### FUEL COMPOSITION TRANSIENTS IN SOLID OXIDE FUEL CELL GAS TURBINE HYBRID SYSTEMS FOR POLYGENERATION APPLICATIONS

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A Thesis Submitted to the School of Graduate Studies in Partial Fulfilment of the Requirements for the Degree of Doctor of Philosophy

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### ABSTRACT

The potential of Solid Oxide Fuel Cell Gas Turbine (SOFC/GT) hybrid systems for fuel flexibility makes this technology greatly attractive for system hybridization with various fuel processing units in advanced power generation systems and/or polygeneration plants. Such hybrid technologies open up the possibility and opportunities for improvement of system reliabilities and operabilities. However, SOFC/GT hybrid systems have not yet reached their full potential in term of capitalizing on the synergistic benefits of fuel cell and gas turbine cycles.

Integrating fuel cells with gas turbine and other components for transient operations increases the risk for exposure to rapid and significant changes in process dynamics and performance, which are primarily associated with fuel cell thermal management and compressor surge. This can lead to severe fuel cell failure, shaft overspeed, and gas turbine damage. Sufficient dynamic control architectures should be made to mitigate undesirable dynamic behaviours and/or system constraint violations before this technology can be commercialized. But, adequate understanding about dynamic coupling interactions between system components in the hybrid configuration is essential.

Considering this critical need for system identification of SOFC/GT hybrid in fuel flexible systems, this thesis investigates the dynamic performance of SOFC/GT hybrid technology in response to fuel composition changes. Hardware-based simulations, which combined actual equipment of direct-fired recuperated gas turbine system and simulated fuel cell subsystem, are used to experimentally investigate the impacts of fuel composition changes on the SOFC/GT hybrid system, reducing potentially large inaccuracies in the dynamic study.

The impacts of fuel composition in a closed loop operation using turbine speed control were first studied for the purpose of simplicity. Quantification of safe operating conditions for dynamic operations associated with carbon deposition and compressor stall and surge was done prior to the execution of experimentation. With closed loop tests, the dynamic performance of SOFC/GT hybrid technology due to a transition in gas composition could be uniquely characterized, eliminating the interactive effects of other process variables and disturbances. However, for an extensive system analysis, open loop tests (without turbine speed control) were also conducted such that potential coupling impacts exhibited by the SOFC/GT hybrid during fuel transients could be explored. Detailed characterization of SOFC/GT dynamic performance was performed to identify the interrelationship of each fuel cell variable in response to fuel composition dynamics and their contributions to operability of the system.

As a result of lowering LHV content in the fuel feed, which involved a transition from coal-derived syngas to humidified methane composition in the SOFC anode, the system demonstrated a dramatic transient increase in fuel cell thermal effluent with a time scale of seconds, resulting from the conversion of fuel cell thermal energy storage into chemical energy. This transient was highly associated with the dynamics of solid and gas temperatures, heat flux, heat generation in the fuel cell due to perturbations in methane reforming, water-gas shifting, and electrochemical hydrogen oxidation.

In turn, the dramatic changes in fuel cell thermal effluent resulting from the anode composition changes drove the turbine transients that caused significant cathode airflow

fluctuations. This study revealed that the cathode air mass flow change was a major linking event during fuel composition changes in the SOFC/GT hybrid system. Both transients in cathode air mass flow and anode composition significantly affected the hybrid system performance. Due to significant coupling between fuel composition transitions and cathode air mass flow changes, thermal management of SOFC/GT hybrid systems might be challenging. Yet, it was suggested that modulating cathode air flow offered promise for effective dynamic control of SOFC/GT hybrid systems with fuel flexibility.

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# TABLE OF CONTENTS

Abstra	act			iii
Ackno	wledge	ments		v
Table	of Cont	ents		vi
List of	Figure	s		ix
List of	Tables			xiv
List of	Abbre	viations	and Symbols	XV
Declar	ation o	f Acader	nic Achievement	xvii
1	Introd	uction		1
	1.1	Emergin Sustain	ng Solid Oxide Fuel Cell Technologies Toward Energy ability	1
	1.2	Role of	Solid Oxide Fuel Cell Gas Turbine Hybrid in Meeting Future	1
	1.3	Researce Cell Gas	heeds h Motivation: Potential and Challenges in Solid Oxide Fuel Turbine (SOFC/GT) Hybrid Systems for Fuel Flexible	4
		Operati	ons	6
	1.4	Problen	n Statement	8
	1.5	Researc	h Objective	8
	1.6	Thesis (	Jutline	9
	1.7	Referen	ces	11
2 Fuel C		ompositi	on Transients in Fuel Cell Turbine Hybrid for Polygeneration	
	Applic	ations		14
	2.1	Publica	tion Highlights	14
	2.2	Abstrac	t	15
	2.3	Introdu	ction	15
	2.4	Method	ology	17
		2.4.1	1D-Real Time Fuel Cell Dynamic Model	17
		2.4.2	SOFC Fuel Composition Scoping Study	19
		2.4.3	Hardware-based Hybrid Test Facility	21
		2.4.4	Hardware-based Simulation Procedures	21
	2.5	Results	and Discussion	22
		2.5.1	The Dynamic Response of Thermal Effluent	22
		2.5.2	The Impact of Thermal Effluent on Turbine Load	24
		2.5.3	The Response of Turbine Inlet Temperature and SOFC	
			Cathode Inlet Temperature	26
		2.5.4	The Dynamic Behaviour of the System Air Mass Flow	29
		2.5.5	The Transient Impact on the Fuel Cell Performance	31
	2.6	Conclus	ion	32
	2.7	Acknow	vledgement	33
	2.8	Referen	ices	33

