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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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 CellsTM (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 PlusTM 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.

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

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NOMENCLATURE

V_{cell}	cell voltage (V)	<i>Greek letters</i>	
V_{stack}	stack voltage (V)	η_{ohm}	ohmic polarization (V)
V_{ocv}	open-circuit voltage (V)	η_{act}	activation polarization (V)
n_{cells}	number of fuel cells per stack	$\eta_{\text{conc,a}}$	anode concentration polarization (V)
F	Faraday's constant (C mol^{-1})	$\eta_{\text{conc,c}}$	cathode concentration polarization (V)
$\bar{R}$	universal gas constant ($\text{J mol}^{-1} \text{K}^{-1}$)	θ	leakage coefficient
E_n	Nernst potential (V)	α	symmetry factor
E°	standard electrode potential (V)	σ_L	component conductivities (S cm^{-1})
n	number of electrons transferred	ε	component emissivities
X	mole fraction of each species (-)	σ	Stefan-Boltzmann constant ($\text{W m}^{-2} \text{K}^{-4}$)
T	temperature ($^\circ\text{C}$)	$\mathcal{E}_{\text{elec}}$	electrical efficiency (%)
i	current density (A cm^{-2})	$\mathcal{E}_{\text{heat}}$	heating efficiency (%)
i_o	exchange current density (A cm^{-2})	$\mathcal{E}_{\text{CHP}}$	combined heat and power efficiency (%)
i_L	limiting current densities (A cm^{-2})	β	empirical fraction of net heat flux
$\bar{h}_j$	molar enthalpy of each species j (kJ kmol^{-1})	<i>Subscripts</i>	
P_o	pre-exponential term (A cm^{-2})	st	stack
E_{act}	activation energy (J mol^{-1})	an	anode
$\mathbb{R}$	charge-transfer resistance ($\Omega \text{ cm}^2$)	cat	cathode
t	component thickness (μm)	el	electrolyte
P	pressure (kPa)	ic	interconnect
P_L	partial pressures (kPa)	$comb$	combustor unit
D_L	binary diffusion coefficients ($\text{m}^2 \text{s}^{-1}$)	ih	inner annulus housing
$\bar{h}$	heat transfer coefficients ($\text{W m}^{-2} \text{K}^{-1}$)	oh	outer annulus housing
$\bar{\text{Nu}}$	Nusselt numbers	rad	radiation heat transfer
D	component diameter (m)	$conv$	forced convection heat transfer
k_{air}	thermal conductivity of air ($\text{W m}^{-1} \text{K}^{-1}$)	exp	experimental data
A	component surface area (m^2)	sim	model simulation result
$\dot{Q}_{\text{geo}}$	heat transfer to geology (W)		
$\dot{Q}_{\text{gas}}$	heat convected out via exhaust gas (kW)		
$\dot{Q}_{\text{loss}}$	heat flux to geology (kW m^{-1})		
R_{total}	equivalent heat transfer resistance (K W^{-1})		
$\dot{E}_{\text{air}}$	total flow of energy in air inlet (kW)		
$\dot{E}_{\text{fuel}}$	total flow of energy in fuel inlet (kW)		
$\dot{E}_{\text{ann}}$	total flow of energy in annulus exhaust (kW)		
$\dot{E}_{\text{chem}}$	chemical energy flow in stream (kW)		
$\dot{E}_{\text{sens}}$	sensible energy flow in stream (kW)		
$\dot{W}_{\text{elec}}$	GFC module electric power output (kW)		
LHV	lower heating value (kJ kmol^{-1})		
GFC	Geothermic Fuel Cell		
SOFC	solid oxide fuel cell		

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 to 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 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-CO₂-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 ($< 350\text{ }^{\circ}\text{C}$) [17, 18, 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:
 - Brandt et al. estimate life-cycle carbon emissions for SOFC-based in situ oil-shale upgrading processes to be 64% lower than Shell’s ICP process and 49% lower than conventional oil [21];
 - Cleveland et al. estimate the GFC energy ratio to be greater than 15:1 [22];
- Unlike most SOFC-CHP applications, the GFC application places higher value on high-grade thermal-energy generation at the expense of electricity generation:
 - The objective of the system is to reject high-grade heat from the GFC assembly at temperatures greater than $500\text{ }^{\circ}\text{C}$ to the surrounding geology;
- The GFC system is continuously operated over a four-year period, with the SOFCs held at a single steady-state condition for months at a time. In this application, there are no load-following or transient-demand constraints that necessitate dynamic-power and thermal-cycling conditions. This extends stack lifetime and consequently reduces system costs.

In this work, we present a model of the Geothermic Fuel Cell prototype shown in Figure 1a. The module is designed and built by Delphi Powertrain Systems [23, 24, 25, 26, 27], and consists of three 1.5 kW_e SOFC stack-and-combustor assemblies packaged within a stainless-steel casing. The stacks are placed in a 1.8

m tall, 0.3 m diameter cylindrical housing and vertically distributed to promote uniform housing surface temperature and heat rejection.

Fuel and air reactants are fed to the stacks in a parallel configuration, and are electrochemically converted into electricity and product gases. Both products and unutilized reactants can mix and burn within a combustor located below each stack. Alternately, the anode exhaust can vent to the atmosphere through “anode-return” plumbing (not shown); mechanical valving is used to regulate anode-return flow. This anode return enhances operational flexibility by reducing thermal-energy generation with only a modest impact to electrochemical performance. Hot product gases exit the combustors and flow upwards through an annular space between two stainless steel housings, rejecting heat to the surroundings before being exhausted above ground.

The experimental testing and performance of this Geothermic Fuel Cell module is described in Anyenya et al. [28], where electrochemical and thermal performance were quantified over a wide range of operating conditions. In this paper, we present a computational model that simulates GFC thermo-electrochemical behavior. The model is validated using experimental data from laboratory testing presented in Anyenya et al. [28]. A thermal-resistive network simulates heat rejection from the stack and burner components to the surrounding outer wall. Following validation, the model is exercised over a far-wider range of conditions than could be demonstrated experimentally. The physics underlying the observed experimental performance is presented, and GFC operational characteristics are reviewed.

The novel contributions of this modeling work include:

- The first detailed thermo-electrochemical model of a novel SOFC system architecture that is designed to reject high-temperature / high-quality process heat;
- Model and simulate the thermally integrated design as a means to characterize the stack-combustor units’ performance in this application;
- Explore operating conditions that favor thermal energy output to electricity production, contrary to other SOFC-CHP applications.

2. Computational model development

A model of the GFC system is used to capture the gross transport of chemical, thermal and electrical energy through the module. Developed in Aspen PlusTM, the model utilizes mass and energy balances, chemical equilibrium, and reaction kinetics to simulate thermo-chemical system processes. As shown in Figure 2, the GFC operating condition to be simulated is defined by nine input parameters: stack operating current I , stack temperature T_{st} , operating pressure P , fuel utilization U_{fuel} , stoics of air λ , air inlet temperature T_{air} , fuel inlet temperature T_{fuel} and fuel composition. Using these inputs, the stack voltages and

Figure 1: a) Schematic of the Geothermic Fuel Cell module. b) Control volume analysis around single 3-stack module and thermocouple locations for temperature measurements used.

