Energy Conversion and Management 140 (2017) 247–259

Contents lists available at ScienceDirect

Energy Conversion and Management

journal homepage: www.elsevier.com/locate/enconman

Modeling and simulation of a novel 4.5 kW$_e$ multi-stack solid-oxide fuel cell prototype assembly for combined heat and power

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ARTICLE INFO

Article history:
Received 26 July 2016
Received in revised form 19 February 2017
Accepted 23 February 2017

Keywords:
Solid oxide fuel cell (SOFC)
SOFC system model
Geothermic Fuel Cell
In situ oil shale processing
Combined heat and power
Fuel cell commercial application

ABSTRACT

The United States Geological Survey estimates that over four trillion barrels of crude oil are currently trapped within U.S. oil shale reserves. However, no cost-effective, environmentally sustainable method for oil production from oil shale currently exists. Given the continuing demand for low-cost fossil-fuel production, alternative methods for shale-oil extraction are needed. Geothermic Fuel Cells™ (GFC) harness the heat generated by high-temperature solid oxide fuel cells during electricity generation to process oil shale into "sweet" crude oil. In this paper, a thermo-electrochemical model is exercised to simulate the performance of a 4.5 kW$_e$ (gross) Geothermic Fuel Cell module for in situ oil-shale processing. The GFC analyzed in this work is a prototype which contains three 1.5 kW$_e$ solid oxide fuel cell (SOFC) stack-and-combustor assemblies packaged within a 0.3 m diameter, 1.8 m tall, stainless-steel housing. The high-temperature process heat produced by the SOFCs during electricity generation is used to retort oil shale within underground geological formations into high-value shale oil and natural gas. A steady-state system model is developed in Aspen Plus™ using user-defined subroutines to predict the stack electrochemical performance and the heat-rejection from the module. The model is validated against empirical data from independent single-stack performance testing and full GFC-module experiments. Following model validation, further simulations are performed for different values of current, fuel and air utilization to study their influence on system electrical and heating performance. The model is used to explore a wider range of operating conditions than can be experimentally tested, and provides insight into the competing physical processes at play during Geothermic Fuel Cell operation. Results show that the operating conditions can be tuned to generate desired heat-flux conditions as needed across applications.

1. Introduction

This paper presents a steady-state system model that simulates the electrochemical performance and thermal-energy generation of a multi-stack solid-oxide fuel cell assembly. This novel assembly is termed a "Geothermic Fuel Cell" (GFC). As first presented in Sullivan, et al. [1], the GFC concept entails placement of a network of GFC modules within oil-shale formations hundreds of meters below the earth's surface. The high-temperature solid oxide fuel cells contained in the GFC release thermal energy to the surrounding geology, resulting in conversion of the kerogen within the shale into liquid oil and natural gas at ~350 °C [2,3]. Fueled by natural gas, the SOFCs contained in the GFC modules continuously generate electricity that can be used to serve plant processes at the surface or be fed back to the electrical grid.

Oil is traditionally extracted from oil shale through ex situ methods. The kerogen rock is mined and then fed to retort vessels where it is pyrolyzed using various heating methods [4,5]. Such ex situ oil-shale processing leads to adverse environmental impacts and is not cost competitive [6]. Bolonkin et al. quantifies the economic viability of oil shale as an energy resource through the ratio of energy contained within the extracted oil to the energy used in mining and processing that oil [7]. The Alberta Taciuk processor provides an example of an ex situ oil-shale upgrading plant. Brandt et al. have projected the rate of greenhouse-gas emissions from this plant to be 1.5–1.75 times larger than that from conventional production, at a modest energy ratio of 2.6–6.9: 1 [8]. To help alleviate the adverse environmental impacts and high energy costs of ex situ processing, researchers are developing in situ oil-shale processing techniques whereby the formation is directly heated within the geology to retort the oil shale in the absence of direct mining [9]. Current methods of in situ oil shale extraction rely on resistive heaters, radio waves and hot gas injection to supply heat

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http://dx.doi.org/10.1016/j.enconman.2017.02.071
0196-8904/