3 Open Loop and Closed Loop Performance of Solid Oxide F		Loop and Closed Loop Performance of Solid Oxide Fuel Cell Turbine		
	Hybri	id Systems during Fuel Composition Changes	35	
	3.1	Publication Highlights		
	3.2	Abstract	86	
	3.3	Introduction	86	
	3.4	SOFC/GT Hybrid Test Facility	88	
	3.5	5 Hardware-based Simulation of SOFC/GT Hybrid		
	3.6	Test Procedure	ŀ1	
	3.7	Result and Analysis	13	
		3.7.1 Fuel Cell Thermal Effluent, O. and Turbine Temperatures 4	13	
		3.7.2 Cathode Inlet Mass Flow	16	
		3.7.3 Cathode Inlet Pressure 4	17	
		37.4 Cathode Inlet Temperature	17	
		3.7.5 Analysis of Mitigating versus Pronagating Effects 4	19	
		3 7 5 1 Open Loon Transients	19	
		3 7 5 2 Closed Loon Transients	50	
	3.8	Conclusions and Future Work	;0	
	3.0	Acknowledgement	;1	
	3.7	References 5	;2	
	5.10			
4	Impa	ct of Fuel Composition Transients on SOFC Performance in Gas		
	Turbi	ine Hybrid Systems	53	
	4.1	Publication Highlights5	53	
	4.2	Abstract	54	
	4.3	Introduction	54	
	4.4	Methodology	56	
		4.41 Hardware System 5	56	
		4.4.2 Model Description 5	57	
		4.4.3 Hardware-based Simulation of SOFC Fuel Composition		
		Transient	59	
	4.5	Results and Discussions	50	
		4.5.1 Distributed Analysis for the Initial Steady State with Coal-		
		Derived Syngas Feed	50	
		4.5.2 Transient Analysis of Fuel Composition Change Impacts 6	52	
		4.5.2.1 Compositional Gradient and Localized Fuel Utilization 6	52	
		4.5.2.2 Current Density, Nernst Potential, and		
		Electrochemical Losses	57	
		4.5.2.3 Fuel Cell Thermal Performance	71	
		4.5.2.4 Dynamic Response of Fuel Cell Thermal Effluent 7	77	
	46	Conclusions 7	78	
	4.7	Acknowledgement 7	78	
	4.8	References 7	79	
	1.0		,	
5	Coup	ling Effects of Fuel Composition Transition and Cathode Air Mass Flow		
	on Dy	vnamic Performance of SOFC/GT Hybrid Systems	32	
	5.1	Publication Highlights	32	

5.2	Abstra	act	
5.3	Introd	Introduction	
5.4	Backg	round	
5.5	Metho	odology	
	5.5.1	Description of Hardware-based Simulation System	
	5.5.2	Open Loop and Closed Loop Test Procedures	
5.6	Result	ts and Discussion	
	5.6.1	Turbine Speed and Cathode Air Mass Flow Transient Responses	
	5.6.2	Transient Characterization of Fuel Cell Thermal Performance	
		Spatial Cradient of Eucl Call Solid Temperature	
		Spatial Gradient of Fuel Cen Sond Temperature	
		Fuel Cell Cathode Gas Temperature	
		Cathode Solid and Gas Temperature Difference and Heat	
		Flux	
	562	ruei Cell Heat Generation	
	5.6.3	ITANSIENT ANALYSIS OF FUEL COMPOSITIONS	
		Methan Eucl Composition Credients and Eucl Utilization	
	E 6 4	Current density	
	5.6.4	Transient Analysis of Eyel Coll Thermal Energy Storage and	
	5.6.5	Fuel Cell Thermol Effluent	
	Canal	Fuel Cell Thermal Ellivent	
5./ E 0	Defer	usions	
D			
Degr Svste	adation	Analysis of SOFC for Various Syngas Compositions in IGFC	
6.1	Public	ation Highlights	
62	Ahstra	act	
6.3	Introd	luction	
6.4	SOFC	Model	
65	Test P	Procedure	
6.6	Result	ts and Discussion	
0.0	661	Composition Cradiants	
	0.0.1		
	662	Fuel Utilization	
	6.6.2	Fuel Cell Solid Temperature	
	6.6.2 6.6.3	Fuel Utilization Fuel Cell Solid Temperature	
	6.6.2 6.6.3 6.6.4	Fuel Utilization Fuel Cell Solid Temperature Nernst	
	6.6.2 6.6.3 6.6.4 6.6.5	Fuel Utilization Fuel Cell Solid Temperature Nernst Current Density Degradation Pate	
67	6.6.2 6.6.3 6.6.4 6.6.5 6.6.6	Fuel Utilization Fuel Cell Solid Temperature Nernst Current Density Degradation Rate	
6.7 6 8	6.6.2 6.6.3 6.6.4 6.6.5 6.6.6 Conclu	Fuel Utilization Fuel Cell Solid Temperature Nernst Current Density Degradation Rate Isions	
6.7 6.8	6.6.2 6.6.3 6.6.4 6.6.5 6.6.6 Conclu Refere	Fuel Utilization Fuel Cell Solid Temperature Nernst Current Density Degradation Rate usions	
6.7 6.8 Conc	6.6.2 6.6.3 6.6.4 6.6.5 6.6.6 Conclu Refere	Fuel Utilization Fuel Cell Solid Temperature Nernst Current Density Degradation Rate ences	
6.7 6.8 Conc 7.1	6.6.2 6.6.3 6.6.4 6.6.5 6.6.6 Conclu Refere	Fuel Utilization Fuel Cell Solid Temperature Nernst Current Density Degradation Rate usions	
6.7 6.8 Conc 7.1 7.2	6.6.2 6.6.3 6.6.4 6.6.5 6.6.6 Conclu Refere	Fuel Utilization Fuel Cell Solid Temperature Nernst Current Density Degradation Rate usions ences	

# LIST OF FIGURES

### Chapter 1:

Figure 3.5:

Chapter 1:	
Figure 1.1:	Basic configuration of an SOFC unit2
Figure 1.2:	Innovation of Brayton cycle to SOFC/GT hybrid systems4
Figure 1.3:	Bypass configuration in the SOFC/GT hybrid system5
Figure 1.4:	Hybrid test facility at NETL9
Chapter 2:	
Figure 2.1:	Flow diagram of the hardware-based hybrid test facility at NETL18
Figure 2.2:	Results of scoping studies (a) real response during the entire course of offline
	simulation (b) normalized plot for the first 10 second transient period20
Figure 2.3:	Transition in fuel heating values (LHV) between syngas to humidified methane
	of three different compositions20
Figure 2.4:	Block diagram of the load-based speed controller22
Figure 2.5:	Real-time dynamic response and estimated steady state profile23
Figure 2.6:	Dynamic profiles of thermal effluent, turbine speed and turbine load (a) The
	real response over 7,000 seconds, (b) normalized plot of (a), and (c) the real
	response over 1,050 seconds25
Figure 2.7:	Normalized profiles of thermal effluent, turbine speed, and turbine load over
	10 seconds after the step time25
Figure 2.8:	The effect of thermal effluent on turbine temperatures and SOFC cathode inlet
	temperature (a) the real response over 7,000 seconds, (b) the normalized plot
	of (a), and (c) normalized plot for the response over 1,050 seconds27
Figure 2.9:	Normalized plots of thermal effluent, turbine temperatures and SOFC cathode
	inlet temperature over the first 50 seconds28
Figure 2.10:	Turbine cycle efficiency
Figure 2.11:	The SOFC cathode inlet flow and the compressor intake air flow transients (a)
	the real response over 7,000 seconds (b) normalized plot of (a)30
Figure 2.12:	SOFC performance during fuel composition dynamics (a) the real response
-	over 7,000 seconds (b) normalized plot of (a)31
Chapter 3:	
Figure 3.1:	The recuperated SOFC/GT hybrid test facility at NETL [1]37
Figure 3.2:	Hardware-based simulations of SOFC/GT hybrid system40
Figure 3.3:	Load based speed control scheme [1]42
Figure 3.4:	Turbine speed and turbine load responses for open and closed loop
	configurations

ix

o nd (b)
45
7ersus 46
ressure ow, 47
ersus 48
en loop oop 48
n versus 49
56
58
steady zed 61
itial ues62
1 of local me 1 s, 63
lot, as uted 63
:, as uted 64
cal me 1 s, 65
oosition 50 s, 66

Figure 4.10:	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
Figure 4.11:	Local current density, (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.
Figure 4.12:	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
Figure 4.13:	Activation loss 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
Figure 4.14:	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
Figure 4.15:	Transient profile of diffusion loss, (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 change70
Figure 4.16:	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 change71
Figure 4.17:	Fuel cell cathode inlet conditions72
Figure 4.18:	Spatio-fuel cell temperature gradient, $dT/dx$
Figure 4.19:	Average solid temperature profile, (a) average solid temperature profile as a function of time, and (b) temporal changes of average solid temperature, $dTave/dt$
Figure 4.20:	Cathode gas temperature profiles, (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 change74
Figure 4.21:	Fuel cell heat generation, (a) a 3D mesh plot, as function of local position along the cell node and time, and (b) distributed profiles at time 1s, 250 s, 1,500 s, and 7,000 s after the step change
Figure 4.22:	The profile of solid-gas temperature difference $(Tsolid - Tgas)$ , (a) distributed temperature profile across the cell at different time, and (b) average temperature difference as function of time
Figure 4.23:	(a) Fuel cell model thermal effluent transient, (b) Dissipation of fuel cell thermal energy storage77
<b>Chapter 5:</b> Figure 5.1:	Basic flow diagram of a SOFC/GT hybrid system84

Figure 5.2:	Comparison of fuel cell solid temperature performance, (a) between the open loop and closed loop with 13.6% CH <sub>4</sub> content, and (b) between the open loop
	(13.6% CH <sub>4</sub> ) and the closed loop (14% CH <sub>4</sub> )86
Figure 5.3:	The layout of SOFC/GT testing facility at NETL
Figure 5.4:	Comparison of variations in turbine speed and cathode air mass flow for open loop and closed loop
Figure 5.5:	Fuel cell solid temperature as a function of time, (a) open loop (b) closed loop91
Figure 5.6:	Comparison of fuel cell solid temperature performance, between the open loop and the closed loop tests (a) distributed data as a function of time, and (b) the response of solid temperature difference at selected fuel cell nodes
Figure 5.7:	Cathode inlet temperature profiles for the open loop and closed loop systems using 13.6% $CH_4$ content and for the closed loop operation using 14% $CH_4$ content
Figure 5.8:	Spatial temperature gradient as a function of time, (a) open loop transient response (b) comparison of open loop and closed loop solid temperature gradients at critical nodes
Figure 5.9:	The difference in solid temperature gradient at critical nodes
Figure 5.10:	Fuel cell gas temperature as a function of time, (a) open loop transient response content (b) comparison of open loop and closed loop transients95
Figure 5.11:	Crossover points in fuel cell gas temperature difference between the open loop and the closed loop for selected local fuel cell positions
Figure 5.12:	Fuel cell solid-gas temperature difference as a function of time, (a) open loop transient response, (b) comparison of open loop and closed loop transients
Figure 5.13:	Heat flux of a fuel cell stack as a function of time, (a) open loop transient response, (b) comparison of open loop and closed loop transients97
Figure 5.14:	Normalized profiles of total heat flux in a fuel cell stack for open loop and closed loop, (a) over 5,500 s of test period, (b) over the first 200 s after fuel composition transition
Figure 5.15:	Fuel cell heat generation as a function of time, (a) open loop transient response (b) comparison of open loop and closed loop transients
Figure 5.16:	Methane mole fraction as a function of time, (a) open loop transient response (b) comparison of open loop and closed loop transients100
Figure 5.17:	Carbon monoxide mole fraction as a function of time, (a) open loop transient response (b) comparison of open loop and closed loop transients
Figure 5.18:	Carbon dioxide mole fraction as a function of time, (a) open loop transient response (b) comparison of open loop and closed loop transients
Figure 5.19:	Hydrogen mole fraction as a function of time, (a) open loop transient response (b) comparison of open loop and closed loop transients