Figure 2: Computational flow-chart of the simulation model.

GFC electric power are predicted through an electrochemical model configured as a user-defined subroutine (Section 2.1).

The model uses gas stream temperatures, electric current, fuel composition and utilization to predict the required reactant flow rates and the total energy in the inlet streams. The composition of anode and cathode exhaust streams are determined from equilibrium calculations. Energy and mass balances are solved for the chemical, thermal and electrical energy flows into and out of the module as shown in Figure 1b. The heat to the surrounding and the temperature of the module's outer housing are predicted by a heat-transfer subroutine described in Section 2.3. Electrochemical and heating performance of the module is calculated from the resulting electric power and heat loss. This model provides insight on the physical phenomena underway during GFC operation, and guidance regarding operating conditions for optimal CHP performance.

2.1. Electrochemical model

Following the approach of Trendewicz et al.[29], Leah et al.[30] and Keegan et al.[31], a zero-dimensional computational model simulates the electrochemical performance of an SOFC unit-cell. The single-cell performance is then extrapolated to a full 1.5 kW_e stack by assuming that the stack is comprised of identical repeating unit cells n_{cells} arranged in electrical series

$$V_{\text{stack}} = n_{\text{cells}} \cdot V_{\text{cell}}. \quad (1)$$

The model is used to predict the stack voltage V_{stack} , and GFC electric power $\dot{W}_{\text{elec}}$ for a given current I , stack temperature T_{st} and fuel utilization U_{fuel}

$$\dot{W}_{\text{elec}} = n_{\text{stacks}} \cdot V_{\text{stack}} \cdot I. \quad (2)$$

The single cell voltage V_{cell} is given as

$$V_{\text{cell}} = V_{\text{ocv}} - \eta_{\text{ohm}} - \eta_{\text{act}} - \eta_{\text{conc,a}} - \eta_{\text{conc,c}} \quad (3)$$

with the open-circuit voltage V_{ocv} , the activation losses η_{act} , the ohmic losses η_{ohm} , and the concentration losses $\eta_{\text{conc,a}}$ and $\eta_{\text{conc,c}}$ at the anode and cathode, respectively.

The Nernst potential E_n is a function of the stack temperature T_{st} , the universal gas constant $\bar{R}$, Faraday's constant F , number of electrons transferred in the reaction n , mole fractions of steam $X_{\text{H}_2\text{O}}$, hydrogen X_{H_2} and oxygen X_{O_2} at the stack outlets and the standard electrode potential E°

$$E_n = E^\circ - \frac{\bar{R}T_{\text{st}}}{nF} \ln \left(\frac{X_{\text{H}_2\text{O}}}{X_{\text{H}_2} \cdot \sqrt{X_{\text{O}_2}}} \right). \quad (4)$$

The standard electrode potential is calculated using Equation 5 as used in Becker et al.[32]

$$E^\circ = 1.2723 - 2.7645 \cdot 10^{-4} \cdot T_{\text{st}}. \quad (5)$$

An empirical leakage coefficient θ is used to account for the deviation of the observed open-circuit voltage from the Nernst potential as in Bove et al.[33] and Lisbona et al.[34]

$$V_{\text{ocv}} = E_n \cdot \theta. \quad (6)$$

This leakage coefficient was determined from experiments executed on a similar Delphi 1.5 kW_e stack, where $\theta = 0.9827$.

The activation, ohmic and concentration over-potentials are calculated using the ‘‘SOFC spreadsheet-based unit-cell model’’ developed by Pacific Northwest National Laboratories (PNNL) [35]. In this work, the original PNNL model is calibrated using experimental data collected from early generation Delphi SOFC unit-cell tests under H₂/N₂ fuels across a wide range of temperatures. The model predicts ohmic losses through cell components, charge-transfer overpotential at the electrodes, and losses due to diffusion of reactants into and products out of the porous electrodes. The model also takes into account cell parameters such as component thicknesses, porosities and tortuosities. These losses are dependent on the current density i , fuel and air compositions, cell operating temperature T_{st} and pressure P . These inputs are assumed to be homogeneous over a small electrochemically active area.

The activation polarization η_{act} is given by an approximation of the Butler-Volmer equation

$$\eta_{\text{act}} = \left(\frac{\bar{R}T_{\text{st}}}{\alpha F} \right) \sinh^{-1} \left(\frac{i}{2i_o} \right) \quad (7)$$

where α is the symmetry factor, F is Faraday's constant. The exchange current density i_o is a function of the pressure-dependent pre-exponential term P_o , the cell temperature T_{st} , the universal gas constant $\bar{R}$ and the activation energy for charge transfer E_{act}

$$i_o = P_o \cdot \exp \left(-\frac{E_{\text{act}}}{\bar{R}T_{\text{st}}} \right). \quad (8)$$

139 The adjustable Butler-Volmer parameters (α , P_o , E_{act}) are calibrated to fit experimental data collected from
 140 single-stack electrochemical-performance measurements.

The ohmic polarization η_{ohm} is given by

$$\eta_{ohm} = i \cdot \mathbb{R} \quad (9)$$

where $\mathbb{R}$ is the sum of the charge-transfer resistances of the anode, cathode, electrolyte and interconnect layers

$$\mathbb{R} = \frac{t_{an}}{\sigma_{an}} + \frac{t_{cat}}{\sigma_{cat}} + \frac{t_{el}}{\sigma_{el}} + \frac{t_{ic}}{\sigma_{ic}}. \quad (10)$$

141 The electronic conductivity values σ are calculated using the porosity, cell temperature and empirical con-
 142 stants from cell experiments. The thicknesses t_i are obtained from the cell manufacturer (Delphi Powertrain
 143 Systems). The formulation above assumes negligible contact resistances, cross-plane charge flow and series
 144 connection of resistances, as discussed in Aguiar et al.[36].

145 The cathode concentration polarization ($\eta_{conc,c}$) is given by

$$\eta_{conc,c} = -\frac{\bar{R}T_{st}}{4F} \ln \left(1 - \frac{i}{i_{O_2}} \right) \quad (11)$$

146 where i_{O_2} is the oxygen limiting current density

$$i_{O_2} = \frac{4FPD_{O_2-N_2}}{\bar{R}T_{st}t_{cat}} \ln \left(\frac{P}{P - P_{O_2}} \right) \quad (12)$$

147 and is a function of the cathode thickness t_{cat} , effective binary diffusion coefficient between oxygen and
 148 nitrogen $D_{O_2-N_2}$, the partial pressure of oxygen in the bulk gas P_{O_2} , the total pressure in the cathode P
 149 and the cell operating temperature T_{st} . Similarly, the anode concentration polarization $\eta_{conc,a}$ is given by

$$\eta_{conc,a} = -\frac{\bar{R}T_{st}}{2F} \left[\ln \left(1 - \frac{i}{i_{H_2}} \right) - \ln \left(1 + \frac{i}{i_{H_2O}} \right) \right] \quad (13)$$

150 where i_{H_2} and i_{H_2O} are the hydrogen and steam limiting current densities, respectively

$$i_{H_2} = \frac{2FP_{H_2}D_{H_2-H_2O}}{\bar{R}T_{st}t_{an}} \quad (14)$$

$$i_{H_2O} = \frac{2FP_{H_2O}D_{H_2-H_2O}}{\bar{R}T_{st}t_{an}}. \quad (15)$$

151 These are functions of the anode thickness t_{an} , effective binary diffusion coefficients of H_2 and H_2O in the
 152 anode $D_{H_2-H_2O}$, the partial pressures of hydrogen and steam in the bulk gas of the anode P_{H_2} and P_{H_2O} ,
 153 and the cell operating temperature T_{st} .

