## ELECTROLYSER TECHNOLOGY ADVANCEMENT: SOLID OXIDE ELECTROLYSIS USING GDC AS ELECTROLYTE

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#### Abstract:

This study centres on the simulation of Solid Oxide Electrolyser Cells (SOEC) for hydrogen production using Gadolinium-Doped Ceria (GDC) as the electrolyte. The SOEC model was created and its electrochemical performance, hydrogen output, and system efficiency at high temperatures were simulated in COMSOL Multiphysics and Aspen Plus. Simulation results for GDC were benchmarked against Yttria-Stabilized Zirconia (YSZ) literature. GDC showed better ionic conductivity at lower operating temperature, thus improving efficiency, reducing energy consumption, and increasing hydrogen production compared to conventional systems that utilized YSZ. This research illustrates the benefits of utilizing GDC as an electrolyte material towards lower cost and higher efficiency sustainable hydrogen production while showcasing the use of multi-software simulations for the design of advanced electrochemical systems.

#### **Keywords:**

Solid Oxide Electrolyser Cell (SOEC), Gadolinium-Doped Ceria (GDC), Green Hydrogen Production, High-Temperature Electrolysis, Electrochemical Performance, Renewable Energy Integration

## **INTRODUCTION:**

The global pursuit of sustainable and carbon-neutral energy solutions has intensified interest in hydrogen as a clean energy carrier. Among the various hydrogen production methods, Solid Oxide Electrolysis Cells (SOECs) have emerged as a promising technology, offering high efficiency in converting steam into hydrogen and oxygen at elevated temperatures (typically 600–900 °C) [1].

A critical component influencing SOEC performance is the electrolyte material. Yttria-Stabilized Zirconia (YSZ) has been the conventional choice due to its chemical stability and ionic conductivity [2]. However, Gadolinium-Doped Ceria (GDC) has gained attention for its superior ionic conductivity at intermediate temperatures. Recent studies have explored multi-doped GDC composites, incorporating elements like lithium, bismuth, and copper, to enhance ionic conductivity and reduce sintering temperatures, achieving conductivities up to 29.6 mS/cm at 750 °C [3].

Advancements in computational modelling have further propelled SOEC research. Tools like COMSOL Multiphysics facilitate detailed simulations of electrochemical and thermal behaviours within the cell, while Aspen Plus enables system-level analyses to assess process efficiency and integration. These modelling approaches are instrumental in optimizing SOEC designs and operating conditions for enhanced hydrogen production [3].

The fundamental electrochemical reactions in SOECs involve the reduction of steam at the cathode to produce hydrogen and the evolution of oxygen at the anode. The overall reaction is endothermic, benefiting from high-temperature operation to enhance efficiency. Innovations in electrode materials, such as the infiltration of Sm<sub>0.5</sub>Sr<sub>0.5</sub>CoO<sub>3-</sub> $\delta$  (SSC) into LSCF-GDC air electrodes, have demonstrated significant improvements in cell durability, reducing degradation rates by up to 90% [4] [5]. This research aims to investigate the performance of SOECs employing GDC as the electrolyte, utilizing COMSOL and Aspen Plus for comprehensive modelling. The study focuses on evaluating ionic

conductivity, electrolysis efficiency, and hydrogen production rates, contributing to the advancement of efficient and sustainable hydrogen generation technologies [6].

# LITERATURE REVIEW:

### Introduction to SOEC Technology:

Solid Oxide Electrolysis Cells (SOECs) are next-generation high-temperature electrochemical devices capable of converting water and/or carbon dioxide into hydrogen or syngas using renewable electricity. Operating at temperatures ranging from 600°C to 1000°C, SOECs offer thermodynamic advantages due to partial thermal energy contribution, leading to significantly lower electrical energy demands compared to low-temperature technologies like Proton Exchange Membrane (PEM) and Alkaline Electrolysis (AEL) cells [7] [8].

