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Impact of Fuel Composition Transients on SOFC Performance in Gas Turbine Hybrid Systems

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- 27

41

28 Abstract

29 This paper presents a dynamic study of fuel cell gas turbine (SOFC/GT) hybrid systems, focusing on the 30 response to a drastic transient in anode fuel composition for constant turbine speed operations. This work is 31 motivated by the potential of fuel cells for fuel flexibility, which could extend the opportunities for sustainability and profitability in energy conversion systems. A combination of hardware and numerical models 32 in a hybrid simulator is used to investigate the transient trajectories of fuel cell process variables as well as the 33 34 consequent impacts of fuel cell thermal effluent on the integrated gas turbine engine. The conversion of thermal 35 energy stored in the fuel cell stack to chemical energy during the reforming at the beginning of the cell resulted in a 17% increase in thermal effluent from the fuel cell to the turbine in the first few seconds of the transient. 36 37 Fuel cell solid temperature gradients increased by 39% at 250 s from the initiation of the transient. The 38 distributed dynamic performance of the fuel cell in terms of the fuel composition gradient, thermal and 39 electrochemical performance across the fuel cell length was carefully characterized, considering their 40 interactions and their impacts on the total system performance.

- Keywords: Fuel cell gas turbine hybrid; fuel composition transients; fuel flexibility; hardware-based
 simulations
- 45 Nomenclature

| 46 | | |
|----|---------------------------|--|
| 47 | SOFC | Solid oxide fuel cell |
| 48 | GT | Gas turbine |
| 49 | NETL | National Energy Technology Laboratory |
| 50 | APU | Auxiliary power unit |
| 51 | SMR | Steam methane reforming |
| 52 | WGS | Water-gas shift |
| 53 | LHV | Low heating value [kW] |
| 54 | TPB | Triple-phase boundary |
| 55 | Q | Fuel cell waste heat/fuel cell net thermal effluent [kW] |
| 56 | V _{Nernst} | Nernst potential [V] |
| 57 | $\Delta G^{\circ}_{H_2O}$ | Standard Gibbs free energy [kJ] |
| 58 | \bar{F} | Faraday's constant [C/mol] |
| 59 | R_u | Ideal gas constant [J/mol-K] |
| 60 | Т | Temperature [K] |
| 61 | р | Partial pressure [atm] |
| 62 | α | charge transfer coefficient |
| 63 | n | number of electrons transfer per reaction |
| 64 | i | current density [A/cm ²] |
| 65 | i_0 | exchange current density [A/cm ²] |
| 66 | bulk | anode/cathode stream |
| | | |

67 1. Introduction

Hybridization of high temperature fuel cells, such as solid oxide fuel cells (SOFCs), with gas turbines has been widely recognized as a compelling advanced power system for high efficiency energy production with low emissions. [1-4]. In particular, the SOFC gas turbine hybrid system offers an improvement of system efficiency by recovering high temperature waste heat from the fuel cell for additional power production from the gas turbine. In addition, it is discovered through research and development efforts initiated by the U.S Department of Energy using a pilot-scale system that the operating envelope of fuel cell gas turbine (SOFC/GT) hybrid systems has an opportunity to achieve 85% turndown [5]. This suggests that this hybrid system can possibly provide attractive solutions for sudden load excursions on the fuel cells, reducing impacts to both fuel cell and gas turbine during transient events or off-design operations [6].

77 The ability of high temperature fuel cells to directly use various types of fuels also greatly extends the 78 interest in applications of fuel cell gas turbine (SOFC/GT) hybrid systems. Theoretically, it is feasible to run the 79 SOFC/GT system using non-hydrogen fuels such as methane or biogas and even liquid fuels at selected 80 operating conditions [7-10]. Furthermore, there are several potential applications where it might be very 81 beneficial to have a power system that can handle drastic changes in the type of fuel used. First, if the market 82 prices of fuels experiences sudden shifts, or, perhaps new regulations place environmental restrictions on the fuel type, it may be beneficial to switch the fuel used to take advantage of the new economic situation [1, 11]. 83 84 For example, suppose a power plant uses primarily gasified coal, but the price of natural gas suddenly drops, or, 85 a new carbon tax takes effect; it could be more profitable to switch the main fuel from coal to natural gas.

Second, recent studies have shown that flexible polygeneration systems which co-produce electricity with 86 87 fuels or chemicals can take advantage of monthly or even daily shifts in energy prices (such as electricity) by 88 changing the mixture of products that it produces in response to these changing market conditions. [1, 11, 89 12]. For example, one may want to produce more electricity and less fuels during the day when power prices are 90 high, and then switch to producing more fuels and less electricity at night when power prices are low. To 91 maximize efficiency, flexible polygeneration are designed to tightly integrate the chemicals/fuel production and 92 electricity production sections such that when these transitions occur, the feed rates, heating value, and 93 composition to the power generation system changes significantly [11, 13].

In either case, SOFC/GT systems are potentially a very suitable technology to use as the power generation mechanism since they are highly efficient and fuel-flexible. Although SOFC/GT hybrids can be used in both the power plant and polygeneration plant contexts, this study focuses on the former kind of transition (coal to natural gas) because it is the more extreme of the two.

98 However, SOFC/GT hybrid systems are not yet commercially ready due to practical problems associated 99 with dynamic operations [3, 7, 14, 15]. The highly interactive effects between fuel cell systems and turbine 100 cycles during transient events always lead to complicated process dynamics that require problematic control development [16, 17]. For instance, although methane fueled systems can provide means to cool the fuel cell 101 102 stack due to the endothermic reforming reaction [8, 9], a dramatic temperature gradient across the fuel cell must 103 be avoided to limit the thermal stress in the material [18]. Also, any variations in the fuel cell thermal effluent 104 (which is the thermal energy of the SOFC exhaust streams) caused by transients in fuel composition can upset 105 the stability of the turbine cycle, which in turn affects the fuel cell stacks [19, 20]. Fuel starvation could be 106 another potential failure in the system arising from the effects of transient behaviour [15, 21]. The result is that 107 transient effects can cause complicated impacts to the fuel cell system and materials.

108 Despite many promising simulation studies that explore the operability of SOFCs using different type of 109 fuels, there has been no prior published experimental data and/or detailed analyses of SOFC/GT system 110 performance during fuel composition transients [22, 23]. To the best of our knowledge, almost all existing studies focus on steady state operations that are solely dependent on numerical simulations [7-9, 24-28]. 111 112 However, if effective controls are to be developed to take advantage of the extensive operating envelope offered by SOFC/GT hybrids [5, 29], a dynamic characterization of fuel cell parameters is essential. Our understanding 113 114 of the risks and challenges of fuel flexible SOFC/GT hybrid systems must be expanded through evaluation of the actual response and the coupling interactions of each component in the hybrid system. This effort requires 115 116 more than prediction via simulations only.

Therefore, in this work, the dynamics of fuel composition changes in the recuperated direct-fired 117 118 SOFC/GT hybrid system were experimentally investigated using a hybrid test facility with real recuperated 119 turbomachinery equipment. This method was very beneficial to reduce high cost of using a real solid oxide fuel cell and to minimize large inaccuracies in simulating very fast turbomachinery dynamics. For instance, stall and 120 surge in compressor/gas turbine could happen drastically during transient operations, in an order of 121 milliseconds, which could cause catastrophic failure of both fuel cell and gas turbine/compressor. From the 122 123 experience of researchers at National Energy Technology Laboratory (NETL), the real complexity of 124 turbomachinery dynamics could not be sufficiently captured by simulation only.

While our prior work outlined the coupling effects on turbine portion of the system [30], this work characterized the detailed fuel cell dynamic trajectories in response to fuel transitions (specifically from coalderived syngas to humidified methane). As the first step in characterizing the distributed profile of key fuel cell variables, this paper was aimed at evaluating the overall contributions and linking effects of each fuel cell parameter to operability and controllability of the hybrid systems during fuel composition transitions. Emphasis of this work was placed upon the dynamic characterization of the hybrid system during fuel composition changes via hardware-based simulations using the existing real-time model of an SOFC.

132 2. Methodology

133 2.1. Hardware system

134 A public testing facility of SOFC/GT at the U.S Department of Energy, National Energy Technology 135 Laboratory (NETL), Morgantown, West Virginia, was used to carry out the test on fuel composition changes. As shown in a simplified flow diagram in Figure 1, this system combined a real-time fuel cell dynamic model 136 (shown in the dashed-line box) and the balance of the plant for a potential recuperated SOFC/GT hybrid system 137 138 [31, 32]. The balance of the hybrid system was designed using real equipment and piping systems. With such 139 configuration, this facility served as a valuable research tool in steady state or dynamic studies to explore the 140 key operational challenges and opportunities of the SOFC/GT hybrid system in terms of dynamic control 141 development for future system commercialization [3, 29, 33-37].

142



143 144 145

159

166

Figure 1: The physical system of SOFC/GT hybrid test facility at NETL. Reproduced from Harun et. al (2014)

A 120 kW auxiliary power unit (APU) consisting of a single shaft turbine (T-101) attached to a two-stage compressor (C-100), a 400 Hz gear-driven generator (G-102), and two primary surface heat exchangers (E-300 and E-305) were among the major parts of the hardware system. Air plenums were also used to emulate cathode volume (V-301) and post combustor volume (V-304) for a real direct-fired SOFC/GT system. In a constant turbine-speed operation, an adjustable 120 kW load bank system (E-105) was also connected to the system as an independent system variable to maintain the turbine speed.

In this work, the effect of the fuel cell waste heat was embedded in a fuel cell model output variable, which was the fuel cell model net thermal effluent, Q. The definition of Q was simplified by the following equation, Eq. 1 [30], where ΔH_1 and ΔH_2 were the sensible heats of the cathode feed stream before preheating and the postcombustion exhaust after cooling with a reference to standard conditions, as shown in Figure 1. Meanwhile, \dot{m}_1 and \dot{m}_2 were the mass flow rate of the respective streams.

158
$$Q = \dot{m}_2 \Delta H_2 - \dot{m}_1 \Delta H_1$$

(1)

During a fully coupled SOFC/GT test, a complete interaction cycle between the fuel cell model and the hardware system was achieved in real-time (as fast as 80 ms) by feeding the sensor measurement of a real cathode feed stream in the hardware system to the software part as model inputs. To close the system loop, a model output (the fuel cell net thermal effluent) relevant to the study was fed to the hardware system in feedforward fashion. The *Q* value was used to manipulate the natural gas flow through a real fuel valve (% FV432) simulating the energy input for turbomachinery.

167 2.2. Model Description

168 To achieve the objective of the case study presented herein, a previously developed one-dimensional (1D) 169 real-time distributed fuel cell model was modified to enable fuel composition changes in the simulated SOFC fuel feed [31]. The implementation of fuel composition transitions in the emulator of solid oxide hybrid systems is graphically shown in Figure 2. The fuel cell model was based on an anode-supported fuel cell system with the standard material using 441SS interconnects and co-flow configuration [31]. The thermal behaviour of the materials used was characterized via curve fits based on temperature-dependent thermophysical properties at a broad temperature range (300K to 1800K) [31]. This model was verified with IEA benchmarking data sets and the result from other studies [31, 38, 39].

- 176
- 177



Figure 2: 1D-Real time fuel cell dynamic model.

This model was developed by considering the occurrence of both steam methane reforming and watergas shift reactions, in addition to electrochemical oxidation of hydrogen component only. This assumption was reasonable since it was shown that direct chemical oxidation of CH_4 and CO resulted in negligible differences [38, 40-42]. The characterization of steam methane reformation was based on first order reaction kinetics as described in Eq. 2, where A_{rx} is a pre-exponential factor, T_{PEN} is the fuel cell solid temperature, and R_u is the ideal gas constant [38, 43].

189
$$r_{SMR} = 4274 \frac{mol}{s.m^2.bar} p_{CH_4} exp \left[\frac{-82,000^{J}/mol}{R_u T_{PEN}} \right] A_{rx}$$
 (2)
190

191 Meanwhile, water-gas shift was presumed to occur at equilibrium at the selected operating range, and 192 its equilibrium constant was empirically resolved as a function of temperature, as presented in Eq. 3, where p_i is 193 the partial pressure of component *i*, x_i is the mole fraction of component *i*, and *T* is temperature in Kelvin[31]. 194

195
$$K_{P,WGS} = \frac{P_{H_2}P_{CO_2}}{P_{H_2O}P_{CO}} = \frac{x_{H_2}x_{CO_2}}{x_{H_2O}x_{CO}} = exp\left[\frac{4276}{T} - 3.961\right]$$
 (3)

196 197

198 Given the initial operating condition as described in Table 1, at a desired set of fuel cell configuration 199 parameters (Table 2) [30], the model simulated the distributed fuel cell profiles as function of time and local 200 position for 20 nodes along the length of the cell in real-time based on the sensor measurements of recuperated 201 compressed air being delivered to the cathode inlet (mass flow rate-FT380, temperature-TE326, and pressure-202 PT305). Sensitivity studies showed that using 20 nodes provides the optimum balance in measurement speed 203 and accuracy in capturing the fuel cell dynamics, particularly for millisecond time scales [44, 45]. It was shown that increasing the number of nodes above 20 did not improve the solution accuracy but increased the 204 205 computational time exponentially [45].

The model evaluated most of the key fuel cell process variables, in terms of thermal performance including solid and gas temperature on the cathode side, axial heat generation within the cell, partial pressures of major components in the anode side, Nernst potential, polarization losses, and local current density [31, 44]. Implicit/explicit finite difference was the key methods used to determine the thermal performance along the fuel cell length. This also considered conductive heat for the solid material, convective heat transfer between the oxidant and the SOFC, and heat generation in the fuel cell as a result of chemical kinetics (i.e. water gas shift and steam methane reforming reactions) and electrochemical operations.

The model of temperature profile resolution is given in Eq. 4. β is the fractional weighting of implicit formulation, k is the effective thermal conductivity of solid, A_s is the cross-sectional area for conduction heat 215 transfer, while A_g is the cross-sectional area for convective heat transfer. The term Δx represents the spatial 216 distance between the nodes, Δt is the time step for each iteration, n is the node, and i is the iteration. The 217 HG_{cell} , HG_{WGS} , and HG_{SMR} respectively represent heat generated by the fuel cell due to electrochemical 218 reactions, water gas shift, and steam methane reforming. 219

220 Temperature profile:

221

 $\beta \left[\frac{kA_s}{(\Delta x)^2} (T_{i+1}^{n+1} - 2T_i^{n+1} + T_{i-1}^{n+1}) + hA_g (T_{\infty} - T_i^{n+1}) \right] + (1 - \beta) \left[\frac{kA_s}{(\Delta x)^2} (T_{i+1}^n - 2T_i^n + T_{i-1}^n) + hA_g (T_{\infty} - T_i^n) \right] + (HG_{cell} + HG_{WGS} + HG_{SMR})A_s(\Delta x) = \rho C_P(\Delta x) \left[\frac{T_i^{n+1} - T_i^n}{\Delta t} \right]$ (4) 222 223

224

225 The cell voltage was ultimately calculated using Eq. 5, where V_{NERNST} is the Nernst potential, η_{dif} , η_{act} , and η_{ohm} respectively represent the diffusion loss, the activation loss and the ohmic loss. The polarization 226 227 losses were calculated using Eq. 6 to Eq. 8. Detailed work on model development including model assumptions, 228 validations, and challenges of real-time fuel cell model applications in hardware-based simulations were 229 discussed in a previous publication [31]. 230

231
$$V_{cell} = V_{NERNST} - \eta_{dif} - \eta_{act} - \eta_{ohm}$$
(5)

232
233
$$\eta_{dif} = \frac{R_u T}{2F} \left(\ln \left(\frac{x_{H_2, bulk, x_{H_2, 0, TBP}}}{x_{H_2, 0, bulk, x_{H_2, TBP}}} \right) + \frac{1}{2} \ln \left(\frac{x_{O_2, bulk}}{x_{O_2, TBP}} \right) \right)$$
(6)
234

235
$$\eta_{act} = \frac{R_u T}{anF} \sinh^{-1}\left(\frac{i}{2i_0}\right)$$
(7)

236 237

 $\eta_{ohm} = R \cdot i$

The detailed fuel cell parameters and initial operating conditions used in this study are shown in Table 238 1. It was assumed that the initial fuel cell temperature was around 800°C. As such, for simplification, the feed 239 240 temperature of fuel was also at the same temperature. In this study, fuel manifolds for the fuel cell system were 241 not modeled. Thus, autoreforming of methane was not considered.

(8)

242

243 Table 1 Inlet conditions for fuel cell cathode and anode streams. Based on Harun et.al [30] Measured cathode inlet condition at initial steady

| state | |
|--------------------|-----------|
| Air mass flow rate | 1.04 kg/s |
| Air temperature | 705 °C |
| Air pressure | 346 kPa |
| 1 | |

| Simulated anode inlet condition | ı |
|---------------------------------|---------|
| Fuel mass flow rate | 145 g/s |
| Fuel temperature | 800 °C |
| Fuel pressure | 346 kPa |
| | |

244

| 245 | Table 2 Specification of SOF | C system parameters. Based on Harun et.al [30]. |
|-----|-------------------------------|---|
| | Fuel cell load | 220 A |
| | Anode recycle | 0% |
| | Initial fuel cell temperature | 800 °C |
| | Initial cell voltage | 0.83 V |
| | Total cell area | 200 mm x 200 mm |
| | Anode thickness | 0.5 mm |
| | Electrolyte thickness | 0.008 mm |
| | Cathode thickness | 0.05 mm |
| | Oxidant/fuel channel size | 2 mm x 2 mm |
| | Stack size | 2500 cells |
| | Total stack mass | 3500 kg |
| | Total stack heat capacity | 2625 kJ/K |

246 2.3. Hardware-based Simulation of SOFC Fuel Composition Transient

The recuperated turbine cycle was first brought up to a nominal turbine speed at 40,500 rpm without the 247

248 fuel cell model in the loop. Before integrating the fuel cell model into the test facility, the startup step was continued by heating the hardware system for about two hours to a thermally steady state condition, approaching
 0.1 K/min in the skin temperature gradient post combustor (V-304). During this period, a 40 kW turbine load
 and different bleed air bypass valve openings were used to accelerate the heating up process.

252 For this initial system steady state, the model input parameters for the fuel feed to the SOFC were specified 253 to be CH₄ 0%, CO₂ 12%, CO 28.6%, H₂ 29.1%, H₂O 27.1%, N₂ 3.2% (mole fraction). This coal-derived syngas was selected based on previous studies and because the SOFC/GT hybrid system properties are well known 254 255 under these conditions [46, 47]. It was assumed that air composition in the cathode stream was O_2 21% and N_2 79%. Since it has been shown that the overall SOFC/GT system efficiency of direct fired configurations was 256 insensitive to fuel utilization in the fuel cell [48], a lower initial fuel utilization of 67% was chosen. However, 257 the overall fuel utilization was not kept constant. Instead, the test was run at a constant fuel mass flow rate (145 258 259 g/s) and a constant fuel cell load (220 A). Thus, the impacts of fuel composition variations could be decoupled 260 from the interaction of the changes in the mass flow and fuel cell load.

The integration of the real-time fuel cell model into the hybrid test facility was initiated once steady state conditions in both the recuperated hardware and the virtual SOFC system were achieved. The fuel feed was then switched from the initial steady state with the syngas composition to a methane rich fuel composition (CH₄ 14% and H₂O 86%) at the same fuel mass flow rate (145 g/s). This step change represented a 17% reduction in the overall heat input (i.e. lower heating value of fuel) of SOFC system (Figure 2). No change was made in any other operating parameters during the fuel composition transition. This means that the operation using humidified methane was continued with the resulting steady state condition for syngas.

268 In a prior work, this composition was determined as a tolerable transition to ensure safe heat change in 269 turbomachinery system in the hybrid configuration, and with this humidified methane mixture, no chance for the 270 occurrence of carbon deposition [30]. Fuel diffusion effects were not taken into account. The step change from coal-derived syngas to this methane-rich fuel represented the "worst case possible" because this transition 271 272 involved significant changes in each fuel constituent. It was expected that the effects of each fuel component 273 could provide broad generality in terms of qualitative assessment, but the sensitivity of methane content could 274 not be neglected. In a previous study, it was found that switching from coal-syngas to humidified methane with 275 more than 14% methane could not be tolerated due to the transient limitations in the turbine cycle [30]. For 276 transitions to fuels with larger than 14% methane, the fuel cell dynamics caused a rapid and extreme transient 277 increase in the turbine speed which could destroy the turbine.

In this paper, the step time was indicated as time zero in the result plots. The transient profiles were observed for approximately 7,000 s after the step time. Based on operator experience, no significant transient response beyond 7,000 s of the experimental test was expected. The test was run at a constant fuel mass flow rate (145 g/s) and a constant fuel cell load (220 A). Thus, the impacts of fuel composition variations could be decoupled from the interaction of the changes in the mass flow and fuel cell load.

283 **3. Results and Discussions**

285

284 3.1. Distributed Analysis for the Initial Steady State with Coal-Derived Syngas Feed

286 Due to the absence of methane (CH_4) content in the coal-derived syngas used in this study, as shown in 287 Figure 3, the composition gradient of each gas component was primarily driven by the water-gas shift (WGS) kinetics (Eq. 9) and the electrochemical hydrogen (H₂) oxidation (Eq. 10). The direct electrochemical oxidation 288 289 of CO and CH₄ was assumed to be negligible, since (1) there is excess water in the system; (2) the kinetics of 290 CO and CH_4 oxidation are significantly slower than H_2 oxidation; (3) less surface area is available for 291 electrochemical oxidation at the three-phase-boundary as compared to the area available for catalytic reforming 292 and WGS along the anode channel; and (4) CO and CH_4 has slower mass transfer to the triple-phase boundary 293 [40].

As clearly illustrated in Figure 3, the most rapid reduction in CO appeared to be at the first two nodes or 10% of the cell length, diminishing by 20%. The sharp initial decline in CO partial pressure was due primarily to the shifting of CO to obtain the equilibrium condition. This was followed by the slow almost linear decline in CO towards the exit of the fuel cell as hydrogen was consumed, driving the shift reaction to consume the CO to the final mole fraction of 0.09.

300 Water-gas shifting:

$$301 CO + H_2O \rightleftharpoons H_2 + CO_2 (ΔH° = −41 kJ/mol) (9)
 302 (9)$$

303 Hydrogen oxidation:

304
$$H_2 + \frac{1}{2}O_2 \to H_2O \ (\Delta H^\circ = -286 \ kJ/mol)$$
 (10)
305

306 Figure 3 also shows the resulting changes in carbon dioxide (CO_2), increasing from 0.120 at node 1 to 307 approximately 0.310 at node 20. Intuitively, the mole fraction gradient of CO_2 was completely controlled by the 308 CO mole fraction as well as the WGS kinetics. Thus, it reflected closely the CO conversion along the fuel 309 channel.

As the results of both WGS and H_2 oxidation in the fuel cell, higher H_2 mole fraction at the entrance of the 310 311 cell and lower H_2 mole fraction at the end of the cell were observed. As shown in Figure 3, an initial increase in 312 H_2 mole fraction was evident between the first two nodes, from 0.291 to 0.334, before decreasing through the remaining cell length. This suggested that there were strong impacts of WGS kinetics at the beginning of the 313 cell, whereas the electrochemical activities had greater influence on the downstream path. 314

315 The change in H₂ mole fraction was reflected by the change in water (H₂O) mole fraction. As opposed to 316 the maximum level of H_2 , the minimum H_2O mole fraction (0.228) was observed at the same location shortly 317 after the cell entrance. This was due to H_2O consumption in WGS to yield H_2 in the system, which also 318 stimulated the remarkable decrease in CO. Starting from node 2, H_2O mole fraction steadily increased to the 319 highest level of 0.461 at the cell outlet as the hydrogen oxidation outweighed the effects of other reactions.





321 Figure 3: Distributed profiles of composition gradient in the anode at the initial steady state using syngas feed 322

323 The Nernst potential was quantified using an expression shown in Eq. 11. This function reveals that the 324 Nernst potential is correlated to fuel cell temperature, as well as the partial pressure of H_2 and H_2O in the anode 325 and O_2 in the cathode. There is no significant change in O_2 mole fraction in since the air mass flow rate in the 326 cathode coming from the recuperated hybrid system is very high, so the effect of O_2 on the Nernst potential transient is negligible. The O2 utilization was maintained very low, approximately at 19%, with the maximum 327 328 variation less than 3% over the entire course of experiment. In Eq. 11, the net value of the first term, which 329 consists of the Gibbs free energy of water at the standard condition, is a positive value. Meanwhile, as the 330 consequence of operating in excess water condition, the net value of the second term, as a function of 331 temperature and component partial pressure is a negative value. In this case, there is a reversed effect of fuel cell 332 temperature on the Nernst potential.

(11)



Figure 4: Nernst potential, current density, and electrochemical losses at the initial steady state using syngasfeed

The corresponding effects on Nernst potential, current density, and polarization losses for a steady state with syngas feed are presented in Figure 4. Regardless of increased polarization losses at the entrance of the fuel cell, a 1% increase in Nernst potential from the initial condition was identified in the H_2 concentrated region, as expected. Likewise, current density also increased significantly within the first two nodes. However, the highest current density (0.720) was found at around node 6.

The significant reduction in H_2 partial pressure in the downstream region decreased Nernst potential by 13% to its lowest value at the cell outlet. This response was also influenced by the increasing fuel cell temperature. On the other hand, the electrochemical losses reduced substantially with the increasing temperature. The greater discrepancy in the transients between the Nernst potential and the electrochemical losses (increased voltage) eventually caused the significant decrease in current density (60% from the inlet) at the cell outlet.

350

338

351 3.2. Transient Analysis of Fuel Composition Change Impacts

- 353 3.2.1. Compositional Gradient and Localized Fuel Utilization
- 354 355

352

The transient CH_4 mole fraction profile after the step change in fuel composition is presented in Figure 5. Figure 5 shows that rapid conversion of CH_4 occurred in the first six nodes. With respect to the selected initial conditions and the fuel cell configuration, the residence time of the fuel cell subsystem was on the order of hundreds of milliseconds (approximately 500 ms), which was slower than the resolution of 1 s captured by the dynamic model used in this study. Zero to very low CH_4 mole fraction was observed at approximately halfway down the fuel cell length immediately after the transient, approaching a complete CH_4 conversion.

The analysis suggests that the behaviours in the fuel cell upstream would be strongly affected by the steam methane reforming (SMR) kinetics (Eq. 12) due to the observed significant variations. This reaction was initially stimulated by the elevated fuel cell thermal condition. Owing to the aggressive CH_4 conversion in this region, the fuel cell solid temperature was expected to decrease in the long run, which would cause undesirable changes in the spatial temperature gradient and deceleration of the SMR kinetics.

The effects of reduced fuel cell solid temperature were clearly demonstrated by slower CH_4 consumption at the end of the test. At the final state (at time 7,000 s), as presented in Figure 5b, the system exhibited a fairly distributed CH_4 profile along the cell. The CH_4 conversion was still incomplete until the fuel cell outlet. Overall, the result suggests that future control strategies of SOFC/GT hybrid system will need to include thermal management of fuel cell temperature.



Figure 5: Variations in methane partial pressure, (a) a 3D mesh plot, as function of local position along the cell
node and time, and (b) distributed profiles at time 1 s, 250 s, 1,500 s, and 7,000 s after the step change

The profile of the CO composition gradient is shown in Figure 6. As shown in Figure 6, CO steeply increased to the highest point at node 7 and reduced at the end of the cell.

Changes in CO mole fraction gradient along the fuel cell length were highly reflected by the presence of CH₄ in the system, as expressed in Eq. 12. The dramatic accumulation of CO in the fuel cell upstream (Figure b) was correspondingly promoted by the rapid consumption of CH₄ (Figure 5b). The highest CO mole fraction was achieved when almost all CH₄ was converted to SMR products. The complete CH₄ consumption subsequently initiated the depletion in CO in the downstream region, which was due to WGS reactions (Eq. 9).

However, the maximum CO reduced by about half and shifted to node 16 within 7,000 s. The shift of the maximum CO from node 7, 35% from the inlet, downstream to node 16 at 7,000 s was strongly motivated by the reduction of cell temperature. As the test progressed, decreasing fuel cell solid temperature decreased SMR kinetics. This ultimately reduced the formation of CO, and thus, moved the region of high CO concentration to the end of the fuel cell.



Figure 6: Transient response of carbon monoxide composition, (a) a 3D mesh plot, as function of local position
along the cell node and time, and (b) Distributed profiles at time 1 s, 250 s, 1,500 s, and 7,000 s after the step
change

397 The change in the H_2 content over the entire course of the experiment is shown in Figure 7. The coupled effects from WGS, H₂ oxidation as well SMR, as shown in Eq. 9, Eq. 10, and Eq. 12, have determining 398 399 influence on the H_2 mole fraction profile. The initial transient increased in H_2 mole fraction in the first half of 400 the cell length followed closely the dramatic reformation of methane. As the result of the high production of H_2 401 as well as the decreasing SMR kinetics and WGS reaction, the impact of H₂ oxidation became more noticeable 402 in the second half region. Within this region, H₂ was consumed faster than its formation. As such, significant 403 reduction in H_2 mole fraction level was observed. Theoretically, increasing H_2 consumption should have shifted 404 the equilibrium of WGS process further to product side, and so moderating the H_2 reduction. However, this 405 effect was insignificant due to diminishing CH₄ content that restricted CO generation from methane reforming.

406 Due to the corresponding effects of SMR on the fuel cell solid temperature over 7,000 s time studied, the 407 local maximum of H_2 mole fraction gradually shifted to the end of the cell to a lower level (0.220), featuring a 408 more even distribution curve. It is also interesting to note that the H_2 concentration at the exit was effectively the 409 same during the entire transition, despite the shifting internal profiles. This illustrates the usefulness of a model 410 which can predict shifting internal profiles that could not otherwise be detected by experiment since spatial 411 measurements are very difficult to obtain inside the SOFC.



Figure 7: Hydrogen mole fraction gradient, (a) a 3D mesh plot, as function of local position along the cell node and time, and (b) distributed profiles at time 1 s, 250 s, 1,500 s, and 7,000 s after the step change

416 The corresponding change in H₂O mole fraction is illustrated in Figure 8. As shown in Figure 8, the 417 resulting variations in H_2O mole fraction were inversely correlated to H_2 dynamic response (Figure 7). 418 Substantial reduction in H_2O partial pressure was more apparent at the beginning of the cell, between node1 to node 6, following the rapid methane reformation and WGS reactions. Similarly, the shifting in the local 419 minimum points of H₂O was attributed to the effect of slower methane conversion indicated in Figure 5. 420 421 Significant formation of H₂O due to electrochemical reactions was identified at node 6 onwards when H₂O mole 422 fraction started to increase up to its final level at the fuel cell outlet. Over 7,000 s, the final H₂O mole fraction at 423 the fuel cell exit was about 0.740, slightly lower than the inlet mole fraction (0.860).

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426 Figure 8: Water mole fraction gradient, (a) a 3D mesh plot, as function of local position along the cell node and 427 time, and (b) distributed profiles at time 1 s, 250 s, 1,500 s, and 7,000 s after the step change

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430 Fuel Utilization

431 The changes in localized fuel utilization in response to fuel composition transition are shown in Figure 9. 432 Localized fuel utilization, U_{i} , for each node across the fuel cell length is defined in Eq. 13, where x_i is the partial 433 pressure for fuel component i, j represents a current node, while j+1 represents the exit of the current node. As 434 can be seen in Figure 9a, fuel utilization at the initial steady state was almost uniformly distributed across the cell but with a lower level at both cell inlet (node 1) and outlet (node 20). After switching the anode feed to 435 humidified methane, the highest peaks were found at node 2 at 1 s, and at node 19 after 7,000 s (Figure 9b). The 436 437 highest fuel utilization at the beginning of the cell at the initial transition phase was likely due to rapid SMR 438 reaction that led to significant variations in localized H_2 availability. Intuitively, this was promoted by the 439 elevated initial fuel cell solid temperature.

442

441
$$U_F(j) = \frac{x_{H_2}(j+1) + x_{CO}(j+1) + 4x_{CH_4}(j+1)}{x_{H_2}(j) + x_{CO}(j) + 4x_{CH_4}(j)}$$
(13)

443 At the beginning of the cell, fuel utilization reduced gradually over the course of the experiments, but these 444 dynamics were reversed at the end of the cell. The analysis indicates that the variations at the beginning of the 445 cell were significantly driven by the reduction of fuel cell temperature, which was also reflected by the 446 reduction in CH_4 consumption over time studied. Meanwhile, as methane was almost completely consumed at 447 the downstream region, the trends of fuel utilization were strongly related to the activities of electrochemical 448 reactions.

At the end of the cell, fuel utilization increased over time with increasing current density and less available fuel. This is clearly illustrated because the hydrogen concentration in the last half of the cell was not significantly changing, as seen in Figure 7, while current density was increasing at the end of the cell. The overall fuel utilization increased from 67% to approximately 71% as fuel was switched to humidified methane and remained constant until the test was terminated.



Figure 9: Localized fuel utilization, (a) a 3D mesh plot, as function of local position along the cell node and time, and (b) distributed profiles at time 1 s, 250 s, 1,500 s, and 7,000 s after the step change

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458 3.3. Current Density, Nernst Potential, and Electrochemical Losses

460 *Current Density*

The local current density profiles are illustrated in Figure 10. As the result of switching the fuel to humidified methane at a constant fuel cell load, higher current density was observed at the end of the cell, as opposed to the profile at the initial steady state of syngas operation (Figure 10a).

As shown in Figure 10b, at 1 s after the transient, current density increased to the highest value (0.73) at around node 8, 40% of the cell length, before slowly decreasing through the remaining fuel cell length. However, decreasing solid temperature over 7,000 s test subsequently shifted the maximum current density towards the end of the cell, resulting in the highest peak (0.83) at node 18. The distributed profile at the end of the test was mirrored the performance at the initial steady state.

469 The dynamics of current density were greatly coupled with the effects of H_2 partial pressure and Nernst 470 potential. As expected, higher current density region was achieved in the elevated solid temperature segments 471 (Figure 15) at a relatively higher partial pressure of H_2 (Figure 5), as well as higher Nernst potential (Figure 11). 472 Increasing current density at the end of the cell also promoted the fuel cell heat generation, as indicated in 473 Figure 20.





477

478 Nernst Potential

The resulting variation in Nernst potential is plotted in Figure 11. Over 7,000 s, a rapid increase in Nernst potential with insignificant variations with time was observed at the beginning of the cell, as illustrated in Figure 11b. This was due to dramatic increase in the H_2 mole fraction to 31% (Figure 7), which was also correlated to evenly distributed profiles in the local solid temperature gradient over time (Figure 15), and a 30% reduction in H_2O (Figure 8).



Figure 11: Nernst potential distribution, (a) a 3D mesh plot, as function of local position along the cell node and
time, and (b) distributed profiles at time 1 s, 250 s, 1,500 s, and 7,000 s after the step change

488 Meanwhile, the Nernst potential dynamics in the second half of the cell was most likely influenced by the 489 fuel cell temperature changes rather than the partial pressures of H_2 and H_2O . As presented in Figures 7 and 8, 490 the H_2 and H_2O contents did not change significantly. Although the H_2 mole fraction reduced over the time 491 studied, the Nernst potential of the cell increased with decreasing fuel cell temperature. Over 7,000 s, the peaks 492 of the Nernst potential were scattered between node 5 and node 8 (20% to 40% of the cell length) from 493 approximately 0.93 V to 0.96 V.

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5 Electrochemical Resistance

The variations in activation loss in response to the fuel composition change are shown in Figure 12. The activation loss represents the polarization resistance due to the required activation energy to initiate electrochemical reactions [24]. In this test, as presented in Figure 12b, the cell initially exhibited a very low activation resistance at node 1 in the absence of H₂ molecules. But, it steeply increased with time to a higher resistance at around node 4 to node 8 (20% to 40% from the fuel cell inlet), followed by a steady decrease to the outlet shortly after the maximum point.

502 The analysis indicates that higher activation loss was obtained at higher H_2 partial pressure (Figure 7), 503 current density (Figure 10), and Nernst potential (Figure 11). As expected, the significant reduction in fuel cell 504 temperature over 7,000 s test substantially increased activation loss. However, it was expected that the influence 505 of partial pressure changes was greater than the impacts of temperature in determining the activation loss at the 506 beginning of the cell.

507



508 Figure 12: Activation loss distribution, (a) a 3D mesh plot, as function of local position along the cell node and 509 time, and (b) distributed profiles at time 1 s, 250 s, 1,500 s, and 7,000 s after the step change

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As shown in Figure 13 due to similar correlation to fuel cell temperature, changes in ohmic loss closely followed the trend observed in activation loss distribution. Figure 13b shows that over the entire course of the transient, ohmic loss increased with the decreasing fuel temperature. Overall, the distributed ohmic resistance varied between 0.01 V to 0.057 V with respect to the variations in the fuel cell temperature, approximately between 660 °C to 900 °C.



Figure 13: Ohmic loss profile, (a) a 3D mesh plot, as function of local position along the cell node and time,
and (b) distributed profiles at time 1 s, 250 s, 1,500 s, and 7,000 s after the step change

The transient response of diffusion loss is shown in Figure 14. Theoretically, this loss results from the resistance associated with the transportation of chemical compounds to the reaction sites [24]. Intuitively, diffusion loss is strongly correlated to the mole fraction gradients across the cell. However, variations in the local current density and the fuel cell temperature also contribute some impacts on the changes in this polarization resistance.

In comparison to other polarization resistance, the diffusion loss had the least impact on the fuel cell, since a thin electrode was used. Overall, over 7,000 s of test, the system started at very low diffusion resistance at the cell inlet, and sharply increased at node 2, as shown in Figure 14b. The diffusion loss at node 2 increased with time, reflecting the increase in localized H₂O mole fraction or the reduction in H₂O consumption (Figure 8) when the fuel cell solid temperature dropped. Toward the end of the test, the increase at node 2 was more significant, with a substantial decrease immediately after node 2.

In the first 250 s of the transient, the maximum diffusion resistance was demonstrated at node 10, and gradually shifted to the cell exit to higher values over 7,000 s. Without significant variation in H_2O mole fraction, the diffusion loss at the end of the cell increased with decreasing fuel cell temperature, and increasing current density (Figure 10).





- 539
- 540 3.3.1. Fuel Cell Thermal Performance541
- 542 Solid Temperature

The result of solid temperature distribution is presented in Figure 15. During the initial steady state, as shown before time 0 s in Figure 15a, the solid temperature inclined from node 1 to node 20, in a range of 780 °C at the inlet, to 903 °C at the outlet, with an average temperature of 857 °C. This resulted from an initial operating temperature of 800 °C using coal-derived syngas feed. In response to the fuel composition switch, the local solid temperature decreased significantly afterwards, except just a slight increase at the cell outlet during the first few minutes after the transient.

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The slight increase in the solid temperature at the end of the cell occurred at the first 250 s is clearly illustrated in Figure 15b. This dynamic was driven by the increase in fuel utilization (Figure 9), current density 551 (Figure 10), and heat generation (Figure 19). In a short-term period, due to the large heat capacity of the fuel 552 cells, the increase in fuel cell temperature was not offset by the temperature reduction promoted by the steam 553 methane reforming reactions.

554



555 Figure 15: The dynamic profiles of fuel cell temperature, (a) a 3D mesh plot, as function of local position along the cell node and time, and (b) distributed profiles at time 1 s, 250 s, 1,500 s, and 7,000 s after the step change 556 557

558 Unlike the end of the cell, the substantial reduction in solid temperature at the beginning of the cell was 559 highly correlated to the drastic localized methane reforming as indicated in Figure 5, and heat flux, as reflected by the solid-gas temperature difference in Figure 20. As the consequence, 33% of the total temperature change 560 561 at the cell entrance region took place in 250 s after the transient, and about 60% temperature drop occurred within the first 1,500 s (Figure 15b). This cooling impact was remarkable even though there was a 2% decrease 562 in cathode air mass flow during the first 1,500 s of test (Figure 16), which should have mitigated the impact on 563 564 the solid temperature. Due to the control action taken by the system to maintain constant turbine speed at 40, 565 500 rpm, a 40% increase in turbine load caused a 1% increase in compressor discharge pressure. This resulted in 566 a 4% reduction of compressor inlet flow which eventually reduced the cathode air flow by 2% [30].



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570 As presented in Figure 15b, despite the small temperature changes observed around the first and the 571 last few nodes, the solid temperature across the cell increased to the maximum temperature region near the 572 outlet. The increase in solid temperature occurred in the downstream region where CH₄ mole fraction was 573 almost complete, while significant H₂ oxidation was observed. Hence, it resulted in less heat consumption in the 574 reforming reaction. In addition, higher current density was also localized at the downstream region.

575 As the test progressed, the cell exit eventually cooled off to the point where the new steady state 576 temperature profile was identical to the initial steady state profile (i.e. before fuel composition switch), but at a 577 lower average temperature (715 °C). Decreasing the solid temperature decelerated the SMR kinetics that 578 ultimately led to a more gradual CH₄ conversion. At the end of the test, the fuel cell temperature was distributed 579 more evenly between 661 °C at node 1, and 778 °C at node 20. Due to shifted localized SMR towards the end of the cell, greater temperature reduction occurred at the cell outlet between time 1,500 s and 7,000 s. However, after 7,000 s, the fuel cell temperature difference between the initial and the final steady state at the cell inlet was about 120 degrees, similar to that observed at the cell exit.

583 Figure 17 presents the relevant solid temperature gradient between fuel cell nodes, dT/dx, for selected critical nodes. For control system development, fuel cell temperature gradient is a critical control variable 584 585 because uneven temperature changes across the fuel cell length during transient processes can lead to dramatic localized thermal stress on the material, which contributes to fuel cell material destruction. As the result of the 586 initial average temperature of 857 °C with a 113 °C temperature difference across the cell before the fuel 587 composition change, the maximum dT/dx of 11.5 K/cm occurred at node 5, 25% down the cell inlet. The 588 589 maximum temperature gradient remained at the same location over 100 s after the step change, featuring an 590 increasing value up to 15.8 K/cm. Unfortunately, over the 7,000 s test period, the greatest change in the 591 localized fuel cell temperature of 16 K/cm was indicated at node 7, 250 s after the fuel transition. The highest peak of dT/dx was then shifted node by node towards the cell outlet as the test continued. However, beyond 592 593 3,100 s, the maximum dT/dx remained at node 13, with a lower final value (10 K/cm) at the end of the test. 594





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598 The profile of average solid temperature in Figure 18a shows that there was a gradual change over the 599 7,000 s test period. Meanwhile, Figure 18b illustrates that the most extreme transient in average solid 600 temperature gradient as a function of time, dT_{ave}/dt , was not more than 0.10 K/s. 601





Figure 18: Average solid temperature profile, (a) Average solid temperature profile as a function of time, and (b) Temporal changes of Average solid temperature, dT_{ave}/dt

603 604

605 Cathode Gas Temperature

The associated dynamic response in the gas temperature is highlighted in Figure 19. Overall, the profile of cathode gas temperature features gradual decay characteristics toward its final value, with a slight increase at the cell outlet within the first few minutes, similar to the fuel cell solid temperature trends. However, as shown in Figure 19a, the cathode gas temperature at the fuel cell inlet did not follow the drastic decrease observed in the solid temperature (Figure 15a). In contrast, the profile of cathode gas temperature at the cell entrance was 612

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611 dominated by the 40 °C increase in cathode inlet air temperature (Figure 17) over the first 600 s after the initiation of the fuel composition change, due to the integrated system effects on the gas turbine system.



Figure 19: Cathode gas temperature profiles, (a) a 3D mesh plot, as function of local position along the cell 614 615 node and time, and (b) distributed profiles at time 1 s, 250 s, 1,500 s, and 7,000 s after the step change

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617 As depicted in Figure 19b, the cathode gas temperature at the initial steady state monotonically increased from 704 °C at node 1 to 902 °C at the last node, approaching a 200°C difference across the cell. After the fuel 618 transition, an increasing gas temperature towards the end of the cell was locally distributed in S-shaped curves 619 620 with the lowest temperature observed at around nodes 4 and 5. Correspondingly, over 7,000 s, the changes in gas temperature closely followed the distribution of fuel cell solid temperature. The detailed analysis suggests 621 622 that the dynamic response at the beginning of the fuel cell was driven by the heat flux, unlike the changes 623 occurred at the exit of the cell. At the final state, gas temperature difference across the cell length reduced by 624 about 50% with the decreasing local gas temperature, in comparison to the initial steady state. 625

Heat Generation

627 The dynamic trajectory of heat generation in the fuel cell unit per given length of each node is shown in Figure 20. As the consequence of operating the fuel cell at 220 A total current with 67% fuel utilization using 628 629 syngas, a maximum of 17 W/cm of heat was generated at the inlet, decreasing to a minimum of 3 W/cm at the 630 outlet (Figure 20a). More heat was accumulated in the region in which contained higher current density (Figure 631 4), as expected.





635

636 After shifting the syngas feed to methane-rich gas, a detrimental reduction in heat generation was evident at the beginning of the cell, resulting in an immediate drop of 53 W/cm at the first node from 17 W/cm 637 at the initial state to a -36 W/cm at 1 s after the step change. But, heat generation increased gradually towards 638 639 the maximum region at the fuel cell downstream.

640 The coupled effects of the sudden decrease in the fuel cell heat generation at the cell inlet (Figure 20) 641 were reflected by the remarkable reduction in solid temperature (Figure 15). This change was due to higher heat 642 consumption in the highly endothermic methane reformation at the cell upstream when the system was fed by

643 14% methane. Meanwhile, as the highly exothermic H_2 oxidation significantly took place in the second half of 644 the cell length, the solid temperature started to increase, as shown in Figure 15.

In a longer experimental run, the contribution of deceleration in steam methane reforming was demonstrated clearly at the cell entrance, in which heat generation at the first node increased gradually with decreasing rate in methane conversion. Beyond more than 7,000 s after the step change, the heat generation across the cell moderately fluctuated, but its highest peak shifted from the centre to the end of the cell.

650 Solid-Gas Temperature Difference

The fuel cell thermal performance was further analyzed by quantifying the local temperature difference between solid and cathode gas temperatures ($T_{solid} - T_{gas}$), as provided in Figure 21. The local and the overall temperature difference are shown in Figure 21a and 21b respectively. As shown in Figure 21a, the profile of temperature difference in the first half of the cell length was quite distinct from the dynamic response in the second half of the cell, indicating appreciable changes in the beginning of the cell, and insignificant transient response at the end of the cell. Variations of temperature difference at the cell exit were between 1°C to 10 °C over 7,000 s.

At the initial transient period that is denoted as time 0.08 s in Figure 20a, the temperature difference reduced dramatically by about 80%, from 75 °C to 14.5°C, within the first 5 nodes (25% of the cell length), following by a slow decrease to 1 °C gap at the cell exit. Such a transient implies that the cathode airflow was initially cooling the fuel cell, mostly at the first 25% of the cell length. Decreasing the temperature gap across the fuel cell length reduced the heat exchange from the solid to the air flow. Therefore, the cooling process progressed slowly as the air delivered through the end of the cell. Likewise, reducing the temperature difference at 100 s after the fuel transition also lowered the cooling impact of air flow at the inlet region.

The results in Figure 22a also show that as soon as 250 s after the transient, the cathode inlet airflow was being used to heat the beginning of the cell. This occurred once the solid temperature dropped below the gas temperature due to the rapid heat consumption in SMR, reducing the temperature difference to negative values. The thermal effects of cathode airflow was far more complicated in the period between 1,500 s after the transient to the final state, in which the heating and the cooling effects of cathode airflow alternated as moving from the inlet down through the cell outlet. But in this period, the airflow cooled the downstream region more than in the initial steady state.

672 As such, this work reveals the real challenges in modulation of airflow for thermal management of 673 SOFC/GT hybrid system for fuel composition changes. Alternative strategies might need to be considered to 674 compensate for the variations in solid temperature due to methane reforming and the impact of cathode airflow. 675





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679 3.4. Dynamic Response of Fuel Cell Thermal Effluent

Previous studies of the SOFC/GT hybrid system show that the fuel cell waste heat in the direct fired
 SOFC/GT hybrid configuration is a very important process variable for system performance controls and safety
 [30].

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Figure 22: (a) Fuel cell model thermal effluent transient, (b) Dissipation of fuel cell thermal energy storage

687 When the humidified methane was fed into the anode, methane reformation occurred immediately, as 688 observed in Figure 5. This reaction was initially driven by the elevated fuel cell thermal energy provided in the cathode stream as well as the available chemical energy level contained in the fuel mixture. However, the 689 available energy state was insufficient to facilitate the reactions while maintaining the fuel cell temperature. As 690 such, the fuel cell thermal energy storage was extracted, resulting in a sudden initial increase in fuel cell thermal 691 effluent in a short term period, as highlighted in Figure 22. As shown in Figure 22b, the dissipation rate of 692 693 thermal energy stored in the fuel cell was 260 kW immediately after the fuel transition. This thermal energy was transformed to chemical energy via the reforming reaction which increased the low heating value (LHV) of the 694 695 anode effluent. This subsequently increased the fuel cell thermal effluent, which then increased the thermal 696 energy entering the turbine by 120 kW, or about 17%. This in turn caused an increase in turbine exhaust 697 temperature, which caused a higher heating duty in E300 and E305, which finally caused the rise in cathode inlet temperature discussed previously (Figures 16 and 19). 698

The total mass-heat capacity contained in the simulated 2500 cell-stack with a total mass of 3500 kg was approximately 2625 kJ/K. Under the nominal operating condition, the fuel cell itself stored approximately 2.1 GJ of thermal energy. Theoretically, reducing the temperature of the fuel cell average temperature by 142 °C over the 7,000 s test (Figure 18) would significantly decrease the total thermal energy storage in the fuel cell by about 18%. Approaching the new steady state, Q decreased gradually, following the reduction in LHV of the fuel feed. As the result of highly coupled interactions in SOFC/GT hybrid system, this dynamic transient subsequently reduced the thermal effluent that ultimately decreased the cathode inlet temperature.

706 4. Conclusions

707 This work presented the detailed analysis of fuel cell dynamic performance in SOFC/GT hybrid system during a transition from syngas-fuelled to methane-fuelled operation, including the interactive effects among the 708 key operating variables. It was found that it was feasible to suddenly switch from a coal-derived syngas to a 709 humidified methane fuel (with 14% methane content) and transition to a new steady state within two hours 710 without causing compressor stall or surge, violating SOFC safe operating constraints, or otherwise adversely 711 712 affecting the hardware or functionality of the SOFC/GT system. It might also be possible to transition from coal-713 syngas to humidified methane fuels with an even higher energy content if the transition was gradual instead of a 714 step change, although this was a subject for future research.

715 It was found that the fuel transition exhibited a rapid transient increase of fuel cell thermal effluent by 716 17% in the time scale of milliseconds. The primary driver for the dramatic change in thermal effluent was the 717 conversion of thermal energy stored in the fuel cell stack to chemical energy. Over the course of the 7,000 s 718 period studied, 18% of the total thermal energy stored in the fuel cell stack itself was extracted.

In the initial period after the transient, methane was all used up by node 8 (40%), but node 20 by 7,000 s. As a consequence of the cooling effects of methane reformation, the maximum spatial temperature gradient, dT/dx, increased from 11 K/cm to 16 K/cm at around 35% from the cell inlet 250s after initiation of the transient. Maximum current density also increased by 15%, indicating a shift from node 5 (25%) to node 18 (90%).

Thermal management using modulation of cathode air flow could be a potential strategy to mitigate this unfavorable transient impact. However, due to alternating cooling and heating transient effects of cathode air flow observed across the cell, advanced control strategies may be required to mitigate the unfavorable transient impact as well as to increase the flexibility of SOFC/GT hybrid system.

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