Figure 5.20:	Water mole fraction as a function of time, (a) open loop transient response (b) comparison of open loop and closed loop transients
Figure 5.21:	Fuel utilization in open loop and closed loop cases
Figure 5.22:	Fuel cell current density as a function of time (a) open loop transient response
	(b) comparison of open loop and closed loop transients106
Figure 5.23:	Dissipation of fuel cell thermal energy storage and fuel cell thermal effluent
	and for the open loop and the closed loop tests107
Chapter 6:	
Figure 6.1:	Distributed profiles of CH <sub>4</sub> mole fraction for the five fuel compositions studied 
Figure 6.2:	Distributed profiles of CO mole fraction for the five fuel compositions studied
Figure 6.3:	Distributed profiles of $H_2$ mole fraction for the five fuel compositions studied
Figure 6.4:	Distributed profiles of CO <sub>2</sub> mole fraction for the five fuel compositions studied
Figure 6.5:	Distributed profiles of $H_2O$ mole fraction for the five fuel compositions studied
Figure 6.6:	Distributed data of fuel utilization for the five fuel compositions studied
Figure 6.7:	Distributed data of fuel cell solid temperature for the five fuel compositions
	studied121
Figure 6.8:	Distributed data of fuel cell solid temperature gradient, dT/dx for the five fuel compositions studied
Figure 6.9:	Distributed data of Nernst potential for the five fuel compositions studied
Figure 6.10:	Distributed data of current density for the five fuel compositions studied
Figure 6.11:	Distributed data of degradation rate impacts for the five fuel compositions studied

# LIST OF TABLES

Chapter 2:			
Table 2.1: SOFC operating conditions and parameters			
Cable 2.2: Coal-derived syngas and humidified methane compositions on mole basis			
Chapter 3:			
Table 3.1: SOFC parameters and initial operating conditions40			
Table 3.2: Coal-derived syngas and humidified methane compositions			
Table 3.3: Summary of open loop and closed loop transient response			
Chapter 4:			
Table 4.1: Inlet conditions for fuel cell cathode and anode streams			
Table 4.2: Specification of SOFC system parameters			
Chapter 5:			
Table 5.1: SOFC parameters and initial operating conditions      89			
Chapter 6:			
Table 6.1: Fuel compositions studied for SOFC systems (mole %)			
Table 6.2: Fuel cell stack inputs for different fuel compositions			
Table 6.3: Average fuel cell solid temperature 122			
Table 6.4: The maximum and overall degradation rate			

# LIST OF ABBREVIATIONS AND SYMBOLS

Abrreviations:	
1D	One dimensional
act	Activation
APU	Auxiliary power unit
BGL	British Gas Lurgi
dif	Diffusion
DC	Direct current
DOE	Department of Energy
GT	Gas turbine
HiLS	Hardwar e-in the loop-simulations
IEA	International Energy Agency
IGFC	Integrated gasification fuel cell
LHV	Low heating value
NETL	National Energy Technology Laboratory
ohm	Ohmic
PEMFCs	Proton exchange membrane fuel cells
PID	Proportional-Integral-Derivative (controller)
TET	Turbine exhaust temperature
TIT	Turbine inlet temperature
TPB	Triple phase boundary
SECA	The Solid State Energy Conversion Alliance
shift	Water-gas shift
SMR	Steam methane reforming
SOFC	Solid oxide fuel cell
SOFC/GT	Solid oxide fuel cell gas turbine hybrid technologies
WGS	Water-gas shift

### Symbols:

Areact	Area of reaction, m <sup>2</sup>
F	Faraday's constant, C/mol
FU	Fuel utilization
i	Current density, A/cm <sup>2</sup>
i <sub>0</sub>	Exchange current density, A/cm <sup>2</sup>
j	Node number
n	Number of electrons transfer per reaction
$K_p$	Equilibrium constant
Т	Temperature, K
р	Partial pressure, atm
Q	Model predicted fuel cell thermal effluent, kW
R	Area specific resistance, $\Omega$ -m $^2$
$r_d$	Degradation rate, %/1000hr
r <sub>sr</sub>	Reformed methane rate [mol/s]

$R_u$	Ideal gas constant, J/mol-K
α	Charge transfer coefficient
η	Turbine cycle efficiency, ratio (Chapter 2)
dT/dx	Temperature gradient between fuel cell nodes, K/cm
$dT_{ave}/dt$	Temporal changes of average solid temperature, K/s
$T_{solid} - T_{aas}$	Solid-gas temperature difference, °C
V	Voltage, V
V <sub>Nernst</sub>	Nernst potential, V
Δ	Variation
$\Delta G_{H_2O}$	Standard Gibbs free energy, kJ
$\Delta H^{\circ}$	Heat of reaction at a reference condition, kJ/mol
$\Delta H_1 \text{ or } \Delta H_2$	Sensible heat, kW
X	Mole fraction
η	Electrochemical loss, V (Chapter 6)

### **DECLARATION OF ACADEMIC ACHIEVEMENT**

The majority of the work described in this thesis, including experimental design and execution, data collection and analysis, as well as thesis writing, were completed by the author of this thesis, with the following exceptions.