	Alkaline water electrolysis	AEM	PEM	SOEC
Electrolyte	KOH/NaOH	KOH/NaOH	Solid polymer	Solid oxide
	(1M)	(1M)	electrolyte	
Operating	70-90	40-60	50-80	700-850
temperature (C)				
Nominal current	0.2-0.8	0.2-2	1-2	0.3-1
density (A-cm <sup>-2</sup> )				
Voltage range (V)	1.4-3	1.4-2	1.4-2.5	1-1.5
Cell pressure (bar)	<30	<35	<70	<10
Efficiency	50%-78%	57%-59%	50%-83%	89% (Laboratory)
Lifetime (thousand	60	>30	50-80	20
hours)				
H <sub>2</sub> purity	99.5%	99.99%	99.99%	99.99%
Development	Mature	R&D	Commercialized	R&D

Table 1. Technical characteristics of different water electrolysis technologies [7]

## THERMODYNAMIC AND ELECTROCHEMICAL PRINCIPLES:

SOECs operate via the electrochemical splitting of H<sub>2</sub>O and/or CO<sub>2</sub>. The core reactions are [9]:

• At the cathode (fuel electrode):	
$H_2O + 2e^- \rightarrow H_2 + O^{2-}$	(1)
$\mathrm{CO}_2 + 2\mathrm{e}^- \rightarrow \mathrm{CO} + \mathrm{O}^{2-}$	(2)

- At the anode (oxygen electrode):
- $2O^{2-} \rightarrow O_2 + 4e^-$

The overall cell voltage decreases with increased temperature, making high-temperature operation energetically favourable. Thermoneutral voltage ( $\Delta$ H/nF) defines the ideal cell potential at which electrolysis is neither endothermic nor exothermic [10] [11].



Figure 1: Working Principle of SOECs [7]

(3)

# MATERIALS AND COMPONENT DEVELOPMENT:

## **Electrolytes:**

- YSZ (Yttria-stabilized zirconia) remains the dominant electrolyte due to high oxygen-ion conductivity and mechanical stability at 800–1000°C.
- GDC (Gadolinium-doped ceria) shows better conductivity at intermediate temperatures (~600°C), but reduction under cathodic polarization remains a limitation.
- LSGM  $(La_{1-x}Sr_xGa_{1-\gamma}Mg_{\gamma}O_3)$  offers even higher conductivity and is chemically stable with electrodes.

#### **Electrodes:**

#### **Cathode (Fuel Electrode):**

Nickel-YSZ cermet is standard due to excellent catalytic activity and conductivity. Issues include Ni coarsening and carbon deposition during CO<sub>2</sub> electrolysis.

### Anode (Oxygen Electrode):

LSM-YSZ is widely used but suffers from interfacial delamination. LSF and LSCF have emerged as promising alternatives with better mixed conductivity [12] [7].

#### **MODELLING AND SIMULATION TOOLS:**

#### **Aspen Plus:**

Aspen Plus is widely used to simulate SOEC processes thermodynamically. It enables parametric studies of voltage, temperature, and pressure effects. Mathematical models show that increasing temperature reduces cell voltage, improving efficiency.

COMSOL Multiphysics

COMSOL allows detailed simulation of heat, mass, and charge transport, including the implementation of Butler-Volmer kinetics and concentration overpotentials. It helps identify optimal operating conditions and temperature distributions [13] [14].

## **RECENT ADVANCES AND FUTURE OUTLOOK:**

According to Hauch et al. (2020), recent advancements have doubled the electrochemical performance and improved durability 100-fold. Emerging trends include [8]:

- Nanostructured electrodes with in-situ exsolution catalysts
- Advanced stack sealing for longer lifetimes
- Integration with Fischer-Tropsch, methanol, and ammonia synthesis plants
- Use of renewable electricity in gigawatt-scale SOEC systems

## **METHODOLOGY:**

#### **Overview of Research Approach:**

This study adopts a comprehensive computational modeling approach to analyze and compare the performance of Solid Oxide Electrolysis Cells (SOECs) using two different electrolyte materials: Gadolinium-doped Ceria (GDC) and Yttria-stabilized Zirconia (YSZ). The primary goal is to evaluate the hydrogen production efficiency of GDC-based SOEC systems under high-temperature electrolysis conditions and benchmark it against the more conventional YSZ-based systems to determine whether GDC presents a superior alternative.

# TO ACHIEVE THIS, A DUAL SIMULATION FRAMEWORK IS EMPLOYED: Aspen Plus–MATLAB Integrated Model:

A process-level simulation of the SOEC system was developed in Aspen Plus, using custom electrochemical subroutines written in MATLAB. This hybrid setup allows dynamic and parametric control over electrochemical variables such as current density, operating temperature, and gas composition. The MATLAB module computes polarization behavior and voltage losses based on

electrolyte properties, while Aspen Plus handles mass and energy balances, syngas separation, and hydrogen quantification.

# **COMSOL Multiphysics Model :**

A detailed multiphysics model of the SOEC was created using COMSOL's built-in SOEC template, which simulates electrochemical, thermal, and transport phenomena within the cell. The following modifications were made:

- Electrolyte Material: YSZ was replaced with GDC to assess its effect on ionic conductivity, potential distribution, and hydrogen output.
- Electrolyte Thickness: Reduced to improve ionic transport and investigate its influence on ohmic resistance and overall efficiency.
- Operating Conditions: Temperature, pressure, current density, and boundary conditions were kept identical to the baseline YSZ model to ensure a fair comparison.

# MATHEMATICAL MODELLING:

The mathematical model of the Solid Oxide Electrolysis Cell (SOEC) used in this study incorporates key equations governing electrochemical reactions, voltage losses, and material-specific transport phenomena. These models are implemented in MATLAB for process-level simulation and used to configure physics-based simulations in COMSOL. The purpose of this section is to define the set of equations used to describe cell performance under different material conditions (GDC vs. YSZ).

#### a) Cell Voltage Equation

The total operating voltage U of an SOEC is the sum of the thermodynamic reversible voltage and the various losses across the cell:

$$U = U_{rev} + \eta_{act} + \eta_{ohmic} + \eta_{conc} \tag{4}$$

#### b) Reversible Voltage (Nernst Equation)

The Nernst equation calculates the theoretical voltage required for electrolysis based on partial pressures of reactants and products [9]:

$$U_{rev} = U^0 + \frac{RT}{2F} ln\left(\frac{p_{H_2} p_{O_2}^{1/2}}{p_{H_2O}}\right)$$
(5)

#### c) Activation Overpotential (Butler–Volmer Equation)

Activation losses arise from the energy barrier for electron transfer reactions [7]:

$$\eta_{act} = \frac{RT}{\alpha F} sinh^{-1} \left(\frac{j}{2j_0}\right) \tag{6}$$

#### d) Ohmic Overpotential

Ohmic losses are caused by resistance to ion flow through the electrolyte and electron flow through the electrodes [12]:

$$\eta_{ohmic} = j \cdot R_{ohm} = \frac{j \cdot L}{\sigma} \tag{7}$$

#### e) Concentration Overpotential

Concentration losses occur due to limitations in gas diffusion to the reactive sites, especially at high current densities [11]:

$$\eta_{conc} = -\frac{RT}{nF} ln \left( 1 - \frac{j}{j_{lim}} \right)$$
(8)

#### f) Hydrogen Production Rate

The rate of hydrogen production is directly proportional to the cell current [8]:

$$n_{H_2} = \frac{l}{2F} \tag{9}$$

# g) Energy Efficiency

Voltage efficiency is defined as:

$$\eta_V = \frac{U_{rev}}{U_{cell}} \tag{10}$$

## SIMULATION AND SETUP: Aspen Plus integrated with MATLAB:

The simulation of the Solid Oxide Electrolysis Cell (SOEC) was carried out using Aspen Plus V14, integrated with MATLAB to incorporate dynamic electrochemical calculations. The modelling approach was based on a steady-state simulation mode, allowing a consistent analysis of system behaviour under fixed operating conditions. The SOEC was modelled using the Soave–Redlich–Kwong (SRK) property method, which is suitable for high-temperature gas-phase systems like steam electrolysis. The working electrolyte material used in the model was Gadolinium-doped Ceria (GDC), with its key ionic properties (notably higher ionic conductivity than YSZ) defined and embedded in the MATLAB subroutines. The core chemical species considered in the model were hydrogen (H<sub>2</sub>), oxygen (O<sub>2</sub>), steam (H<sub>2</sub>O), and nitrogen (N<sub>2</sub>), representing both reactants and products in the electrolysis process.

## Flowsheet design:



Figure 2: SOEC Flowsheet in Aspen Plus

The figure 2 represents a Solid Oxide Electrolyser Cell (SOEC) system modelled in Aspen Plus for green hydrogen production. The process begins with a steam feed introduced through the FEED stream, which is then preheated in the HEATER to the high operating temperatures (typically 700–850°C) required for solid oxide electrolysis. The heated steam enters the SOEC, where it undergoes high-temperature electrolysis using a ceramic electrolyte (such as GDC or YSZ), producing a gas mixture of hydrogen (H<sub>2</sub>), oxygen (O<sub>2</sub>), and residual steam. This gas mixture then flows into the SEP unit, where hydrogen is separated and exits as H2OUT, while the remaining gases, primarily oxygen and steam, proceed to a mixer or splitter labelled B1. An AIR stream is introduced here to dilute the oxygen for safe venting or further processing, and the final oxygen-rich stream exits as O2OUT. This flowsheet efficiently models the core process of high-temperature steam electrolysis for sustainable hydrogen production.

