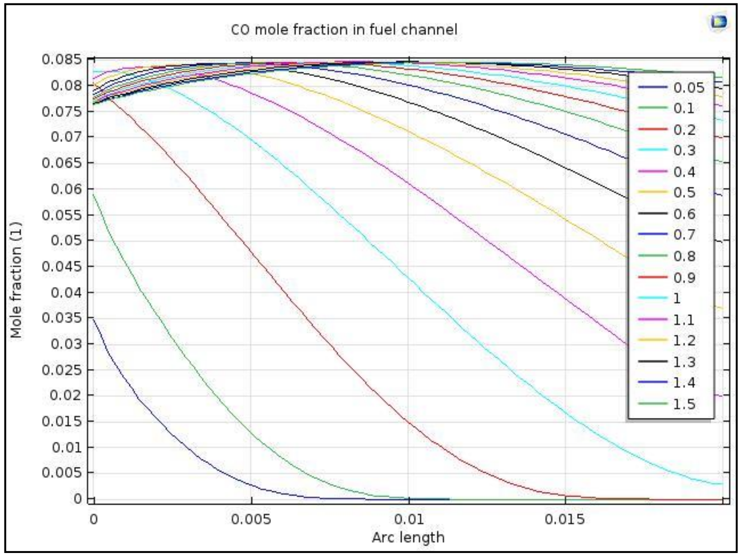
Carbon monoxide mole fraction in anode

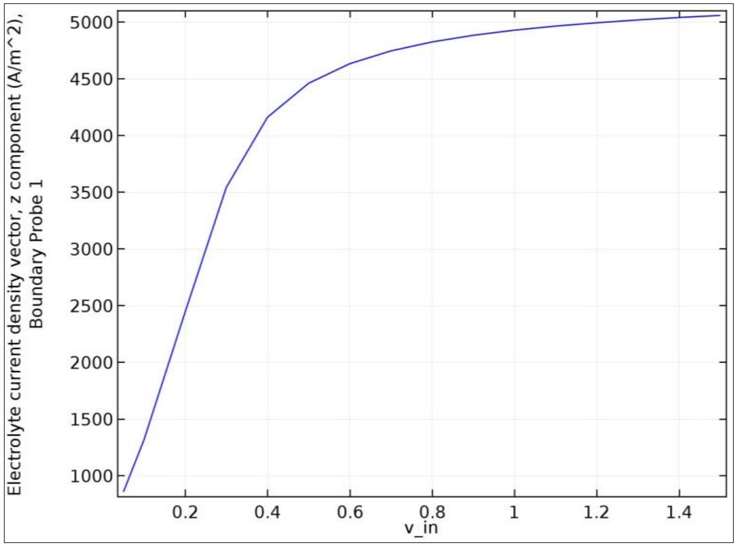
S/C =1, V_{cell} =0.7 V and T=1073 K

- Good utilization of H_2 in fuel
- CO consumption was sluggish

Effect of fuel velocity

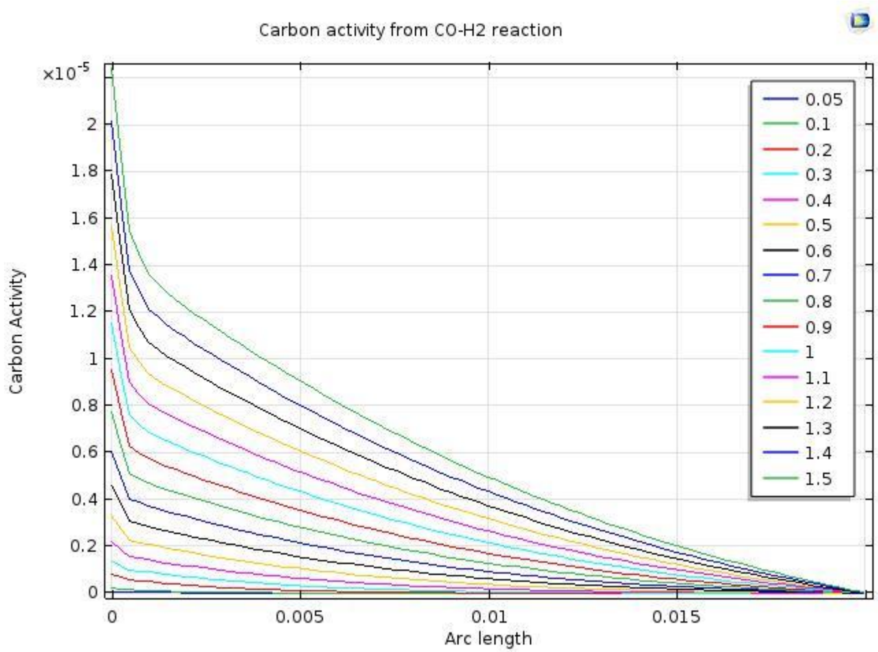