- In general, I had help from the U.S. Department of Energy, National Energy Technology Laboratory (NETL) - a research scientist, Dr. David Tucker, a post graduate researcher/control engineer, Dr. Paolo Pezzini, a visiting scholar, Dr. Nana Zhou (University of Chongqing), and a PhD candidate, Valentina Zaccaria (University of Genoa), a project technician, Dave Ruehl, to execute all the tests. Each test required at least three authorized operators (including myself), due to the complexity of the system and experimental works presented herein. The control strategies used during the test were primarily developed by Dr. Paolo Pezzini and Dr. David Tucker. The integration of the fuel cell dynamic model (software) with hardware part of the system through an interface platform was also accomplished by the author, with some help from Dr. Paolo Pezzini.
- **Chapter 2:** Dr. David Tucker was responsible to guide the experimental design and data analysis since he was the principle investigator of the hybrid test facility at NETL. Dr. Thomas A. Adams II helped to determine the direction of the case study, assisted in the preparation of manuscript, editing and organizing the final version.
- **Chapter 3:** Both Dr. Thomas A. Adams II and Dr. David Tucker helped to finalize the content of the manuscript.
- **Chapter 4:** Dr. David Tucker assisted with data analysis and interpretation, as well as editing and preparation/submission of the manuscript. Meanwhile, Dr. Thomas A. Adams II provided helps in the preparation/revision process of the first draft to strengthen the content of the manuscript.
- **Chapter 5:** Dr. David Tucker provided support for the analysis of system identification. Both Dr Thomas A. Adams II and Dr. David Tucker assisted in the editing and preparation of the manuscript.
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# **1** INTRODUCTION

### 1.1 Emerging Solid Oxide Fuel Cell Technologies Toward Energy Sustainability

The most critical issues associated with power generation today are related to improvement of system efficiency and environmental impacts. Since electricity generation are primarily based on fossil fuel combustion, mostly coal and natural gas electricity generation was claimed as the largest contributor of sulfur compounds and noxious emissions, leading to global warming and pollutions [1, 2]. Yet, with the existing energy infrastructures, fossil based energy systems are unquestionably important and more reliable for heat production for almost all applications including commercial, residential, industries, and transportation [2, 3].

Today, the reliability on clean, efficient, and environmental-friendly energy technologies grows significantly with increasing energy demand and the need for a transition to low-emission and low-carbon world. To address the issues of global climate change and gas emission management, there are a lot of ongoing efforts, involving innovation of the current energy infrastructures or development of new advanced energy systems that are more sustainable [4]. The 'future' energy systems should be able to provide long-terms benefits to society in terms of addressing energy needs, including heat, electricity, and cooling for economic growth, as well as addressing vital requirements for safety, health, and environment.

One such alternative to traditional power generation systems that has the potential to fulfil environmental and economic critical needs is solid oxide fuel cell (SOFC) technology [5, 6]. Solid oxide fuel cells create DC power and heat from direct conversion of chemical energy of a fuel gas via electrochemical reactions (i.e. fuel oxidation) with low noise and vibration. As compared to other fuel cell technologies, such as the proton exchange membrane fuel cells (PEMFCs) that require relatively pure hydrogen and operate at a temperature of below 90 °C, SOFCs operate at higher operating temperature, approximately between 600 °C to 1000 °C. The high operating temperature of SOFCs is mutually beneficial for other power generation technologies, such that SOFCs can be integrated into the current

energy infrastructure such as gas turbines, gasifiers, etc. [7]. In addition, SOFCs are also resistant to CO poisoning. Thus, SOFCs can use various type of fuels including carbon monoxide and hydrocarbon, which can be coal-derived syngas, biomass, natural gas, methanol, and diesel to produce electricity [7, 8]. This increases the flexibility in the choice of fuels. Since no mechanical motion is involved, and potential for greater system flexibilities exist, SOFCs have received considerable attention in wide applications, ranging from stationary power generation (centralized power generation and distributed power generation) to transportation (auxiliary power unit for vehicles) at flexible module sizes [5, 6, 9].

The working principles of SOFCs are similar to batteries but SOFCs can continuously generate electricity if fuel and oxidant (i.e. air or oxygen) are constantly supplied to the system. The basic configuration of planar SOFCs is shown in Figure 1.1. An SOFC unit is generally fabricated with three main layers of solid structures called the anode, ion conducting electrolyte, and cathode. On top of that, there are channels constructed in an SOFC subsystem to deliver fuels and oxidant along the fuel cell length. The anode channels are used for fuel transportation, whereas cathode channels are for oxidant flow [10].



Figure 1.1: Basic configuration of an SOFC unit

During SOFC operations, oxygen anions,  $O^{=}$  generated from the reaction between oxygen and electrons (Eq. 1), travel from the cathode interface through the electrolyte to the anode interface, at which oxygen ions will be consumed to oxidize fuels. Hydrogen oxidation (Eq. 2) takes place in SOFCs, producing heat, electricity, and waste gases H<sub>2</sub>O and CO<sub>2</sub>, depending on the fuel types [10]. For example, steam methane reforming described in Eq. 3

may occur in the high operating temperature SOFCs if methane or methane-content gas is used. With the presence of CO and  $H_2O$  in the system, the formation of  $H_2$  can also be promoted through water-gas shift equilibrium shown in Eq. 4, resulting in the production of waste gas  $CO_2$  from the anode channel.

Oxygen reduction (cathode side):  $1/2 O_2 + 2e^- \rightarrow O^=$  (1)

Hydrogen oxidation (anode side):  $H_2 + 0^= \rightarrow H_2 0 + e^- (\Delta H^\circ = -286 \, kJ/mol)$  (2)

Steam methane reforming:

 $CH_4 + H_2 0 \rightleftharpoons 3H_2 + CO \quad (\Delta H^\circ = 206 \ kJ/mol) \tag{3}$ 

Water-gas shifting:

 $CO + H_2 O \rightleftharpoons H_2 + CO_2 \quad (\Delta H^\circ = -41 \, kJ/mol)$  (4)

The Nernst potential for SOFCs is based on an expression shown in Eq. 5, assuming direct electrochemical oxidation of carbon species is negligible compared to hydrogen oxidation and the reforming and shifting of hydrocarbon fuels at the anode. This function reveals that the maximum voltage of fuel cells is correlated to temperature, as well as the partial pressure of  $H_2$  and  $H_2O$  in the anode and  $O_2$  in the cathode. However, the actual cell voltage is calculated by subtracting cell polarization losses from the Nernst. In Eq. 5, the net value of the first term, which consists of the Gibbs free energy of water at the standard condition, is a positive value. Meanwhile, the net value of the second term, as a function of temperature and component partial pressure is usually a negative value, especially if operating the system in excess water condition. In this case, there is an inverse effect of fuel cell temperature on the Nernst potential.

Nernst potential:

$$V_{Nernst} = -\frac{\Delta G_{H_2O}^{\circ}}{2F} + \frac{R_u T}{2F} ln \left[ \frac{p_{H_2} \cdot p_{O_2}^{0.5}}{p_{H_2O}} \right]$$
(5)

Although Eq. 5 indicates that Nernst potential may reduce with the increase in fuel cell temperature for certain conditions, operating SOFCs at high temperature provides some advantages over the polarization losses, particularly ohmic losses, which reduces with increasing temperature. Operating SOFCs at high temperature also generate high quality of waste heat from its exhaust stream that contains significant amount of energy from some unutilized combustible fuel. However, optimal temperature and fuel utilization must be chosen according the fuel cell fabrication and materials of construction. Technically, it is difficult to operate high temperature SOFCs at high fuel utilization (above 90%) since this can lead to accelerated degradation rate of the fuel cell systems [11]. Unexpected metal oxidation may occur in fuel starvation states, which consequently cause material failure. Delaminating and cracking due to nickel oxidation at the anode side, as well as chromium

deposition and microstructural changes are the potential issues that can inhibit efficient SOFC operations [6, 10, 12].

Considering the material problems with the existing SOFC technologies, the Solid State Energy Conversion Alliance (SECA) program in the United States takes a lead in the development of commercially relevant and robust SOFC systems, with a goal of reducing stack costs, increasing cell efficiency, and increase cell longevity. The undergoing research broadly focuses on degradation process of anode/electrolyte/cathode components, cathode materials and microstructural engineering, catalytic fuel reforming, and many others [8].

# 1.2 Role of Solid Oxide Fuel Cell Gas Turbine Hybrid in Meeting Future Energy Needs

Solid oxide fuel cell gas turbine (SOFC/GT) hybrid systems have been discovered as a promising alternative energy technology to standalone SOFC systems as well as conventional power generation technologies. SOFC/GT hybrid systems offer remarkable potentials that are cost competitive with existing combined cycle energy systems and enhanced efficiency up to 75% LHV on natural gas, or 60% HHV of coal, with minimal emissions [6, 9, 13-15]. Integration of a high temperature SOFC with a gas turbine engine in a recuperated cycle shown in Figure 1.2 is one of the most common hybrid approaches [16, 17]. As configured in Figure 1.2, this hybrid technology is based on a direct thermal coupling scheme, utilizing the net thermal effluent from an SOFC subsystem for additional power generation from a gas turbine to supplement SOFC power. Thus, the system allows for an increase in total system efficiency [9, 13, 14]. The net thermal effluent of an SOFC includes thermal energy of by-product heat generation of an operating SOFC, plus the heat released from the oxidation of SOFC anode off-gas. With this feature, SOFC/GT hybrid systems do not require any combustion in the gas turbine itself.



Figure 1.2: Innovation of recuperated cycle to SOFC/GT hybrid systems

An important aspect of SOFC/GT is the synergistic integration benefits of fuel cells and gas turbines that inherently enhance system reliability and operability. From the design standpoint, this system permits pressurized fuel cell operations in which the compressed air from compressor discharge is channelled to the cathode side of an SOFC fuel subsystem through recuperation of gas turbine exhaust. Operating SOFC systems under pressure offers an improvement in fuel cell efficiency with regard to enhancement of Nernst potential [10, 18]. The preheating of fuel cell cathode air flow will further improve the efficiency of the entire cycle [13, 14].

In the hybrid configuration, high cathode cooling air flow is granted by gas turbine operation without reduction in efficiency, providing means for better fuel cell thermal management [19]. It has been shown that modulation of cathode air flow into SOFC subsystems is critical for fuel cell temperature controls [20, 21]. Small transient changes in cathode air flow can significantly affect the performance of SOFC/GT hybrid systems [22]. Cathode air flow management in SOFC/GT hybrid system can be practically realized using bypass valves. With certain control strategies via bypass modulation, it is also possible for the hybrid system to have turndown rate up to 93%, allowing for load following operations [19, 23]. An example of the SOFC/GT hybrid system with bypass valves is shown in Figure 1.3.



Cold air bypass



Considering the limitation of high fuel utilization in SOFC systems, hybridizing an SOFC and a gas turbine as a bottoming cycle provides solutions to work around this problem. Prior work has shown that the total efficiency of SOFC/GT hybrid was insensitive to fuel utilization (FU) in a range between a 57% to an 85% FU [24]. Interestingly, this implied that it is feasible for the hybrid systems to run at a lower fuel utilization (i.e. by increasing fuel flow) than in the standalone configuration without efficiency penalties in system performance. Since the resulting unspent fuel from an operating SOFC subsystem in SOFC/GT hybrid is eventually used by the gas turbine to power compressor for cathode air supply and cathode air preheating, the final total system efficiency can be maintained at

higher level. Undoubtedly, operating at a lower fuel utilization reduces taxing operating conditions in the SOFC subsystem, which potentially extend the fuel cell lifetime [25]. Furthermore, anode recycle, which is usually employed in SOFC systems to boost the efficiency at low fuel utilization operations, is not necessarily required in SOFC/GT hybrid systems. This leads to less problematic issues in controlling the effects of composition gradients on SOFC performance.

### 1.3 Research Motivation: Potential and Challenges in Solid Oxide Fuel Cell Gas Turbine (SOFC/GT) Hybrid Systems for Fuel Flexible Operations

Mostly, hydrogen can be fed directly to fuel cell systems in which the highest ideal fuel cell potential can be achieved with dry/pure hydrogen. In fact, hydrogen is not readily available to be an ideal fuel for future power conversion systems due to generation and handling issues associated with storage and distribution [26]. However, high temperature fuel cells, including SOFCs relax the dependency on hydrogen as the main fuel, expanding the number of potential fuels that can be used [10, 27]. The elevated temperature allows the system to perform direct internal conversion of hydrocarbon to hydrogen via reactions of CO and  $CH_4$  with  $H_2O$ , respectively in water-gas shift and steam reforming [10].

With the aforementioned features, the potential of SOFC/GT can be further improved through advanced integration cycles with different fuel processing infrastructures. Depending on applications, SOFC/GT hybrid cycles can be integrated to coal gasifiers, biomass gasifiers, and fuel reformers, etc. for fuel supply in larger system operations [16, 28, 29]. But direct utilization of natural gas in SOFC/GT is also possible [30]. However, almost all of fuel coupling schemes are technically susceptible to significant composition fluctuations as a consequence of changes in feedstock quality, operating conditions, or even the fuel processing technologies [31]. This consequently imposes significant perturbations on SOFC systems. As such, the ability of SOFCs to run in fuel flexible environments is beneficial to handle variability in fuel compositions, minimizing the detrimental transient impacts on the system performance and life.

Furthermore, the advantage of SOFC fuel flexibilities can also be capitalized on a power generation plant to take advantage of current economic conditions as well as to meet new environmental restrictions placed. Carbon tax, price of fuels and electricity may require a significant shift in the fuel compositions and/or fuel types used, such that, it could improve the economic viability of the plant [29]. For example, a shift from an initial operation utilizing coal-derived syngas to natural gas is more profitable if the prices of natural gas drops and/or new carbon tax increases.

Another example of potential SOFC/GT applications as the power conversion system is in flexible polygeneration systems, which co-produce electricity with fuels or chemicals [28, 31]. In this polygeneration system, an SOFC/GT hybrid system is coupled with chemicals or fuel production sections, with a goal of maximizing efficiency and plant profit, corresponding to monthly or daily fluctuations in energy prices. More electricity and less fuel are produced during the day when the prices of power prices are high, and the reversed mixture of polygeneration products is produced at night when the power prices are low. To fulfil the production target, significant changes in fuel feed conditions with regard to flow rate, composition, and heating value must be performed to modify the product envelope. In

the worst case, supplementing natural gas as an auxiliary fuel feed to electricity generation subsection might be beneficial in the polygeneration plant when there is maximum utilization of syngas in chemicals or fuel production subsection. These cases demonstrate a critical need for sufficient transient capabilities in SOFC/GT hybrid sections.

Due to high coupling between the fuel cell and other system components, such as a gas turbine and fuel processor, transitioning fuel compositions or fuel types in SOFC subsystem might be very challenging. Since each of the system components has different nonlinear behaviours, effective control architectures must be developed and proven to address potential technical challenges in dynamic operation modes of SOFC/GT hybrid systems. Prior works have shown that there are three major dynamic issues and operational sensitivities associated to the hybrid system.

- Fuel cell thermal management: Small transient changes in cathode air mass flow can cause dramatic effects on the hybrid system performance, leading to problematic fuel cell thermal gradients across the fuel cell length [22]. In turn, changes in cathode mass flow in the hybrid configuration are strongly coupled the speed of turbine shaft and compressor dynamics [21, 32]. The impacts of flow perturbations resulting from turbomachinery dynamics is more significant than the impacts of temperature fluctuations [14]. It is believed that managing cathode air flow during transient events is critical to avoid over-cooling or over-heating the fuel cell stacks.
- **Compressor stall and surge**: Sudden reduction in fuel/thermal input going into gas turbine and introduction of pressure losses between compressor and gas turbine in the hybrid configuration can lead to decrease in compressor surge margin. This subsequently results in compressor stall and surge. Such transient events put the hybrid system at the highest risk of turbine damage because of instability in the dynamics of turbomachinery [33]. The transients of compressor stall and surge can occur very quickly, just within a few seconds. Ultimately, this event can result in catastrophic failure of the fuel cell due to intolerable pressure difference between anode and cathode streams. Turbine damages due to compressor stall and surge during fuel cell hybrid operations have been discovered through the experience of NETL researchers.
- Fuel cell degradation: Degradation mechanisms, such as oxidation of anode material and microstructural changes in fuel cell systems can be accelerated by carbon deposition, high fuel utilization and current density, high anode-cathode pressure difference, etc. This eventually inhibits efficient working performance of the fuel cells as well as reduces the fuel cell lifetime. However, to make the system economically viable, certain control strategies must be developed to mitigate the degradation impacts.

### 1.4 Problem Statement

The tightly interactive effects between each component in SOFC/GT hybrid configuration during transient events always leads to complicated dynamic operability that requires problematic control development. But, it is important to have good control schemes for improvement of transient capabilities and operating flexibilities, rejecting any system disturbance associated with rapid cycling changes that ultimately modify system pressure, mass flow, and pressure in the system. However, if dynamic controls are to be developed to take advantage of the extensive operating envelope offered by SOFC/GT hybrids, detailed system identification is required to adequately develop understanding about dynamic coupling interactions between system components in hybrid configuration, especially the fuel cell, gas turbine, compressor and heat exchangers.

Motivated by the previously mentioned advantages and challenges in SOFC/GT systems, this project investigates transient behaviours of SOFC/GT hybrid cycle with regard to its potential for fuel flexibilities. This study focuses on detailed analyses of SOFC/GT system performance during fuel composition transients. In general, there are a few research questions that are addressed in this study regarding:

- impacts of fuel composition dynamics on the fuel cell and the balance of the plant
- flexibility of the SOFC/GT hybrids to deal with fuel composition variations
- associated operability limitations and technical issues during operations
- potential control strategies that could be implemented to mitigate any negative impacts on the system before catastrophic failure takes place (i.e. due to the compressor and turbine stall and surge as well as fuel cell damage due to material starvation and thermal stress).

SOFC/GT hybrids are complex systems. Real responses due to process perturbations cannot be accurately estimated, and in fact, the ability to prevent failures under real conditions cannot be predicted by simulation only. To the best of our knowledge, almost all existing studies to date focused on steady state operations, with very limited experimental data and/or validated simulation works. Therefore, in this project, the response of SOFC/GT hybrid systems to fuel composition transients was experimentally investigated using hardware-based simulations in real-time. A hybrid test facility of a recuperated fuel cell gas turbine system developed by the U.S department of Energy, National Energy Technology Laboratory (NETL) shown in Figure 1.4 was used. This system incorporated actual equipment of direct-fired recuperated gas turbine and simulated fuel cell subsystem, reducing the drawbacks of potentially large inaccuracies in fully simulation approaches of highly integrated energy system.