	Blocks Used	
Block type	Block name	purpose
Heater	HEATER	Preheats feed gases to SOEC operating temp (800°C)
Rstoic	SOEC	Electrolysis reactor
Separator	SEP	
		Separates gas output stream into H2, O2, H2O
Mixer	B1	
		Combines steam and Air

Table 2: The following Blocks and Streams are used in Aspen plus to model SOEC.

Streams Used						
FEED	FEED					
AIR	AIR					
O2OUT & H2OUT	O2OUT & H2OUT					

#### **PARAMETERS AND COMPONENTS:**

Table 3: Constant values used in Matlab Code

Constants									
Parameter	Description	Value	Unit						
R	Universal gas constant	8.314	J/mol·K						
F	Faraday constant	96485	C/mol						
MO2	Molar mass of O2	31.9988	g/mol						
MN2	Molar mass of N2	28.0135	g/mol						
MH2	Molar mass of H2	2.0159	g/mol						
MH2O	Molar mass of H2O	18.0135	g/mol						

#### Table 4: Cell Parameter Values used in Matlab Code

Cell Parameters								
Parameter	Description	Value	Unit					
	Electrolyte ionic							
SigmaE	conductivity (GDC)	0.05	S/cm					
DeltaE	Electrolyte thickness	0.0000125	m					
DeltaC	Cathode thickness	0.000032	m					
DeltaA	Anode thickness	0.0000175	m					
rOhm	Ohmic resistance	0.0000265	Ohm·m <sup>2</sup>					
А	Cell area	0.01	m <sup>2</sup>					
N	Number of cells	10						

Tables 3 and 4 summarize the constants and SOEC parameters used in the MATLAB model integrated with Aspen Plus. Table 3 includes essential constants such as the universal gas constant, Faraday constant, and molar masses of key species (O<sub>2</sub>, N<sub>2</sub>, H<sub>2</sub>, and H<sub>2</sub>O). Table 4 lists SOEC-specific parameters, including electrolyte ionic conductivity (0.05 S/cm for GDC), layer thicknesses (electrolyte, cathode, anode), and ohmic resistance. The cell area and number of cells define the system size. These parameters are vital for simulating electrochemical behaviour and hydrogen production performance.

) :	Selection Petroleum Nonconventional		Centerprise Database	e Comments		
e	ct components					
Component ID		Туре		Component name	Alias	CAS number
	H2O	120 Conventional		WATER	H2O	7732-18-5
	H2	Conventional		HYDROGEN	H2	1333-74-0
	02	Conventional		OXYGEN	02	7782-44-7
	N2	Conventional		NITROGEN	N2	7727-37-9

Figure 3: Components Selected in Aspen Plus

Figure 3 shows the selection of chemical components used in the Aspen Plus simulation of the SOEC process. The selected components ( $H_2O$ ,  $H_2$ ,  $O_2$ , and  $N_2$ ) are all conventional species essential to the

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electrolysis system. Water  $(H_2O)$  serves as the primary feedstock for hydrogen production, while hydrogen  $(H_2)$  is the desired product. Oxygen  $(O_2)$  is generated as a byproduct, and nitrogen  $(N_2)$  is often used as an inert carrier or purge gas.

	Solid	NC Solid	Flash Opt	tions	EO Options	Costing	Comments	
Specificati	ons							
-lash Type	т	emperature	-	Pres	sure	- Co	mposition ———	
- State variabl	les —					M	ole-Flow	<ul> <li>kmol/hr</li> </ul>
Temperature	9		848	c	•		Component	Value
Pressure			1	bar	-		H2O	
Vapor fraction	on					Þ	H2	
Total flow b	asis	Mole	-			>	02	0.0039177
Total flow ra	ite			kmol	/hr 🔹		N2	0.01473
Solvent								
Reference Te Volume flow Component	emperat v referer C : concer	nce temperat	ture ence tempe	erature				