154 Table 1 lists the parameters used in calculating the cell performance through the set of equations above.
 155 The anode, electrolyte, cathode and interconnect thicknesses (t_{an} , t_{el} , t_{cat} and t_{ic} , respectively), anode and

Table 1: Top: Inputs to the electrochemical model, including cell geometry parameters. Middle: Component conductivities derived from the model. Bottom: Tuned parameters fitted to experimental data.

Input parameters	Value	Units
Cell active area	105.75	cm^2
Anode thickness, t_{an}	500	μm
Cathode thickness, t_{cat}	50	μm
Electrolyte thickness, t_{el}	10	μm
Interconnect thickness, t_{ic}	500	μm
Average cell temperature, T_{st}	750	$^{\circ}\text{C}$
Cell operating pressure, P	1	atm
Fuel composition	48.5% H_2 48.5% N_2 3% H_2O	
Model-determined parameters	Value	Units
Anode conductivity, σ_{an}	$2.44 \cdot 10^2$	S cm^{-1}
Cathode conductivity, σ_{cat}	6.88	S cm^{-1}
Electrolyte conductivity, σ_{el}	$2.99 \cdot 10^{-2}$	S cm^{-1}
Exchange current density, i_o	0.363	A cm^{-2}
Cathode effective binary diffusion coefficients, $D_{\text{O}_2-\text{N}_2}$	0.0215	$\text{cm}^2 \text{s}^{-1}$
Anode effective binary diffusion coefficients, $D_{\text{H}_2-\text{H}_2\text{O}}$	0.144	$\text{cm}^2 \text{s}^{-1}$
Tuned parameters	Calibrated value	Units
Symmetry factor, α	$S \cdot T_{\text{st}} + C$ $S = 1.62 \cdot 10^{-3}$ $C = -1.19$	- K^{-1}
Pre-exponential, P_o	$\exp(L \cdot T_{\text{st}} + K)$ $L = -6.54 \cdot 10^{-3}$ $K = 1.975$	A cm^{-2} K^{-1} -
Activation energy, E_{act}	$1.26 \cdot 10^5$	J mol^{-1}

cathode tortuosities and the anode and cathode porosity are obtained from the cell manufacturer. The average cell temperature (T_{st}), pressure (P) and fuel composition are experimental set points. The resulting values for activation and concentration polarization are within the expected ranges outlined in Mogensen et al.[37] for anode-supported thin-electrolyte SOFCs in the 650-850 °C temperature range.

2.2. Calibration and validation of electrochemical model

Figure 3 illustrates the model calibration to experimental results of stack voltage and power density as a function of current, while holding reactant flow rates and stack temperature constant (~ 740 °C). For these experiments, in-cell fuel utilization ranged from 0-32%. The model-to-experiment comparison at this operating condition resulted in R^2 values of 94.1% and 99.5% for the stack-voltage and power-density curves, respectively.

Figure 3: Comparison of model-predicted and experimentally measured polarization curves for a 1.5 kW_e stack at 743 °C under 48.5% H₂, 48.5% N₂ and 3% H₂O fuel. Experimental data is shown as symbols, while model results are shown as lines.

This calibrated electrochemical model is then validated through experimental data from GFC-module testing. As the GFC assembly contains three stacks operating at slightly different temperatures, module experimentation creates a wealth of data for model validation. Figure 4 shows the comparison between simulation results and experimental stack voltage data at different stack temperatures and electric currents. The top stack (Stack 1, Figure 1a) demonstrated the highest temperature, while the bottom stack (Stack 3, Figure 1a) was the coolest. Constant fuel utilization of $U_F = 63\%$ was maintained across all conditions shown in Figure 4. However, air flow rate was adjusted to maintain stack temperature within constraints. Model predictions match experimental results within an error of 4%. This result shows that the electrochemical model captures the voltage dependence on stack operating temperature and current draw.

2.3. Heat-transfer model development

A heat transfer model is used to predict the heat loss from the hot GFC components to the cooler surroundings at steady-state operating conditions. The radial heat loss is calculated using the equivalent

Figure 4: Comparison of model-predicted and experimentally measured stack voltage in the GFC module as a function of stack operating temperature and current. Experimental data is shown as symbols, while model results are shown as lines.

Figure 5: Thermal resistive network from the stack-combustor assembly to the GFC's outer wall (not to scale).

thermal circuit for a single stack-combustor assembly shown in Figure 5. In this network, heat transfer from the module to the surrounding geology is driven by two mechanisms:

- Radiation heat transfer from the stack, combustor, and inner-housing surfaces;
- Convection heat transfer from the hot exhaust gases to the inner and outer housing;

Uniform/lumped surface temperatures are assumed for each of the components. Given the stack, combustor, and outer-housing temperatures as inputs, the model predicts the heat flux from the module to the surroundings. Values for these inputs are obtained from physical measurements of the GFC module presented in a companion paper.

Several common heat transfer mechanisms are not included in the model. Convective heat transfer within the cavity between the stack-combustor assembly and the inner housing is assumed negligible; no gas is fed through this space, and buoyant-convection heat transfer is generally small in comparison to radiation and forced-convection heat transfer. Conduction heat transfer between GFC components is also assumed negli-

gible. Thermal communication between the stack and the combustor is neglected as physical measurements found the temperature difference between these two components to be below 10 °C. Conduction heat transfer from the gas plumbing to the inner shield is also ignored, as the thickness of the sheet-metal components limits this heat conduction.

There are five thermal resistors shown in Figure 5 to simulate the following heat-transfer mechanisms:

1. Radiation from the stack to the inner housing $(\bar{h}_{\text{rad,st}})^{-1}$;
2. Radiation from the combustor to the inner housing $(\bar{h}_{\text{rad,comb}})^{-1}$;
3. Radiation from the inner to the outer housing $(\bar{h}_{\text{rad,ann}})^{-1}$;
4. Convection between the inner housing and hot exhaust gases $(\bar{h}_{\text{ih}})^{-1}$;
5. Convection between the hot exhaust gases and the outer housing $(\bar{h}_{\text{oh}})^{-1}$.

The radiation heat transfer coefficients $\bar{h}_{\text{rad}}$ are calculated using the engineering approximation formula from Nellis et al.[38] and Lai et al.[39]. The radiation heat transfer coefficient between the stack and inner wall, is

$$\bar{h}_{\text{rad,st}} = 4\sigma\varepsilon_{\text{st}}\varepsilon_{\text{ih}}(\bar{T}_1^3) \quad (16)$$

where ε_{st} and ε_{ih} are the stack and inner-housing emissivities, respectively. $\bar{T}_1$ is the film temperature between the stack and inner-housing temperatures, T_{st} and T_{ih} , respectively

$$\bar{T}_1 = \frac{1}{2} \cdot (T_{\text{st}} + T_{\text{ih}}). \quad (17)$$

Similarly, the radiation heat transfer coefficient between the combustor and inner-housing is given as

$$\bar{h}_{\text{rad,comb}} = 4\sigma\varepsilon_{\text{comb}}\varepsilon_{\text{ih}}(\bar{T}_2^3) \quad (18)$$

where $\varepsilon_{\text{comb}}$ is the combustor emissivity and $\bar{T}_2$ is the film temperature between the combustor T_{comb} and inner-housing temperatures. $\bar{T}_2$ is equal to $\bar{T}_1$ because the combustor temperature is assumed equal to the stack temperature. Finally, the radiation heat transfer coefficient between the inner and outer housing is

$$\bar{h}_{\text{rad,ann}} = 4\sigma\varepsilon_{\text{ih}}\varepsilon_{\text{oh}}(\bar{T}_3^3) \quad (19)$$

where ε_{oh} is the outer-housing emissivity and $\bar{T}_3$ is the film temperature between the inner and outer T_{oh} housing temperatures

$$\bar{T}_3 = \frac{1}{2} \cdot (T_{\text{ih}} + T_{\text{oh}}). \quad (20)$$

Convection heat transfer coefficients are calculated for the inner housing $\bar{h}_{\text{ih}}$, and the outer housing $\bar{h}_{\text{oh}}$

$$\bar{h}_{\text{ih}} = \frac{\overline{\text{Nu}}_{\text{ih}} \cdot k_{\text{air}}}{D_h} \quad (21)$$

$$\bar{h}_{\text{oh}} = \frac{\overline{\text{Nu}}_{\text{oh}} \cdot k_{\text{air}}}{D_h} \quad (22)$$

where the average Nusselt numbers $\overline{\text{Nu}}_{\text{ih}}$ and $\overline{\text{Nu}}_{\text{oh}}$ are derived for fully developed laminar flow in a circular tube annulus from Table 8.3 in Bergman et al.[40]. The thermal conductivity of the exhaust gas k_{air} is taken to be that of air at the exhaust temperature. The hydraulic diameter D_h is given by

$$D_h = D_{\text{oh}} - D_{\text{ih}}. \quad (23)$$

The model assumes $T_{\text{st}} = T_{\text{comb}}$ with negligible loss in model fidelity, resulting in an equivalent heat transfer resistance R_{total}

$$R_{\text{total}} = \left(\bar{h}_{\text{rad,st}} A_{\text{st}} + \bar{h}_{\text{rad,comb}} A_{\text{comb}} \right)^{-1} + \left(\bar{h}_{\text{rad,ann}} A_{\text{ih}} + \left[\frac{1}{\bar{h}_{\text{ih}} A_{\text{ih}}} + \frac{1}{\bar{h}_{\text{oh}} A_{\text{oh}}} \right]^{-1} \right)^{-1} \quad (24)$$

where A_{st} and A_{comb} are the total stack and combustor surface areas exposed to the inner housing, respectively. The inner and outer annulus wall surface areas are given by A_{ih} and A_{oh} , respectively.

The heat flow due to the temperature difference between the GFC outer casing and the stack-combustor assembly $\dot{Q}_{\text{st-comb}}$ is given by

$$\dot{Q}_{\text{st-comb}} = \frac{T_{\text{st}} - T_{\text{oh}}}{R_{\text{total}}}. \quad (25)$$

A fraction of $\dot{Q}_{\text{st-comb}}$ is the thermal energy convected out of the module via hot exhaust gases in the annular spacing $\dot{Q}_{\text{gas}}$ with the remainder transferred to the geology via the outer housing wall $\dot{Q}_{\text{geo}}$

$$\dot{Q}_{\text{st-comb}} = \dot{Q}_{\text{geo}} + \dot{Q}_{\text{gas}}. \quad (26)$$

As discussed in Braun et al.[41], an approximation of $\dot{Q}_{\text{gas}}$ is formulated by assuming equivalence to an empirical fraction β of the net heat flow $\dot{Q}_{\text{st-comb}}$

$$\dot{Q}_{\text{st-comb}} = \dot{Q}_{\text{geo}} + \beta \cdot \dot{Q}_{\text{st-comb}}. \quad (27)$$

This results in the heat transferred to the geology via the outer housing wall $\dot{Q}_{\text{geo}}$ being equivalent to

$$\dot{Q}_{\text{geo}} = (1 - \beta) \cdot \left(\frac{T_{\text{st}} - T_{\text{oh}}}{R_{\text{total}}} \right). \quad (28)$$

Component and gas temperatures vary considerably across GFC operating conditions and state points. This leads to changes in the heat-transfer properties described previously. Table 2 presents measurements

Table 2: Heat transfer model parameters and calculated heat transfer coefficient values for different component temperatures and current conditions.

Input parameters	Values			
Stack emissivity, ε_{st}	0.40			
Combustor emissivity, ε_{comb}	0.58			
Inner wall emissivity, ε_{ih}	0.88 [42]			
Outer wall emissivity, ε_{oh}	0.80 [42]			
Nusselt number, $\overline{Nu}_{ih}$	8.66 [40]			
Nusselt number, $\overline{Nu}_{oh}$	7.90 [40]			
Physical measurements	Values			Units
Current	30	35	45	A
Fuel flow rate	90.1	105.1	135.2	SLPM
Air flow rate	350	315	357	SLPM
Stoics of air, λ	2.9	2.6	2.3	-
Stack temperature, T_{st}	775	786	794	$^{\circ}\text{C}$
Inner housing temperature, T_{ih}	633	611	612	$^{\circ}\text{C}$
Outer housing temperature, T_{oh}	628	592	605	$^{\circ}\text{C}$
Calculated heat transfer properties	Values			Units
$\bar{h}_{rad,st}$	74.9	73.8	74.9	$\text{W m}^{-2} \text{K}^{-1}$
$\bar{h}_{rad,comb}$	109	107	109	$\text{W m}^{-2} \text{K}^{-1}$
$\bar{h}_{rad,ann}$	117	107	109	$\text{W m}^{-2} \text{K}^{-1}$
$\bar{h}_{ih}$	21.3	20.8	21.0	$\text{W m}^{-2} \text{K}^{-1}$
$\bar{h}_{oh}$	19.5	19.0	19.1	$\text{W m}^{-2} \text{K}^{-1}$
R_{total}	0.0144	0.0149	0.0147	K W^{-1}
β	0.64	0.61	0.62	-

Table 3: Comparison of model-predicted and experimentally measured outer housing temperatures at different operating conditions.

Experimental state point data	1	2	3	4	Units
Current drawn, I	25	30	35	45	A
Fuel flow rate	75.1	90.1	105.1	135.2	SLPM
Air flow rate	350	350	315	375	SLPM
Middle stack temperature, T_{st}	787	800	786	809	$^{\circ}\text{C}$
Fuel inlet temperature, T_{fuel}	680	684	695	611	$^{\circ}\text{C}$
Air inlet temperature, T_{air}	700	699	761	611	$^{\circ}\text{C}$
Annulus exhaust temperature, T_{ann}	694	690	637	602	$^{\circ}\text{C}$
Anode exhaust temperature, T_{ar}	712	604	665	654	$^{\circ}\text{C}$
Outer housing temperature, T_{oh}	674	671	590	605	$^{\circ}\text{C}$
Model-predicted outer housing temperature, T_{oh}	675	657	587	606	$^{\circ}\text{C}$
% difference	0.1	2.1	0.5	0.2	%

of component temperatures and electric current at three GFC operational state points, and the associated values of the calculated heat-transfer properties at these state points. Again, the physical measurements of component temperatures and electric current are used as model inputs. The fractional term β is tuned so that $\dot{Q}_{geo}$ calculated from this heat transfer model is in agreement with heat loss $\dot{Q}_{geo}$ determined by control-volume energy-conservation calculations. The observed decrease in inner and outer annulus surface temperatures with increasing stack temperature is perhaps counterintuitive. The observed behavior is tied to the increased air utilization. Higher air utilization leads to less stack cooling, and higher stack temperature. The reduced air flow rates at high utilization also lead to decreased convective heat transfer from the hot exhaust gases to the outer housing. This reduces the housing temperature, though the stack temperature climbs. During laboratory testing, reactant gases are preheated in a furnace that was operated at a constant heat rate which resulted in the varying reactant temperatures with changing flow rates. Following the tuning procedure, the R_{total} and β values are found to deviate by only 0.03% and 1.5% across the three state points, respectively. As a result, the values for $R_{total}=0.015$ and $\beta=0.62$ are assumed to be constant.

This model is validated by comparing the predicted outer-housing temperature T_{oh} calculated by Equation 28 to physical measurements. Table 3 shows this comparison across a range of operating currents. It should be noted that in addition to differences in electric-current draw, the four state points shown in Table 3 also bear differences in stack temperatures, inlet and outlet gas-stream temperatures, and flow rates. The

combined effects of these differences are well captured in the simulations; the model-predicted outer housing temperatures differ from measured values by about 2%, demonstrating close model-to-experiment agreement. This 2% difference is comparable to the measurement error of 1.7% for the Type K thermocouples used in the experiment [43].

Using ground temperature data from in-ground GFC testing presented in Sullivan et al. [1], an empirical equivalent heat transfer resistance R_{geo} from the outer housing wall to the geology is computed. As a result, given GFC stack temperature T_{st} and geology (or ambient) temperature T_{geo} , the expected outer housing temperature T_{oh} when the GFC is placed in the ground, is computed by solving Equation 28 and Equation 29,

$$T_{\text{oh}} = T_{\text{geo}} + R_{\text{geo}} \cdot \dot{Q}_{\text{geo}}, \quad (29)$$

simultaneously.

3. Results and discussion

3.1. Performance evaluation

A “base case” GFC operating condition of 35 A current draw serves for a more-detailed comparison of model predictions to experimental results. Table 4 presents the model inputs used to analyze the performance of the three-stack Geothermic Fuel Cell module at a 35 A operating state point.

The flow of chemical and sensible energy in the streams are determined from thermodynamic properties at measured gas temperatures and measured flow rates and composition

$$\dot{E}_{\text{fuel}} = \dot{n}_{\text{fuel}} \sum_j X_j \cdot ([\bar{h}_j(T_{\text{fuel}}) - \bar{h}_j(T_0)] + LHV_j) \quad (30)$$

where $\dot{E}_{\text{fuel}}$ is the sum of the flow of sensible and chemical energy of the preheated fuel stream flowing at temperature T_{fuel} and molar flow rate $\dot{n}_{\text{fuel}}$. $\dot{E}_{\text{air}}$ is the flow of sensible energy of the preheated air stream entering at temperature T_{air} and molar flow rate $\dot{n}_{\text{air}}$

$$\dot{E}_{\text{air}} = \dot{n}_{\text{air}} \sum_j X_j \cdot [\bar{h}_j(T_{\text{air}}) - \bar{h}_j(T_0)] . \quad (31)$$

Energy outputs include the flow of sensible energy in the exhaust products exiting the GFC annulus $\dot{E}_{\text{ann}}$ at temperature T_{ann}

$$\dot{E}_{\text{ann}} = \dot{n}_{\text{ann}} \sum_j X_j \cdot [\bar{h}_j(T_{\text{ann}}) - \bar{h}_j(T_0)] . \quad (32)$$

Table 4: Summary of system performance simulation inputs and results at the 35 A operating condition.

Input parameters	Input values		Units
Stack temperature, T_{st}	785		$^{\circ}\text{C}$
Current drawn, I	35		A
Fuel utilization, U_F	63		%
Stoics of air, λ	3		-
Fuel composition	48.5% H_2		
	48.5% N_2		
	3% H_2O		
Fuel inlet temperature, T_{fuel}	695		$^{\circ}\text{C}$
Air inlet temperature, T_{air}	761		$^{\circ}\text{C}$
Annulus exhaust temperature, T_{ann}	637		$^{\circ}\text{C}$
Anode exhaust temperature, T_{ar}	665		$^{\circ}\text{C}$
Control volume energy flows	Calculated values		Units
Total flow of energy in reactant streams, $\dot{E}_{\text{fuel}} + \dot{E}_{\text{air}}$	15.09		kW
Total flow of energy in product streams, $\dot{E}_{\text{ann}} + \dot{E}_{\text{ar}}$	7.51		kW
Chemical energy flow in fuel stream, $\dot{E}_{\text{chem},\text{in}}$	8.45		kW
Chemical energy flow in anode exhaust stream, $\dot{E}_{\text{chem},\text{out}}$	2.13		kW
Radial heat loss, $\dot{Q}_{\text{geo}}$	5.08		kW
Thermal-electrochemical model results	Model	Experiment	Units
Total electric power, $\dot{W}_{\text{elec}}$	2.49	2.42	kW
Outer housing temperature, T_{oh}	584	589	$^{\circ}\text{C}$
GFC module performance	Values		Units
GFC electrical efficiency, $\mathcal{E}_{\text{elec}}$	41.14		%
GFC Heating efficiency, $\mathcal{E}_{\text{heat}}$	33.67		%

$\dot{E}_{\text{ar}}$ is the sum of the flow of sensible and chemical energy in the anode return exiting at temperature T_{ar} , molar flow rate $\dot{n}_{\text{ar}}$, and mole fractions $X_{j,\text{ar}}$

$$\dot{E}_{\text{ar}} = \dot{n}_{\text{ar}} \sum_j X_{j,\text{ar}} \cdot ([\bar{h}_j(T_{\text{ar}}) - \bar{h}_j(T_0)] + LHV_j). \quad (33)$$

The mole fractions, molar enthalpy and lower heating values of each species j in the fuel and air streams are given by X_j , $\bar{h}_j$ and LHV_j , respectively. The sensible energy is defined as the amount of energy that can be harnessed by cooling the hot inlet and outlet gases back to ambient temperature (298 K). This is represented by the difference in species enthalpy at the respective stream temperature (T) and the ambient temperature (T_0), i.e. $[\bar{h}_j(T) - \bar{h}_j(T_0)]$.