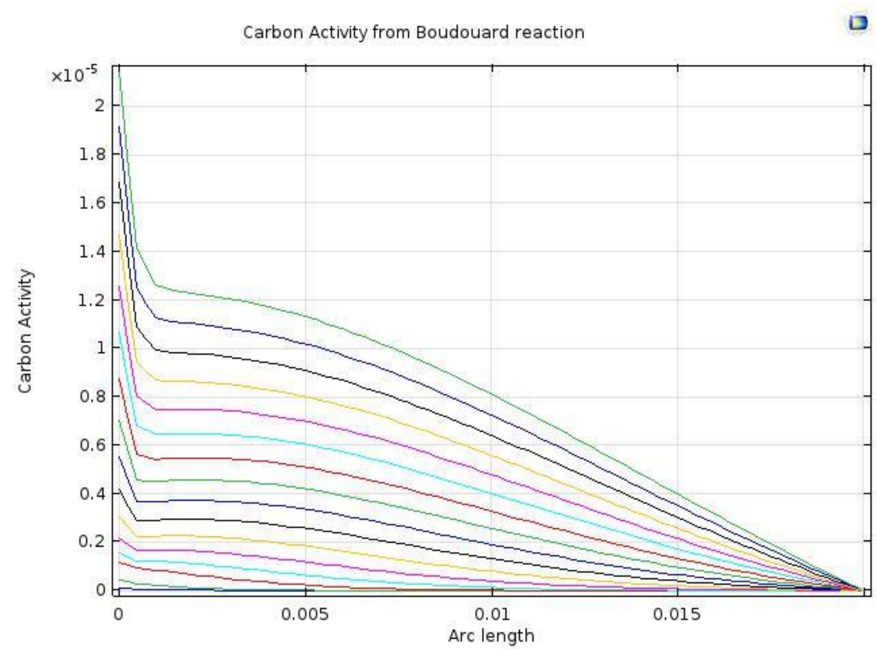


- Fuel utilization decreases with increasing velocity
- CO consumption was affected more than H_2 with increasing velocity
- Fuel velocity of 0.4 m/s had good depletion profile and reasonable current density

Carbon activity



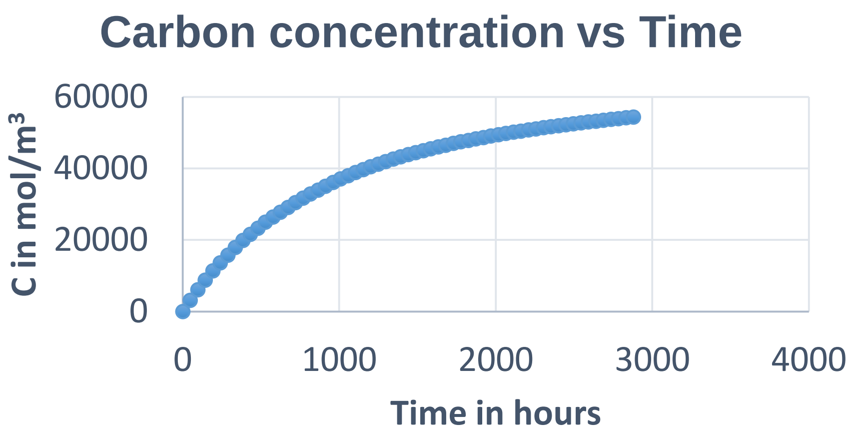
H_2 reduction reaction

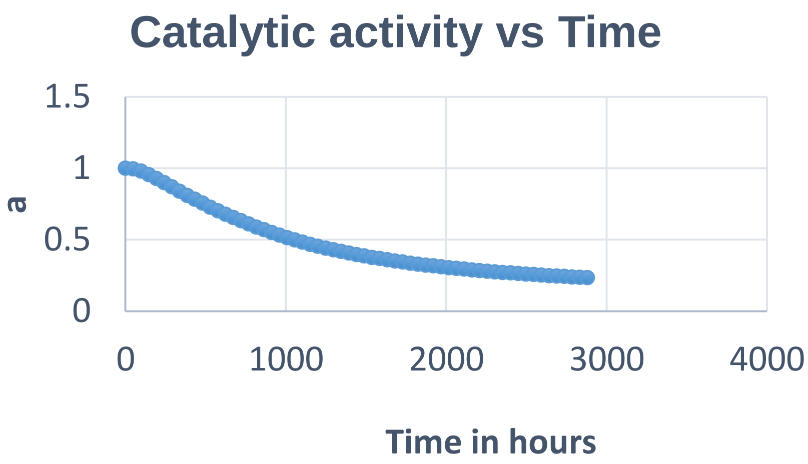


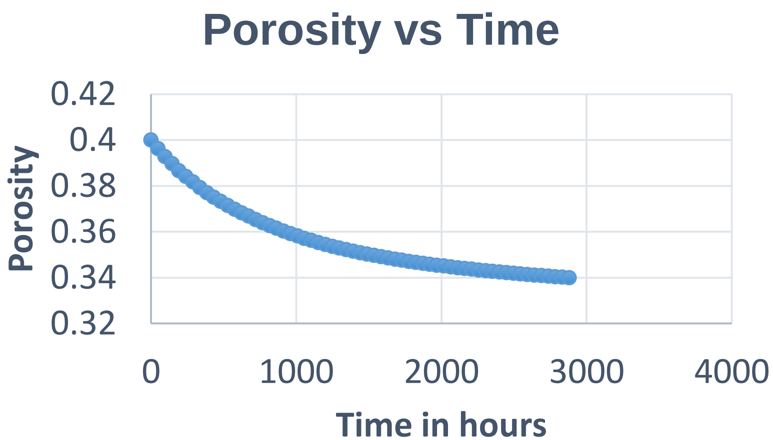
Boudouard reaction

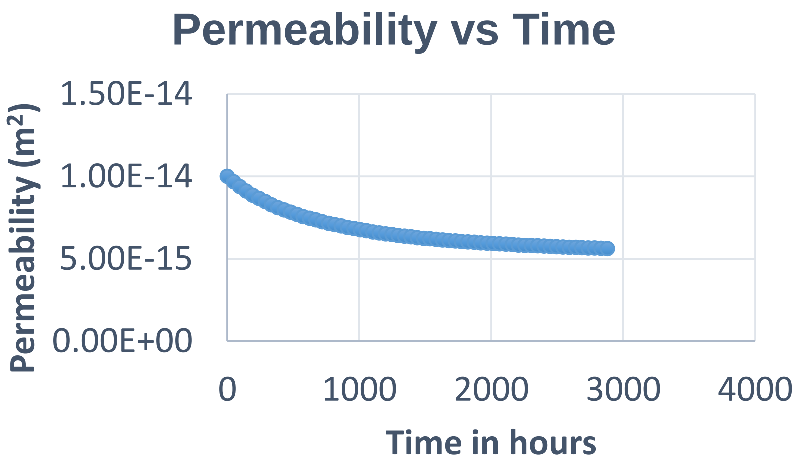
- Carbon activity was <1 up to the fuel velocity of 0.9 m/s
- At higher velocity, the difference in carbon activity between above reactions was much pronounced

Transient Studies





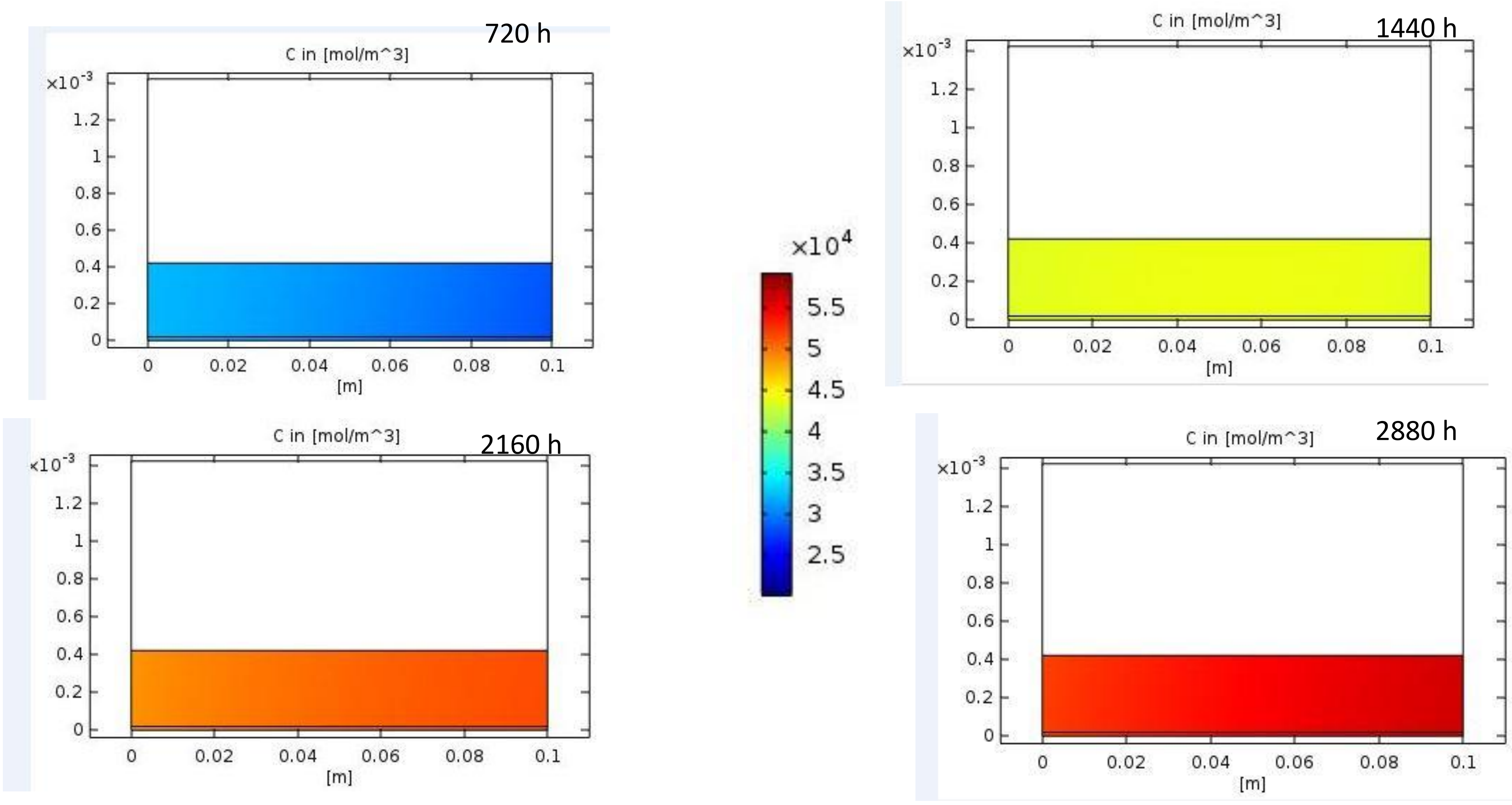




After 120 days of Operation

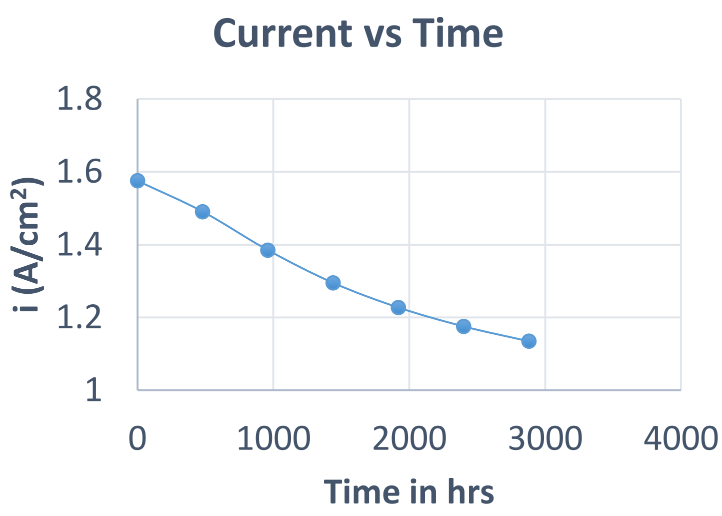
- **15 % reduction in porosity**
- **50 % reduced permeability**

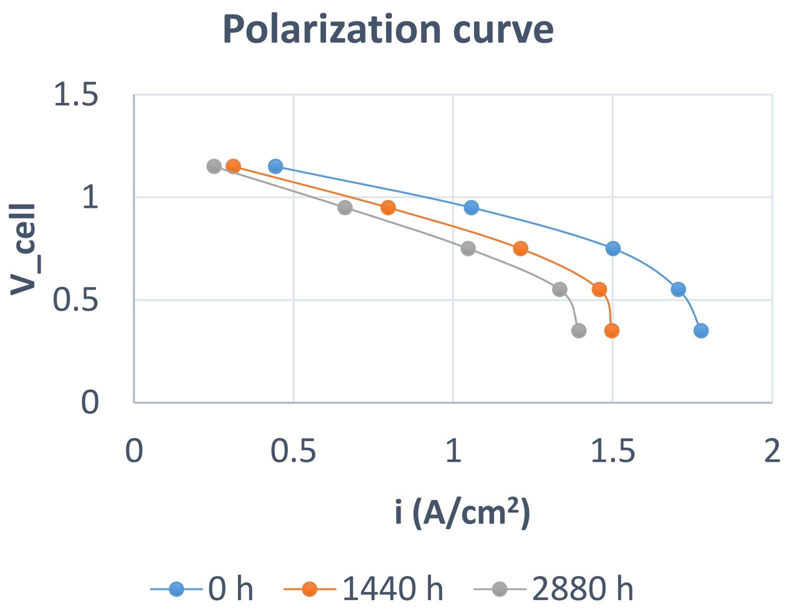
Carbon deposition vs. Time

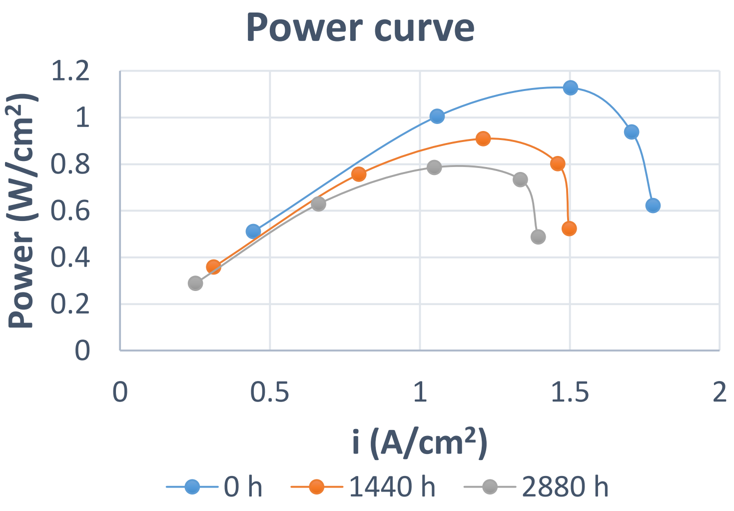


- ➢ Carbon builds-up quickly during the initial days
- ➢ Carbon deposit nears saturation in long duration

Performance Degradation







- 29% drop in performance after 3000 h
- Concentration polarization become much pronounced with time

Conclusions

- S/C ratio of 1 was found to be suitable for SOFC operating temperature of 1073 K
- Fuel velocity of 0.4 m/s found to be suitable in the perspective of fuel utilization and carbon activity
- Transient studies showed 29 % drop in performances over the period of 3000 h due to carbon deposition

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