Figure 4: Stream (AIR) Values

S Mixed	CI Solid	NC Solid	Flash Opt	tions	EO Options	Costing	Comments	
Specifi	ications							
Flash Type		Temperature	•	Press	ure	▼ Cc	mposition ———	
State va	riables —						lole-Flow	kmol/hr
Tempera	ature		848	K	•		Component	Value
Pressure	•		1	atm	•		H2O	0.018655
Vapor fr	action						H2	
Total flo	w basis	Mole	•				02	
Total flo	w rate			kmol/	/hr 🝷	)	N2	
Solvent					*			
Reference	e Tempera	iture						
Volume	flow refere	ence temperat	ure					
	C							
Compor	nent conce	ntration refer	ence tempe	erature				
	С	*					Tota	0.018655

Figure 5: Stream (FEED) Values

Figures 4 and 5 show the input stream values for the AIR and FEED streams used in the SOEC model in Aspen Plus. Both streams operate at a temperature of 848 K and a pressure of 1 atm. The AIR stream consists of 0.0039 kmol/hr of  $O_2$  and 0.0147 kmol/hr of  $N_2$ , representing the oxidant side of the system. The FEED stream supplies the reactant, with 0.0187 kmol/hr of H<sub>2</sub>O as the sole component.

lash specifications			
lash Type	Temperature		-
	Pressure		-
emperature	800	с	-
emperature change		С	-
Degrees of superheating		С	~
Degrees of subcooling		С	-
Pressure	1	bar	-
Duty		Gcal/hr	
apor fraction			
ressure drop correlation parameter			
Always calculate pressure drop co	rrelation parameter		

Figure 6: Heater Specifications

1ain Flowsheet $ imes$	SOEC (RS	toic) × 🕂									
Specifications	Streams	Reactions	Combu	stion   H	leat o	f Reaction	Selectivity	PSD	Component Attr.	Utility	Comments
Operating conditi	ons —										
Flash Type	Те	mperature	Pressu	ire	•						
Temperature		848	3 C		•						
Pressure		1	bar		•						
Duty			Gcal/h	r							

Figure 7: SOEC Operating Conditions

Figures 6 and 7 present the thermal and operational settings for the solid oxide electrolysis process. In Figure 6, the heater is configured to elevate the feed temperature to 800°C at 1 bar, preparing the stream for electrolysis by ensuring it reaches the high-temperature regime necessary for SOEC functionality. Figure 7 shows that the SOEC unit itself operates at a slightly higher temperature of 848°C and 1 bar pressure, which are optimal conditions for promoting the endothermic electrochemical reaction that converts steam (H<sub>2</sub>O) into hydrogen (H<sub>2</sub>) and oxygen (O<sub>2</sub>).

Main	Flowsheet	× SEP (Se	ep) × +			
Øs	pecification	ns Feed Fl	ash Outlet Flash Utility	Comments		
Ou	tlet stream	conditions -				
Ou	tlet stream	5	•			
Sub	ostream	MIXED	•			
	Comp	oonent ID	Specification	Basis	Value	Units
	H2O		Split fraction		0	
	H2		Split fraction		0	
	02		Split fraction		1	
	N2		Split fraction		1	

Figure 8: Separator Conditions

## **COMSOL MULTIPHYSICS:**

The Solid Oxide Electrolysis Cell (SOEC) model used in this study was based on the tutorial provided by COMSOL, which originally employs yttria-stabilized zirconia (YSZ) as the electrolyte material. To investigate the performance of a Gd-doped ceria (GDC)-based SOEC, modifications were made to the model to reflect the distinct material properties of GDC. The electrolyte material was changed from YSZ to GDC, and relevant thermophysical and electrochemical properties were updated accordingly. These included the ionic conductivity, activation energy, and temperature dependence based on literature data for GDC. Furthermore, the electrolyte thickness was adjusted to reflect a more realistic design for GDC-based cells, considering its higher ionic conductivity at intermediate temperatures compared to YSZ. The rest of the cell structure, including the hydrogen and oxygen electrode domains, remained consistent with the reference model to ensure comparability.

## 3.3.2.1 Model Definition:

On the anode, oxygen ions are oxidized to form oxygen gas,

$$0^{2-} \leftrightarrow \frac{1}{2} O_2(\mathbf{g}) + 2e$$
- (11)

whereas on the cathode, water vapor is reduced to form hydrogen gas and oxygen ions:  $H_2O(g) + 2e \leftrightarrow H_2(g) + 0^{2-}$  (12)



#### Figure 9: Model geometry

The transport of hydrogen and water vapor was modelled in both the cathode gas channels and the porous gas diffusion electrode. This was coupled with laminar flow behaviour of the gas mixture using COMSOL's Free and Porous Media Flow interface. The Brinkman equations were applied to simulate fluid flow in the porous electrodes, while the Navier–Stokes equations governed the flow in the nonporous gas channels.