Nomenclature

V_{cell}	cell voltage (V)
V_{stack}	stack voltage (V)
V_{ocv}	open-circuit voltage (V)
n_{cells}	number of fuel cells per stack
F	Faraday's constant (C mol^{-1})
$\overline{R}$	universal gas constant (J mol^{-1} K^{-1})
E_n	Nernst potential (V)
E°	standard electrode potential (V)
n	number of electrons transfered
X	mole fraction of each species (–)
T	temperature (°C)
i	current density (A cm^{-2})
i_o	exchange current density (A cm^{-2})
i_L	limiting current densities (A cm^{-2})
$\bar{h}_j$	molar enthalpy of each species j (kJ kmol^{-1})
P_o	pre-exponential term (A cm^{-2})
E_{act}	activation energy (J mol^{-1})
$\mathbb{R}$	charge-transfer resistance (Ω cm^2)
t	component thickness (μm)
P	pressure (kPa)
P_L	partial pressures (kPa)
D_L	binary diffusion coefficients (m^2 s^{-1})
$\bar{h}$	heat transfer coefficients (W m^{-2} K^{-1})
$\overline{\mathrm{Nu}}$	Nusselt numbers
D	component diameter (m)
k_{air}	thermal conductivity of air (W m^{-1} K^{-1})
A	component surface area (m^2)
$\dot{Q}_{geo}$	heat transfer to geology (W)
$\dot{Q}_{gas}$	heat convected out via exhaust gas (kW)
$\dot{Q}_{loss}$	heat flux to geology (kW m^{-1})
R_{total}	equivalent heat transfer resistance (K W^{-1})
$\dot{E}_{air}$	total flow of energy in air inlet (kW)
$\dot{E}_{fuel}$	total flow of energy in fuel inlet (kW)
$\dot{E}_{ann}$	total flow of energy in annulus exhaust (kW)
$\dot{E}_{chem}$	chemical energy flow in stream (kW)
$\dot{E}_{sens}$	sensible energy flow in stream (kW)
$\dot{W}_{elec}$	GFC module electric power output (kW)
LHV	lower heating value (kJ kmol^{-1})
GFC	Geothermic Fuel Cell
SOFC	solid oxide fuel cell

Greek symbols

η_{ohm}	ohmic polarization (V)
η_{act}	activation polarization (V)
$\eta_{conc,a}$	anode concentration polarization (V)
$\eta_{conc,c}$	cathode concentration polarization (V)
θ	leakage coefficient
α	symmetry factor
σ_L	component conductivities (S cm^{-1})
ε	component emissivities
σ	Stefan-Boltzmann constant (W m^{-2} K^{-4})
$\mathcal{E}_{elec}$	electrical efficiency (%)
$\mathcal{E}_{heat}$	heating efficiency (%)
$\mathcal{E}_{CHP}$	combined heat and power efficiency (%)
β	empirical fraction of net heat flux

Subscripts

st	stack
an	anode
cat	cathode
el	electrolyte
ic	interconnect
comb	combustor unit
ih	inner annulus housing
oh	outer annulus housing
rad	radiation heat transfer
conv	forced convection heat transfer
exp	experimental data
sim	model simulation result

to the shale. Shell Oil's "InSitu Conversion Process" (ICP) and ExxonMobil's "Electrofrac" process consume grid electricity to drive resistive heater elements placed within the geology [10,11]. The electricity supply for these in situ conversion processes may originate from coal-fired power plants that average generation-and-transmission efficiencies near 33%. Following Brandt's analysis [12], these low efficiencies and the coal-based fuel yield full-fuel-cycle emissions that are 21–47% larger than those from conventionally produced, petroleum-based fuels. As a result, the ratio of the energy returned to energy invested for the Shell's ICP conversion process is about 3–4:1; this is not competitive with the 10:1 value estimated for conventional crude oil extraction [7]. In order for unconventional shale-oil extraction to be feasible, there is a need for alternative in situ processing technologies that are capable of rejecting heat above 500 °C and that require minimal energy input from outside sources.

The high operating temperatures required for SOFCs (700–1000 °C), make them suitable for combined heat and power applications when coupled with heat-recovery systems. As shown by Dodds et al. and Elmer et al. [13,14], SOFC-CHP systems can achieve efficiencies of up to 90%, resulting in a low-CO_2-emitting alternative-power and thermal-energy co-generation technology. Current residential and commercial SOFC-CHP systems are used for electricity production and thermal-energy generation for space heating or domestic hot water [15,16]. The primary objective of these systems is electricity generation to meet the building consumer loads; this application results in intermittent part-load operation of the SOFCs and consequently lower efficiencies [13]. These state-of-the-art SOFC-CHP systems generate relatively low-quality heat. Unreacted fuel in the SOFC exhaust is burned within a combustor located downstream of the stack. This high-quality heat is used for reactant-gas processing and preheating. Following reactant heating, the remaining thermal energy available for meeting building space heating or domestic hot water demands is typically of low quality (<350 °C) [17–19]. Studies show that the variations of the operating conditions and thermal cycling of these SOFC-CHP systems cause an overall increase in the mechanical and electrochemical degradation of the SOFC stacks during prolonged use [20].

In contrast, the Geothermic Fuel Cell technology presents critical improvements to the current state-of-the-art oil-shale processing and SOFC-CHP technologies described above:

- The adverse environmental impacts and high costs of ex situ processing are alleviated by placing the GFC modules directly within the geology and utilizing heat from the SOFCs to upgrade the kerogen in situ;
- The high efficiency and lower CO_2-emissions of SOFC-CHP systems provide a potentially efficient and environmentally sustainable alternative to current in situ shale processing methods that rely on centrally generated power to operate buried resistive heater elements: