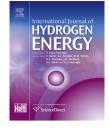


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Elementary reaction modeling and experimental characterization of solid oxide fuel-assisted steam electrolysis cells

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ABSTRACT

A one-dimensional elementary reaction kinetic model for solid oxide fuel-assisted steam electrolysis cell (SOFEC) is developed coupling heterogeneous elementary reactions, electrochemical reaction kinetics, electrode microstructure and transport processes of charge and mass. This model is calibrated and validated by experimental data from a button cell with anode gases of H2, CO and CH4 at 800 °C. After comparisons with solid oxide electrolysis cell (SOEC), the energy demands, performance and efficiency of CO-assisted SOFEC and CH₄-assisted SOFEC are investigated numerically. One important finding is that over 80% of electricity can be saved by SOFEC at a current density of 3000 A m^{-2} . SOFEC assisted by CO or CH₄ for steam electrolysis has better performance than SOEC, especially by CH₄. The efficiencies of 12% CO-SOFEC and 12% CH₄-SOFEC are at least, respectively, 7% and 30% higher than that of SOEC at 800 $^{\circ}$ C with the current density of below 2500 A m⁻². Finally, the effects of type of assisting-fuel, fuel composition and applied voltage are studied. It is found that CO-SOFEC shows higher anode polarization and thus lower performance than CH₄-SOFEC with the same molar fraction of fuel. It is also found that the performance of SOFEC increases with increasing proportion of assisted fuel in anode at high current density.

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Introduction

The use of fossil fuels as the major energy source leads to increasingly more and more serious energy crisis and environmental issues such as global warming, air pollution and acid rain. To address these global issues, it is urgent to adopt clean and sustainable energy technologies. Renewable energies like solar energy and wind energy can perfectly meet our requirements as they are clean, sustainable, and abundant. However, renewable power is restricted in time and space, intermittent and site-specific, thus are not reliable for

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ASR CO-SOFE		S ^{eff} S _{Ni}	Effective reaction area per unit volume, $m^2 m^{-3}$
ASR CO-SOFE			
CO-SOFE	Abbreviation		Ni active surface area per unit volume, $m^2 m^{-3}$
	Area specific resistance	S _{TPB}	TPB active area per unit volume, $m^2 m^{-3}$
CH₄-SOF	C Solid oxide CO-assisted electrolysis cell	Т	Temperature, K
	EC Solid oxide CH ₄ -assisted electrolysis cell	V	Voltage or potential, V
	High-temperature electrolysis	V_k , V_j	Diffusion volume
	Lower heat value, J mol ⁻¹	W	Molecular weight of gas species, kg mol $^{-1}$
LSM	Lanthanum strontium manganate	W_{TPB}	Width of TPB, m
	Methane steam reforming reaction	х	Molar fraction
OCV	Open-circuit voltage	Ζ	Mean coordination number of electron and ionic
ScSZ	Scandium stabilized zirconium		conductor particles
SOEC	Solid oxide electrolysis cell	Z _{elec}	Coordination number of electron conductor
	Solid oxide fuel cell		particles
	Solid oxide fuel-assisted electrolysis cell	Zion	Coordination number of ionic conductor particles
	Triple phase boundary		
	Yttrium stabilized zirconium	Greek le	
	Water-gas shift reaction	α	Charge transfer coefficient
WGJK	water-gas sinit reaction	β_{ca}	Cathode electrochemical kinetics parameter
Roman		γ	Parameter modeling the rate constant from
А	Pre-exponential factor of the Arrhenius form, in		sticking coefficient
	terms of cm, mol and s	Г	Surface sites density, $\Omega^{-1} \mathrm{m}^{-2}$
	Molar concentration of gas-phase species or	ΔS	Entropy change, J $mol^{-1} K^{-1}$
	surface coverage of surface species	ε	Porosity
	The volumetric concentrations of interstitial		Parameter modeling the species coverage
0 (152)	oxygen in the YSZ ionic conductor, mol m^{-3}	e _{ki}	Overpotential, V or efficiency
	The volumetric concentrations of interstitial	$\eta \\ heta$	Contact angle between the electronic and ionic
(102)		0	
	oxygen in the YSZ ionic conductor, mol m^{-3}	,	conductors particles
	The concentration of gaseous species i in the bulk,	ν'	Stoichiometric coefficient of the reactants
	$mol m^{-3}$	$\nu^{''}$	Stoichiometric coefficient of the products
	The concentration of gaseous species i at the TPB,	σ	Electric conductivity, S m ⁻¹
	$mol m^{-2}$	au	Tortuosity
	Activation energy in sticking coefficient	χ	Species symbol
	expression, J mol ⁻¹	$\partial \Omega$	Computational boundary
	Diffusion coefficient, $m^2 s^{-1}$	Subscrip	ate
Е	Active energy, J mol ⁻¹	-	Anode chamber
F	Faraday constant, 96,384 C mol ⁻¹	ac	
i	Current density, A m^{-3}		Anode active layer
i _o	Exchange current density, A m^{-3}	an_sp	Anode support layer
	Reaction rate constant, in terms of m, mol and s	са	Cathode
	Reaction equilibrium constant	ca-el	Interface of cathode and electrolyte
	Length of TPB in anode, m m^{-3}	CC	Cathode chamber
	Length of TPB in cathode, m m ^{-2}	ef	Forward electrochemical reaction
		el	Electrolyte
	Molar mass of gas-phase species i, kg mol^{-1}	elec	Electronic
	Reaction order of the Arrhenius form	er	Reversed electrochemical reaction
	Fraction number of electronic conductor particles	f	Forward reaction
	Fraction number of ionic conductor particles	ion	Ionic
-	Total number of electronic and ionic conductor	ir	Irreversible heat
	particles	Kn	Knudsen diffusion
р	Pressure, Pa	_	Molecular diffusion
	Power density, W m^{-2}	mole	
	Source term of charge balance equations, A m^{-3} or	r	Reverse reaction
	energy flux, W m ⁻²	re	Reversible heat
	Average pore/particle radius, m	Supersci	ripts
	Universal gas constant, 8.314 J $mol^{-1} K^{-1}$	0	Parameter at equilibrium conditions
	Source term of species k for mass balance	bulk	Bulk phase
	equation, kg $m^{-3} s^{-1}$	eff	Effective
	The net molar production rate, in terms of m, mol		Triple phase boundary
		TPB	

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