Electrochemical reactions and charge transport were implemented using the Water Electrolyser interface. This interface enabled the definition of electrochemical reactions, ionic conduction through the electrolyte, and mass transport of gaseous species within the cell. The electrolyte was modelled with a constant ionic conductivity, which was set according to values reported in literature for GDC at the selected operating temperature.

On the cathode side, the reaction kinetics were influenced by the local concentrations of hydrogen and water vapor, incorporating the law of mass action and Nernst equation to determine the local equilibrium potential. For the anode side, a constant oxygen partial pressure was assumed, and a simplified Butler–Volmer expression (independent of oxygen concentration) was used to describe the anodic reaction kinetics. The gas mixture properties and electrochemical potentials were computed using the built-in options of the Water Electrolyser physics interface.

#### **PARAMETERS:**

Figures 10 and 11 present the key geometry and physics parameters used for the SOEC simulation in COMSOL. The cell design incorporates a reduced electrolyte layer thickness of 0.05 mm (5E-5 m), as shown in the parameter H\_el, which enhances ionic transport and lowers ohmic losses. Additionally, the simulation assumes the use of gadolinium-doped ceria (GDC) as the electrolyte material, reflected in the increased electrolyte ionic conductivity value of 5 S/m (sigma\_l). These modifications aim to improve overall SOEC performance by reducing internal resistance and enhancing efficiency at the high operating temperature of 1073.2 K (800°C).

Paramete	ers				
abel: Geo	bel: Geometry Parameters				
<ul> <li>Parame</li> </ul>	eters				
₩ Name	Expression	Value	Description		
W_ch	0.5[mm]	5E-4 m	Channel width		
W_rib	W_ch*3	0.0015 m	Rib width		
L_ch	10[mm]	0.01 m	Channel length		
N_ch	3	3	Number of channels		
H_gde	0.1[mm]	1E-4 m	Gas diffusion electrode thickness		
H_ch	W_ch	5E-4 m	Channel height		
H_el	0.05[mm]	5E-5 m	Electrolyte layer thickness		
D_cell	N_ch*(W_ch+W_rib)	0.006 m	Cell depth (in y-direction)		
W_cell	L_ch+2*W_ch+W_rib	0.0125 m	Cell width (in x-direction)		
H_cell	H_gde*2+H_el+H_ch	7.5E-4 m	Cell thickness (in z-direction)		

Figure 10: Geometry Parameters in COMSOL

Settings Parameters			,		
Label: Physics Parameters					
▼ Paramete	ers				
** Name	Expression	Value	Description		
kappa	1e-10[m^2]	1E-10 m <sup>2</sup>	Electrode permeability		
por	0.4	0.4	Electrode porosity		
I_avg	10^4[A/m^2]	10000 A/m <sup>2</sup>	Average current density		
stoich	1.1	1.1	Inlet steam stoichiometry		
A_cell	W_cell*D_cell	7.5E-5 m <sup>2</sup>	Cell area		
Mflux_in	stoich*18[g/mol]*I_avg*A_cell/(2*F_const)	7.6955E-8 kg/s	Total inlet (steam) mass flux		
Т	800[degC]	1073.2 K	Cell temperature		
sigma_l 5[S/m]		5 S/m	Electrolyte conductivity		
sigma_s	1000[S/m]	1000 S/m	Electrode conductivity		
i0_H2	0.1[A/m^2]	0.1 A/m <sup>2</sup> Reference exchange current density, hydrogen reaction			
i0_02	0.01[A/m^2]	0.01 A/m <sup>2</sup> Reference exchange current density, oxygen reaction			
S	1e9[m^2/m^3]	1E9 1/m	Electrode specific surface area		







Gadolinium-Doped Ceria



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Figure 12 illustrates the implementation of Gadolinium-Doped Ceria (GDC) as the electrolyte material in the SOEC model, replacing the conventional Yttria-Stabilized Zirconia (YSZ). The left panel shows the material settings in COMSOL. The right panel displays the 3D geometry of the SOEC, highlighting the blue region as the electrolyte domain. A significant design improvement is the reduction of electrolyte thickness to 0.05 mm, which enhances ionic transport and overall cell efficiency at high operating temperatures.

# **RESULTS:** ASPEN SIMULATION RESULTS:

		Units	H2OUT -	O2OUT -	FEED -	AIR 👻
Þ	- Mole Flows	kmol/hr	0.0186557	0.0251853	0.0186557	0.0186557
Þ.	H2O	kmol/hr	0.00559672	0	0.0186557	0
1	H2	kmol/hr	0.013059	0	0	0
Þ.	02	kmol/hr	0	0.0104472	0	0.00391771
þ.	N2	kmol/hr	0	0.014738	0	0.014738
P.	- Mole Fractions					
P.	H2O		0.3	0	1	0
P.	H2		0.7	0	0	0
p.	02		0	0.414815	0	0.21
Þ.	N2		0	0.585185	0	0.79
Þ.	- Mass Flows	kg/hr	0.127152	0.747162	0.336089	0.538226
Þ.	H2O	kg/hr	0.100827	0	0.336089	0
Þ	H2	kg/hr	0.0263254	0	0	0
Þ.	02	kg/hr	0	0.334298	0	0.125362
ē.	N2	kg/hr	0	0.412864	0	0.412864
Þ	- Mass Fractions					
Þ	H2O		0.792961	0	1	0
P.	H2		0.207039	0	0	0
Þ.	02		0	0.447424	0	0.232917
P	N2		0	0.552576	0	0.767083
þ.	Volume Flow	cum/hr	1.73927	2.3483	1.29744	1.7395

Figure 13: Results from SOEC Aspen Simulation (GDC as Electrolyte)

Þ.	+ Mole Flows	kmol/sec	5.45833e-07	2.72917e-07
Þ.	- Mole Fractions			
Þ.	WATER		0	0
•	H2		1	0
•	02		0	1
•	+ Mass Flows	kg/sec	1.10033e-06	8.73301e-06
)÷.	+ Mass Fractions			

Figure 14: Results from SOEC Aspen Simulation (YSZ as Electrolyte) [9]

Figures 13 and 14 present the simulation results of a Solid Oxide Electrolysis Cell (SOEC) model in Aspen Plus, with GDC (Gadolinium-doped Ceria) and YSZ (Yttria-stabilized Zirconia) used as electrolytes, respectively. The comparison focuses on the mole and mass flow rates of key species H<sub>2</sub>, and O<sub>2</sub>.

# Mole Flow Comparison:

# GDC Electrolyte (Figure 13):

- H<sub>2</sub> Production (H2OUT): 0.013059 kmol/hr
- O<sub>2</sub> Production (O2OUT): 0.0104472 kmol/hr

## YSZ Electrolyte (Figure 14):

- H<sub>2</sub> Production:  $5.45833e-07 \text{ kmol/sec} \approx 0.001964998 \text{ kmol/hr}$
- O<sub>2</sub> Production: 2.72917e-07 kmol/sec  $\approx$  0.000982499 kmol/hr

Observation: The SOEC using GDC as the electrolyte produces significantly higher amounts of hydrogen and oxygen in mole terms compared to the YSZ-based cell. Hydrogen production is roughly 6.6 times higher with GDC, indicating superior ionic conductivity and overall electrochemical performance.

# **Mass Flow Comparison:**



- I. GDC Electrolyte:
  - H<sub>2</sub> Mass Flow (H2OUT): 0.0263254 kg/hr
  - O<sub>2</sub> Mass Flow (O2OUT): 0.334298 kg/hr

#### **YSZ ELECTROLYTE:**

- H<sub>2</sub> Mass Flow:  $1.10033e-06 \text{ kg/sec} \approx 0.003961 \text{ kg/hr}$
- O<sub>2</sub> Mass Flow: 8.73301e-06 kg/sec  $\approx 0.0310388$  kg/hr

Observation: In terms of mass flow as well, the GDC-based SOEC outperforms the YSZ system. Hydrogen mass flow is over 6.6 times higher and oxygen mass flow is about 10.7 times higher with GDC. This further validates GDC's enhanced ionic conductivity and catalytic activity.

## **COMSOL MULTIPHYSICS RESULTS:**



Figure 15 (a): Concentration, H2, Streamline (tcs) [GDC] Figure 15 (b): Concentration, H2, Streamline (tcs) [YSZ] [15]

Figures 15(a) and 15(b) illustrate the hydrogen concentration streamlines in the SOEC using GDC and YSZ electrolytes, respectively. The GDC-based cell (Figure 15a) demonstrates a more uniform and higher hydrogen molar concentration across the flow channels, with values reaching up to 10 mol/m<sup>3</sup>, indicating efficient hydrogen generation and transport. In contrast, the YSZ-based cell (Figure 15b) shows a slightly higher peak concentration of 11 mol/m<sup>3</sup>, but with greater spatial variation and lower concentrations in key regions of the flow path. This suggests uneven hydrogen distribution and less effective transport. The more consistent and evenly distributed hydrogen flux in the GDC cell highlights its superior electrochemical activity and mass transport characteristics, reinforcing its advantage as an electrolyte material for high-performance SOECs.

Figure 16 (a): Concentration, H2, Surface (tcs) [GDC]

Figure 16 (b): Concentration, H2, Surface (tcs) [YSZ] [15]

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Figures 16(a) and 16(b) present the surface concentration distribution of hydrogen (H<sub>2</sub>) in SOECs using GDC and YSZ electrolytes, respectively. In Figure 16(a), the GDC-based SOEC shows a smooth and gradual gradient in hydrogen concentration, ranging from approximately 2 to over 10 mol/m<sup>3</sup>, with a strong presence of higher concentration values (in the red to yellow range) across most of the active area. This indicates efficient and widespread hydrogen generation throughout the electrolyte interface. In contrast, Figure 16(b) reveals that while the YSZ-based cell reaches similar peak concentrations (just over 10 mol/m<sup>3</sup>), the distribution is less uniform, with more abrupt transitions and lower concentrations observed in broader regions. This disparity suggests that GDC provides better mass transport and reaction kinetics, promoting more effective hydrogen production across the entire cell surface. These findings further support the suitability of GDC as a high-performance electrolyte material for SOEC systems.



Figure 17 (a): Molar Fraction and Flux, H2 [GDC]

Figure 17 (b): Molar Fraction and Flux, H2 [YSZ] [15]

Figures 17(a) and 17(b) display the molar fraction and flux distribution of hydrogen (H<sub>2</sub>) in SOECs with GDC and YSZ electrolytes, respectively. The GDC-based cell in Figure 17(a) shows a well-distributed hydrogen molar fraction, reaching values up to 0.9, with more uniform streamline flow patterns and broader regions maintaining high hydrogen concentrations. In contrast, the YSZ-based cell in Figure 17(b) demonstrates a less consistent distribution, with localized peaks and molar fractions generally remaining below 0.8 in larger areas. The smoother flux distribution and higher hydrogen molar fractions in the GDC model indicate more efficient electrochemical conversion and mass transport, further validating GDC's superior ionic conductivity and overall performance as an SOEC electrolyte compared to YSZ.

## **CONCLUSION:**

In this study, the performance of Solid Oxide Electrolysis Cells (SOECs) using Gadolinium-Doped Ceria (GDC) and Yttria-Stabilized Zirconia (YSZ) as electrolytes was analysed through multi-platform simulations. The results decisively establish that GDC is a superior electrolyte material for SOEC applications. According to Aspen Plus simulations, the GDC-based SOEC produced 0.013059 kmol/hr of H<sub>2</sub> and 0.0104472 kmol/hr of O<sub>2</sub>, compared to only 0.001965 kmol/hr of H<sub>2</sub> and 0.0009825 kmol/hr of O<sub>2</sub> using YSZ (demonstrating that GDC enabled hydrogen production rates over 6.6 times higher). The mass flow comparison further reinforced these findings, with 0.0263 kg/hr of H<sub>2</sub> and 0.3343 kg/hr of O<sub>2</sub> using GDC, versus 0.00396 kg/hr of H<sub>2</sub> and 0.0310 kg/hr of O<sub>2</sub> with YSZ.

COMSOL simulation results provided additional insights. Figures 15–17 revealed that the GDC cell exhibited a more uniform and higher hydrogen concentration distribution (up to 10 mol/m<sup>3</sup>) and molar fraction (up to 0.9) compared to the YSZ cell, which showed inconsistent distribution and lower average performance. Furthermore, the smoother hydrogen flux in the GDC-based system indicates improved mass transport and electrochemical conversion. These advantages stem from GDC's higher ionic conductivity (up to 5 S/m in COMSOL, and 0.05 S/cm in Aspen Plus), which significantly reduces ohmic losses and enhances reaction kinetics even at slightly lower temperatures (~800°C).Overall, the integrated results from Aspen Plus–MATLAB and COMSOL confirm that GDC

not only improves hydrogen yield and system efficiency but also ensures better electrochemical stability and uniformity. Therefore, GDC presents a more efficient, cost-effective, and scalable alternative to YSZ for high-temperature electrolysis applications in sustainable hydrogen production.

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