### 1.5 Research Objective

With the aim of characterizing the SOFC/GT system performance under fuel composition changes, a step change from coal-derived syngas composition to methane-rich gas composition was implemented, representing the worst and most extreme case study of

fuel composition transitions. Details of the research objectives for this study are listed as following:

- a. To determine the operational boundaries of fuel composition changes that could be used without violating the allowable thermal gradient and/or causing carbon deposition in the fuel cell, and causing stalls/surge in the turbomachinery
- b. To investigate the correlation among the key process variables in the fuel cell subsystem and turbomachinery section during fuel composition transition
- c. To evaluate the coupling impacts of fuel cell dynamic performance on the balance of the plant (the recuperated gas turbine cycle)
- d. To clarify the linking events existing in the SOFC/GT hybrid systems that might mitigate or propagate the effects of fuel composition changes on the hybrid system
- e. To identify potential opportunities for dynamic controls of SOFC/GT hybrid systems during fuel composition changes.



Figure 1.4: Hybrid test facility at NETL

### 1.6 Thesis Outline

This thesis is structured based on 7 chapters, led by the *Introduction* in **Chapter 1**, and ending with *Conclusions* in **Chapter 7**. Main contents of the thesis are organized as the following:

# • **Chapter 2**. Fuel Composition Transients in Fuel Cell Turbine Hybrid for Polygeneration Applications:

This chapter presents exploration of dynamic issues associated with fuel composition changes in the case of a transition from coal-derived syngas to humidified methane. Prior to the real experimental works, preliminary tests were required to identify the operational boundaries of fuel compositional changes that could be used without violating the allowable thermal gradient and/or causing carbon deposition in the fuel cell, and causing stalls/surge in the turbomachinery. The step-by-step approach taken to identify the operational restrictions was

explained herein. In favour of simplicity, the hardware-based simulations carried out at this stage were in closed loop mode. As such, the closed loop performance provided valuable insights of relationships among the key process variables in a base condition with very minimal disturbances and risks of system failure. The subsequent impacts of the fuel cell dynamic performance (driven by fuel composition changes) on gas turbine cycle was evaluated thoroughly.

• **Chapter 3**. Open Loop and Closed Loop Performance of Solid Oxide Fuel Cell Turbine Hybrid Systems during Fuel Composition Changes:

This stage attempted to study a different step change in fuel composition, as well as to quantify the difference between open loop and closed loop system performance using the existing control approach. However, the focus up to this point was the investigation of the coupling effects between the fuel cell behaviours and the gas turbine cycle as a result of the step change in fuel composition. The limits for open loop tests were identified, such that the demonstration test could be done safely. A comparison between open loop and closed loop system performance was investigated and the interactions among fuel cell process variables were characterized carefully. The results were discussed in terms of mitigating/propagating influences and the control effects of the case of closed loop test. Therefore, it offered some insight into the real dynamic trajectory of the process variables, and its significance to the system as the result of fuel composition perturbations. This finding is generally not known because dynamic studies of SOFC operations are rare. Hence, this discovery was quite useful for identifying the operational boundaries, which can then lead to better control systems.

 Chapter 4. Fuel Composition Transition Impacts on Dynamic Performance of Fuel Cells in SOFC/GT Hybrid Systems:

As an extension from the investigation presented in Chapter 2, this section primarily focuses on dynamic characterization of fuel cell parameters. The fuel cell parameters discussed in this chapter were related to dynamic 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. The detailed dynamic trajectories of each key fuel cell variables were evaluated thoroughly to quantify their contributions to operability and controllability of the hybrid system. The analyses were based on distributed profiles across the fuel cell length resulted from the closed loop operation.

 Chapter 5. Coupling Effects of Fuel Composition Transition and Cathode Air Mass Flow on Dynamic Performance of SOFC/GT Hybrid Systems:

Chapter 5 is dedicated to a more serious discussion on the dynamic performance of SOFC/GT hybrid systems, leading to system identification of this technology during fuel composition transients. Similarly, the finding obtained in Chapter 3 was

expanded and presented herein. This chapter particularly emphasizes the characterization of linking dynamic events associated with fuel composition changes (i.e. cathode air mass flow variations). Comparison of the open loop dynamic performance and closed loop performance for the important fuel cell parameters was carried out to determine the integration issues that could affect the dynamic performance of SOFC/GT hybrid system as well as to identify potential opportunities for dynamic controls of SOFC/GT hybrid systems during fuel composition changes.

• **Chapter 6**. Degradation Analysis of SOFC for Various Syngas Compositions in IGFC Systems:

This section presents the impacts of fuel composition on fuel cell degradation rate, which was based on various coal-derived syngas resulting from different gasifier technologies. All of the syngas compositions used in this study contained a different level of methane content. The degradation rate was evaluated using the empirical expression, indicating a correlation to three key fuel cell operating parameters; current density, fuel utilization and cell temperature. The performance of fuel cell for each fuel composition was explained and compared to the case of humidified hydrogen to determine their influence on the degradation rate.

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### Impacts of fuel composition changes on SOFC/GT lifetime

For fuel cell degradation studies, there is quite a number of directions that could be further investigated. First, the impacts of switching between syngas and humidified methane or between other sets of compositions on fuel cell degradation rate could be evaluated using hardware-based simulations. The analysis might include detailed economic assessment involving system efficiency and fuel cell lifetime. Development of real-time fuel cell models with degradation rate expressions and incorporation of such dynamic models into the hardware-based simulation are needed to accomplish this goal. Second, degradation studies could also be oriented toward management of fuel cell degradation, which might involve quantification of potential control strategies. Different control configurations could be developed and tested to verify the effectiveness and robustness for fuel cell degradation controls.

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