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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 H_2, CO and CH_4 at 800 °C. After comparisons with solid oxide electrolysis cell (SOEC), the energy demands, performance and efficiency of CO-assisted SOFEC and CH_4-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 CH_4 for steam electrolysis has better performance than SOEC, especially by CH_4. The efficiencies of 12% CO-SOFEC and 12% CH_4-SOFEC are at least, respectively, 7% and 30% higher than that of SOEC at 800 °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 CH_4-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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Nomenclature

Abbreviation

ASR	Area specific resistance
CO-SOFEC	Solid oxide CO-assisted electrolysis cell
CH_4-SOFEC	Solid oxide CH_4-assisted electrolysis cell
HTE	High-temperature electrolysis
LHV	Lower heat value, J mol^{-1}
LSM	Lanthanum strontium manganate
MSRR	Methane steam reforming reaction
OCV	Open-circuit voltage
ScSZ	Scandium stabilized zirconium
SOEC	Solid oxide electrolysis cell
SOFC	Solid oxide fuel cell
SOFEC	Solid oxide fuel-assisted electrolysis cell
TPB	Triple phase boundary
YSZ	Yttrium stabilized zirconium
WGSR	Water–gas shift reaction

Roman

A	Pre-exponential factor of the Arrhenius form, in terms of cm, mol and s
c_i	Molar concentration of gas-phase species or surface coverage of surface species
$c_{O^{2-}(YSZ)}$	The volumetric concentrations of interstitial oxygen in the YSZ ionic conductor, mol m^{-3}
$c_{(YSZ)}$	The volumetric concentrations of interstitial oxygen in the YSZ ionic conductor, mol m^{-3}
c_i^{bulk}	The concentration of gaseous species i in the bulk, mol m^{-3}
c_i^{TPB}	The concentration of gaseous species i at the TPB, mol m^{-2}
d	Activation energy in sticking coefficient expression, J mol^{-1}
D	Diffusion coefficient, m^2 s^{-1}
E	Active energy, J mol^{-1}
F	Faraday constant, 96,384 C mol^{-1}
i	Current density, A m^{-3}
i_0	Exchange current density, A m^{-3}
k	Reaction rate constant, in terms of m, mol and s
K_p	Reaction equilibrium constant
$L_{TPB,an}$	Length of TPB in anode, m m^{-3}
$L_{TPB,ca}$	Length of TPB in cathode, m m^{-2}
M_i	Molar mass of gas-phase species i, kg mol^{-1}
n	Reaction order of the Arrhenius form
n_{elec}	Fraction number of electronic conductor particles
n_{ion}	Fraction number of ionic conductor particles
n_t	Total number of electronic and ionic conductor particles
p	Pressure, Pa
P	Power density, W m^{-2}
Q	Source term of charge balance equations, A m^{-3} or energy flux, W m^{-2}
r	Average pore/particle radius, m
R	Universal gas constant, 8.314 J mol^{-1} K^{-1}
R_k	Source term of species k for mass balance equation, kg m^{-3} s^{-1}
$\dot{s}_k$	The net molar production rate, in terms of m, mol and s
S^0	Initial sticking coefficient
S^{eff}	Effective reaction area per unit volume, m^2 m^{-3}
S_{Ni}	Ni active surface area per unit volume, m^2 m^{-3}
S_{TPB}	TPB active area per unit volume, m^2 m^{-3}
T	Temperature, K
V	Voltage or potential, V
V_k, V_j	Diffusion volume
W	Molecular weight of gas species, kg mol^{-1}
W_{TPB}	Width of TPB, m
x	Molar fraction
Z	Mean coordination number of electron and ionic conductor particles
Z_{elec}	Coordination number of electron conductor particles
Z_{ion}	Coordination number of ionic conductor particles

Greek letters

α	Charge transfer coefficient
β_{ca}	Cathode electrochemical kinetics parameter
γ	Parameter modeling the rate constant from sticking coefficient
Γ	Surface sites density, Ω^{-1} m^{-2}
ΔS	Entropy change, J mol^{-1} K^{-1}
ε	Porosity
ε_{ki}	Parameter modeling the species coverage
η	Overpotential, V or efficiency
θ	Contact angle between the electronic and ionic conductors particles
ν'	Stoichiometric coefficient of the reactants
ν''	Stoichiometric coefficient of the products
σ	Electric conductivity, S m^{-1}
τ	Tortuosity
χ	Species symbol
$\partial\Omega$	Computational boundary

Subscripts

ac	Anode chamber
an_act	Anode active layer
an_sp	Anode support layer
ca	Cathode
ca-el	Interface of cathode and electrolyte
cc	Cathode chamber
ef	Forward electrochemical reaction
el	Electrolyte
elec	Electronic
er	Reversed electrochemical reaction
f	Forward reaction
ion	Ionic
ir	Irreversible heat
Kn	Knudsen diffusion
mole	Molecular diffusion
r	Reverse reaction
re	Reversible heat

Superscripts

0	Parameter at equilibrium conditions
bulk	Bulk phase
eff	Effective
TPB	Triple phase boundary

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