The reactant flow rates are determined by the stack fuel utilization (U_{fuel}) and the desired stoics of excess air (λ) constraints

$$\dot{n}_{\text{fuel}} = \frac{\dot{n}_{\text{H}_2, \text{utilized}}}{U_{\text{fuel}} \cdot X_{\text{H}_2}} \quad (34)$$

$$\dot{n}_{\text{air}} = \frac{\lambda \cdot \dot{n}_{\text{O}_2, \text{utilized}}}{X_{\text{O}_2}}. \quad (35)$$

The total energy into the three-stack assembly is 15.09 kW: 6.64 kW from the sensible energy in the pre-heated inlet gases and 8.45 kW of chemical energy in the fuel mixture. At this 35 A condition, the model predicts 2.49 kW of electric power is continuously generated by the solid oxide fuel cell stacks at 63% fuel utilization and three stoics of air. The GFC module electrical efficiency of 41.14% is calculated as the ratio of electric power output to the chemical energy in the fuel stream

$$\mathcal{E}_{\text{elec}} = \frac{\dot{W}_{\text{elec}}}{\dot{E}_{\text{chem}, \text{in}}}. \quad (36)$$

The module heating efficiency of 33.67% is based on the flow of chemical and sensible energy contained in the fuel and air inlet streams ($\dot{E}_{\text{fuel}}$ and $\dot{E}_{\text{air}}$)

$$\mathcal{E}_{\text{heat}} = \frac{\dot{Q}_{\text{geo}}}{\dot{E}_{\text{fuel}} + \dot{E}_{\text{air}}}. \quad (37)$$

The heat flux to the geology $\dot{Q}_{\text{loss}}$ is the heat transferred via the outer housing wall per unit length of the GFC module

$$\dot{Q}_{\text{loss}} = \frac{\dot{Q}_{\text{geo}}}{\text{GFC length}}. \quad (38)$$

Considerable energy (7.51 kW) exits the GFC module in the form of unreacted fuel and hot products. The GFC module liberates 5.08 kW to the surroundings at a wall temperature of 579 °C at this condition. This results in a heat flux of 2.04 kW m⁻¹ and a combined heat and power efficiency of 74.8%. The effect

of the unconverted chemical energy flow exiting the GFC through the anode return ($\dot{E}_{\text{ar,chem}} = 2.13 \text{ kW}$) on the GFC module performance is exemplified by the low CHP value at this condition. However, since the linear heat flux value exceeds the 1.6 kW m^{-1} target, activating the stack combustors by closing the anode return would lead to higher heating rates. An increase in module performance could instead be realized by increasing the fuel utilization from the modest 63% at this condition. The high radiation heat transfer coefficients show that this is the dominant mode of heat transfer and could be enhanced by increasing the temperature of the solid components.

3.2. Parametric study

An important application of the computational model is to explore how choices of operating conditions can lead to trade-offs in electrochemical and thermal performance. Following calibration and validation of the thermal-electrochemical model, the model is used to simulate the impact of variations in electric current, fuel utilization and stoics of air on GFC-module performance. As noted in Anyenya et al. [28], the Geothermic Fuel Cell was placed within a furnace containing refractory insulation to simulate geology heating within the laboratory setting. The GFC was not subjected to any external heating, as the furnace elements were not activated. When placed within the geology, significant heat will be transported from the module into the surrounding oil shale, resulting in decreased module-surface temperatures.

High-heat-output operating conditions are desirable during down-hole operations (for example, 5.0 kW / m of GFC length). The numerical simulations carried out in this section offer a direct insight into the critical control parameters that ensure that the geology-heating demands are met. The heating requirements for in situ oil shale upgrading vary substantially over the multi-year shale-processing period, as presented in Aouizerate et al.[44]. As geology temperature increases over time, the GFC thermal load drops, and electricity generation becomes more favorable. The objective of this study is to show that the GFC operating window is extensible enough to meet these changing heat demands.

Practical operation and control of a GFC system requires reactant flow and current control, and critical process variable measurements, such as temperature and stack voltage. Table 5 displays representative process variables of a GFC system. As described in Ogunnaike et al. [45], the control parameters represent process variables which can be controlled (e.g., through actuation of a valve) by a system operator. The stack operating current is controlled using programmable load banks, while the reactant flow rates are varied using mass flow controllers. Disturbance variables represent temperature inputs for which we do not have active control but which can be measured. For example, the fuel (anode) and air (cathode) inlet temperatures have been shown to vary with reactant flow rates in Table 3. These variables are measured but not controlled. Measured output variables, such as stack temperature, can be verified by direct on-line measurements and can be used for active control purposes. Unmeasured output variables are those which are difficult to measure, but can be calculated, such as heat loss from the system.

Table 5: Process variables of the GFC system employed in the simulations

Inputs	
Control parameters	Measured disturbance variables
Current drawn, I	Fuel inlet temperature, T_{fuel}
Fuel utilization, U_{F} (or fuel flow rate)	Air inlet temperature, T_{air}
Stoics of air, λ (or air flow rate)	Geology (or ambient) temperature, T_{geo}
Fuel composition	
Outputs	
Measured variables	Unmeasured variables
Stack voltage, V_{stack}	Radial heat flux, $\dot{Q}_{\text{loss}}$
GFC electric power, $\dot{W}_{\text{elec}}$	Reactant energy flows, $\dot{E}_{\text{fuel}}, \dot{E}_{\text{air}}$
Stack temperature, T_{st}	Exhaust energy flows, $\dot{E}_{\text{ann}}, \dot{E}_{\text{ar}}$
Outer housing temperature, T_{oh}	
Annulus exhaust temperature, T_{ann}	

In system simulation, control inputs are more flexible in that air and fuel flow rate control can be substituted with specification of (i.e., input) air stoics and fuel utilization, for instance. Measured disturbance variables listed in Table 5 are inputted to the model. It is important that the stack temperature remain elevated during in-ground operation whereby the GFC will be losing a significant amount of heat to the surrounding geology. Thus, supplying the SOFC stacks with the highest amount of sensible energy in the reactants is desirable. These considerations have motivated our specification of inlet air (cathode) and fuel (anode) temperatures to values of 761 °C and 695 °C, respectively, for the simulations. These temperatures represent the highest reactant inlet temperatures recorded during GFC testing and are indicative of feasible operating conditions. The stack voltage V_{stack} , and GFC electric power $\dot{W}_{\text{elec}}$ are calculated using the electrochemical model described in Section 2.1. The heat loss to the geology $\dot{Q}_{\text{geo}}$ is predicted using Equation 28 from the heat-transfer subroutine described in Section 2.3.

Under nominal solid-oxide fuel cell system operations, the waste heat is transported out of the stack by the cooling power of the cathode air. These systems assume near adiabatic conditions around the stack as conduction and surface radiation play a minor role, Braun et al. and Lisbona et al. both assign empirical percentage values (3-7%) to these thermal losses [46, 34]. As such, conventional SOFC system models assume the stack temperature is equal to either the cathode inlet, exhaust or average temperature depending on the flow configuration [32, 34, 47, 46]. The unique design and application of the Geothermic Fuel Cell modules result in significant heat loss from the stack via radiative heat transfer to the inner housing. For this reason, the stack temperature in these simulations is estimated by the average of the temperature at the cathode inlet to the module and a calculated adiabatic flame temperature at the middle combustor exit. This modeling approach for estimating SOFC stack temperature is in close agreement with measured values [28] for the operating conditions simulated.

A centrally important operating condition is the choice in electric current draw. As shown in Figure 6a, both heat flux and electric power output increase with increasing current. Assuming constant fuel utilization and stoics of air, there is an increase in the mass of reactants being fed to the stacks at higher currents. The power output increases with increasing current as the electrochemical reaction rate is directly proportional to the current. Though the stack voltage decreases by 5.2 volts over the range of current explored, this still results in higher electrical power output at high currents. The observed increase in heat flux to the periphery is credited to the increase in irreversible heat generation within the SOFC stacks at higher currents. The increase in reactant flow rate also generates an increase in the chemical energy of the unutilized fuel exiting the SOFC stack; this fuel is burned in the combustor, releasing yet-more heat.

The heat flux values calculated in this simulation represent the expected heat loss to the periphery given a fixed GFC exhaust temperature of 500 °C. The actual heat flux to the surrounding that is dependent on the temperature difference between the stack and the ambient is also shown in Figure 6a. This result shows that for currents under 20 A, the GFC cannot be operated at the given air and fuel utilization factors

Figure 6: Effect of electric current draw on: (a) Electric power and heat flux ((1) Heat flux values expected when the exhaust temperature is set to 500 °C. (2) Simulated heat flux required for the GFC in ambient temperature (20 °C).) (b) Heat-to-electric power ratio and stack temperature (c) Module heating and electrical efficiencies. The fuel utilization and stoics of air are held constant at 63% and 3, respectively.

without running into the risk of quenching. For instance at 10 A, the GFC would have to dispense 5.5 kW of heat to the surrounding which would result in an exhaust stream temperature of -263 °C. As such, the chemical and sensible energy in the reactant streams is not sufficient to meet GFC heat demands at low current conditions when the geology temperature is at a minimum. Consequently, the GFC should be operated at high current conditions during start up.

Another repercussion of the heightened joule heating is a slight increase in the stack temperature by 29 °C (Figure 6b). This modest increase translates to a rise in radiative heat flux to the geology. Additionally, the trend in heat-to-electric power ratio shown in Figure 6b reveals that the fraction of energy directed towards heating the geology increases substantially with increasing current. During initial start-up when the geology is at very low temperatures (< 150 °C), the heating demands placed on the GFC are far higher than that for electricity generation. In order to keep the SOFC stacks from quenching at these cold-start

conditions, a high-heat-flux operating condition is required.

Improved GFC electrical power and heat output does not translate to a significant increase in the GFC heating and electrical efficiencies. As shown in Figure 6c, the electric efficiency decreases by 9.0% while the heating efficiency climbs modestly by 0.2% at higher currents. The decreasing electrical efficiency is a result of the drop in stack voltage at high currents caused by higher cell-level ohmic and activation polarization values (Equations 7 and 9). Despite the increase in heat flux to the geology, the modest increase in heating efficiency is a result of the increase in the total sensible and chemical energy supplied to the control volume from the higher reactant mass flow rates. The sizable drop in GFC electrical efficiency compared to the modest increase in heating efficiency results in an overall drop in GFC combined heat and power efficiency. This result shows that the stack current draw can be varied to alter the heat flux to the geology, with little to no overall change in GFC performance.

Figure 7: Effect of fuel utilization on: (a) Electric power and heat flux (b) Heat-to-electric power ratio and stack temperature (c) Module heating and electrical efficiencies. The current and stoics of air are held constant at 35 A and 3, respectively. The surroundings are at ambient temperature (20 $^{\circ}\text{C}$).

Increasing the fuel utilization at constant current has the reverse effect on the heat and power outputs.

As shown in Figure 7a, both heat flux and electric power output decrease with increasing fuel utilization. At higher fuel utilization and constant current, there is a decrease in the mass of reactants being fed to the Geothermic Fuel Cell module. The drop in stack voltage at higher fuel utilization leads to a modest decrease in power. The maximum stack voltage is dictated by the Nernst potential calculated by Equation 4. Higher utilization leads to increased steam and decreased hydrogen concentrations at the stack outlet that cause a drop in the Nernst potential. The lower reactant flow rates at higher utilization also lead to increased kinetic and mass-transport limitations that also cause a drop in stack voltage. A slight drop in heat flux is observed due to the decreased amount of energy into the control volume; a much-greater fraction of this energy is directed towards electric-power production.

Figure 7b shows an increase in the stack temperature as a consequence of the reduced reactant mass flow rates at higher fuel utilization. The amount of heat convected from the stack surface by the flowing reactant gases is reduced at low mass flow rates resulting in an increased risk of stack overheating at these conditions. Figure 7b also shows that the fraction of energy directed towards heating the geology decreases slightly with increasing fuel utilization. The heat demand on the GFC module is greatly reduced over the course of operation, once geology temperatures start to exceed 300 °C. By increasing the fuel utilization, the loads on the fuel and air compressors can be reduced due to the lower reactant flow rates, without constraining the amount of heat required. At these low-heat-high-power turn-down conditions, operating at high fuel utilization could potentially result in additional revenue from the surplus electricity production due to the reduced compressor power loads.

Varying fuel utilization has the same effect on both electrical and heating efficiency values. The simulation shows a 17% rise in both heating and electrical efficiencies over the range of utilization factors explored. Consequently, maximum combined heat and power efficiency is achieved at high fuel utilization. This result shows that increasing the fuel utilization can be used in improving the system's CHP performance while decreasing the heat flux to the geology during low-heat, high-power turn-down conditions.

Changing the flow rate of air into the system by varying the stoics of air has a modest effect on the GFC electrical performance, as shown in Figure 8. Despite the change in flow rate of air into the stack, there is very little fluctuation in the concentration of oxygen in the cathode, resulting in little to no effect on the stack electrochemical performance. As shown in Figure 8a, the GFC electric power production is near constant in the range of stoics of air explored. Similarly, Figure 8c shows the GFC electrical efficiency also stays constant, as neither the power production nor the amount of chemical energy into the system changes. The rise in heat flux with stoics of air shown in Figure 8a is as a result of the increase in sensible energy into the system from the increased air flow rates. This sensible energy increase results in the 12% decrease in heating efficiency as seen in Figure 8c.

Contrary to the observations stated above, the flow of excess air is not a trivial operating parameter, as it is used to moderate the temperature of the stack. Figure 8b shows a 111 °C drop in stack temperature

Figure 8: Effect of stoics of air on: (a) Electric power and heat flux (b) Heat-to-electric power ratio and stack temperature (c) Module heating and electrical efficiencies. The fuel utilization and current are held constant at 63% and 35 A, respectively. The surroundings are at ambient temperature (20 °C).

when the stoics of air is increased from two to five. Raising the flow of excess cooling air will reduce the risk of damage to the stacks from overheating and degradation at high temperatures. In contrast, the analyses presented in Figures 6b and 7b show that increasing current and fuel utilization both result in high stack temperatures. During field operation, the GFC modules will be buried over 200 m below the ground surface. Consequently, significant energy demands will be placed on the fuel and air compressors. The greatest impact of the excess air flow rate on the system is the electric power required by the air compressor to drive the air down-hole. The increased flow of excess air into the system during operating conditions that require stack cooling will result in high compressor electric-power demands. This condition could potentially result in the need for an outside source of electric power to supplement GFC electricity generation.

The simulations carried out above depict GFC heating performance when exposed to ambient temperature conditions (20 °C) as in the laboratory experiment. The model is further exercised to characterize the effect of changing geology temperatures on the GFC heat output as well as the outer housing temperature.

Figure 9: Effect of changing geology temperature on the GFC outer housing temperature and heat flux to the geology: (a) and (b) as a function of current, (c) and (d) as a function of fuel utilization. The flow of excess air needed to keep the stack temperature at 750 °C is also shown.

As stated above, the flow of excess air is used to moderate the temperature of the stack. In these simulations, the stack temperature is held constant at the nominal 750 °C by varying the stoics of excess air.

Figure 9a and b show the effect of changing geology temperatures on the GFC outer housing temperature and heat flux, respectively as a function of operating current. Results for three different geology temperatures (35, 150, and 300 °C), which are reflective of different thermal conditions expected in GFC applications throughout its operational life, are shown. The increase in heat flux and surface temperature as a function of current is a result of the increased joule heating and reactant flow rates explained in Figure 6 above. The stoics of excess air flow increases with increasing current as more air is required to cool the hotter stacks (see Figure 6b) at higher currents. The GFC outer housing temperature increases while the heat flux values decrease with increasing geology temperature. The resulting decrease in the temperature difference between the GFC outer housing and geology causes the observed decrease in heat flux values as the geology temperature rises.

Figure 9c and d show the effect of changing geology temperatures on the GFC outer housing temperature and heat flux, respectively as a function of fuel utilization. Contrary to the observations made in simulations carried out in Figure 7 above, the heat flux to the geology increases slightly as a function of fuel utilization

in these simulations. This is a result of the increased cooling air flow rates required to maintain the stack temperature at 750 °C for higher fuel utilization factors. The increased flow rates raise the amount of sensible energy introduced to the GFC control volume. Similarly, the resulting decrease in the temperature difference between the GFC outer housing and geology causes the observed decrease in heat flux values as the temperature of the ambient geology increases.

Figure 10: Effect of varying geology temperature on the GFC outer housing temperature and heat flux to the geology.

It is also useful to directly observe the relationship between geology temperature and housing temperature and heat flux. Figure 10 shows the effect of varying geology temperature on the outer housing temperature and the heat flux to the geology at a single GFC operating condition. The GFC operating current, fuel utilization, stoics of air and stack temperature are specified. As stated above, the flow of excess air is used to moderate the temperature of the stack. In this simulation, the stack temperature is held constant at 750 °C by flowing 3.8 stoics of excess air. As expected, the GFC outer housing temperature increases by 86 °C with increasing geology temperature. The resulting decrease in the temperature difference between the GFC outer housing and geology causes the observed 0.89 kW m⁻¹ decrease in heat flux values at this operating condition.

Since the GFC application targets heat as the more valuable resource over electricity, a high-heat-flux, low-electric-power operating condition is generally desirable. However, in subsequent years of operation, the heat flux (kW m⁻¹ value) from the GFC assembly to the geology must be turned down significantly in order to increase the quality of the oil produced. The simulation model and the subsequent parametric study will prove useful in determining ideal operating conditions for start-up, steady-state and turn-down conditions.

4. Conclusions

Geothermic Fuel Cell technology entails the harnessing of heat that is generated by high-temperature solid-oxide fuel cells during electricity generation for the liberation of crude oil and natural gas from oil shale. This paper describes a thermal-electrochemical model of a Geothermic Fuel Cell module containing

three 1.5 kW_e solid-oxide fuel cell stacks. The model is used to simulate the electrochemical performance of the stacks and heat loss from the GFC module at different operating conditions under a hydrogen fuel blend. The heat rejection from the GFC module is simulated using a thermal-resistive network from the stack and burner components to the surrounding outer housing. The model is validated against experimental data obtained from laboratory testing of a three-stack GFC module. Simulation results serve as a tool to understanding the system combined-heat-and-power efficiency and for developing strategies for varying the heat flux to the geology during GFC operation.

A parametric study reveals:

- The electric current can be used to increase the module electric power and heat flux while keeping the combined heat and power efficiency of the system nearly constant;
- The fuel utilization can be used to increase system efficiency and to decrease the heat flux to the geology during turn-down conditions;
- The stack temperature can be controlled by varying the flow of excess cooling air. However, increased air flow rates will result in high compressor electric power demands.

The Geothermic Fuel Cell thermal-electrochemical model can be used by in-situ oil-shale developers to simulate a wide range of operating conditions during GFC operation, and inform dispatch of the Geothermic Fuel Cell system in the field. Using the Aspen Plus optimization tool, the current, fuel utilization and stoics of air were varied simultaneously within the ranges explored above. The stack temperature is constrained to values below 800 °C to avoid overheating. The heat flux to the geology is constrained to values above the required average of 1.5 kW m⁻¹. The objective is to maximize the system combined heat and power efficiency. A maximum CHP efficiency of 79.3% is achieved at the following operating conditions: $I = 27.5$ A, $\dot{W}_{\text{elec}} = 1.9$ kW, $\lambda = 3.1$ and $U_F = 70\%$. However, this elementary optimization is strictly energetic in nature and does not consider economical and other operational constraints that will govern the system dispatch. A dispatch optimization model would require detailed cost equations, and economic and operational constraints with an objective function that seeks to maximize the system heating and electrical efficiency while minimizing costs. Such a model is the subject of future work.

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