AN INVESTIGATION TO RESOLVE THE INTERACTION BETWEEN FUEL CELL, POWER CONDITIONING SYSTEM AND APPLICATION LOADS

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CONTENTS

1. LIST OF FIGURES ............................................................................................................................................. 5
2. LIST OF TABLES .................................................................................................................................................. 10
3. INTRODUCTION ............................................................................................................................................... 11
4. EXECUTIVE SUMMARY ................................................................................................................................... 15
5. MODELING, ANALYSIS AND EXPERIMENTAL VALIDATIONS ........................................................................ 20
   5.1 COMPONENT AND SYSTEM MODELING ............................................................................................................... 20
      5.1.1 SOFC Stack Subsystem (SOFCSS) Model ........................................................................................................ 21
      5.1.1.1 TSOFC Model ............................................................................................................................................. 22
      5.1.1.2 PSOF Model ............................................................................................................................................... 33
      5.1.2 PES Model ...................................................................................................................................................... 39
         5.1.2.1 Environment for PES Model Development ............................................................................................ 42
         5.1.2.2 PES Topologies ....................................................................................................................................... 43
      5.1.3 BOPS Modeling .......................................................................................................................................... 47
         5.1.3.1 Fuel Processing Subsystem (FPS) .............................................................................................................. 49
         5.1.3.2 Thermal Management Subsystem (TMS) and Work Recovery and Air Supply Subsystem (WRAS) ........... 49
         5.1.3.3 BOPS Model Description ........................................................................................................................ 50
         5.1.3.4 Reduced Order Model ........................................................................................................................... 55
      5.1.4 Comprehensive System Modeling .............................................................................................................. 60
         5.1.4.1 Comprehensive System Model and Methodology on Multi-software Platform ........................................ 60
         5.1.4.2 Low-cost System Modeling Framework ................................................................................................. 62
         5.1.4.3 Modeling Approaches to Resolve Effect of Multiple Time Scales ............................................................ 63
      5.2 SYSTEM-INTERACTION ANALYSIS ........................................................................................................... 67
      5.2.1 Effects of PES and AL on SOFC Stack .......................................................................................................... 67
         5.2.1.1 Effects of AL .......................................................................................................................................... 68
         5.2.1.2 Effects of PES ....................................................................................................................................... 80
      5.2.2 Experimental Work ....................................................................................................................................... 82
         5.2.2.1 Experimental Prototype Design of the Ripple Eliminating PES ................................................................. 82
            5.2.2.1.1 Zero-ripple Boost Converter (ZRBC) ................................................................................................. 82
            5.2.2.1.2 High Frequency (HF) Inverter ............................................................................................................. 84
            5.2.2.1.3 AC-AC Converter ............................................................................................................................. 85
         5.2.2.2 Experimental Stack Prototype .................................................................................................................. 91
            5.2.2.2.1 Stack Construction ........................................................................................................................... 91
         5.2.2.3 Validation of PES Feedbacks on PSOFCS ................................................................................................. 93
            5.2.2.3.1 Characterization of the PSOFCS Stack .............................................................................................. 95
            5.2.2.3.2 Study of Load Transient ............................................................................................................... 95
            5.2.2.3.3 Low-frequency Ripple Study ......................................................................................................... 95
            5.2.2.3.4 Stack Impedance Measurement ...................................................................................................... 95
         5.2.2.4 Long-term Degradation Study ................................................................................................................ 97
            5.2.2.4.1 Long-term Effect of Ripple ........................................................................................................... 97
            5.2.2.4.2 Long-term Effect of Load-transient ............................................................................................... 97
      5.3 CONTROL DESIGN AND PARAMETRIC OPTIMIZATION .............................................................. 99
         5.3.1 Design of Power Management Control ................................................................................................. 100
            5.3.1.1 Control Objectives ............................................................................................................................. 101
            5.3.1.2 Control Architecture ........................................................................................................................... 102
            5.3.1.3 Proposed Topology .................................................................................................................................. 102
         5.3.2 BOPS Control Design .............................................................................................................................. 106
            5.3.2.1 Control Objectives ............................................................................................................................. 106
            5.3.2.2 Control Parameters and Control-variable Set Definitions ....................................................................... 107
            5.3.2.3 Fuel and Energy Buffering .................................................................................................................... 107
            5.3.2.4 Control Laws and Strategies ................................................................................................................. 108
         5.3.3 Parametric Optimization of BOPS .......................................................................................................... 111
            5.3.3.1 System-level Dynamic Synthesis/Design Optimization Problem Definition .................................... 111
            5.3.3.2 Decomposition and Coupling Function Definitions ............................................................................. 114
6. RESULTS AND DISCUSSION

6.1 Validation Result of Electrical Feedback Effects ................................................................. 122
   6.1.1 Validation of Stack Characteristics .................................................................................. 122
   6.1.2 Validation of Load Transients ......................................................................................... 122
   6.1.3 Validation of the Ripple Effect ....................................................................................... 124
6.2 Analysis of Stack Degradation Result ................................................................................. 125
6.3 Parametric Study of the Effect of Electrical-feedbacks ......................................................... 127
   6.3.1 Effects of Load-transients ............................................................................................... 127
   6.3.2 Effects of Load Power Factor ....................................................................................... 132
   6.3.3 Effects of Load Harmonics ......................................................................................... 133
   6.3.4 Effects of Ripple ......................................................................................................... 135
6.4 Power Management Control Results ................................................................................. 136
6.5 Optimization and Control of BOPS .................................................................................... 140
   6.5.1 Cost Optimization Results ............................................................................................ 142
   6.5.2 Start-up Results ........................................................................................................... 145
   6.5.3 System Dynamic Response ......................................................................................... 149
   6.5.4 System Efficiency ....................................................................................................... 158
   6.5.5 Design Variable Effects on System Dynamics and Operational Costs ......................... 160
6.6 Experimental Result of the Novel PES Prototype ................................................................. 163
   6.6.1 Performance of ZRBC .................................................................................................. 163
   6.6.2 Performance of the DC-AC Converter ......................................................................... 164

7. CONCLUSIONS ......................................................................................................................... 170

8. LIST OF ACRONYMS ............................................................................................................. 174

REFERENCES ............................................................................................................................. 175

APPENDICES ............................................................................................................................. 179

A. PES MODELS ......................................................................................................................... 179
   A.1 PES SIMULINK AND SIMPOWERSYSTEMS SCHEMATIC MODELS ............................................ 179
   A.2 FLOW CHART OF THE MULTI-CONVERTER CONTROL FOR POWER MANAGEMENT SYSTEM ................ 183
B. BOPS MODEL CODES ............................................................................................................ 186
   B.1 Main Processing Routine .................................................................................................. 186
   B.2 Modeling the Master Interface ......................................................................................... 190
   B.3 Modeling the Master Model ........................................................................................... 192
   B.4 Modeling the Methane Reformer ................................................................................... 203
   B.5 Modeling the Compact Heat Exchanger ......................................................................... 211
   B.6 Modeling the Reformer Mixer ........................................................................................ 214
   B.7 Modeling the Combustion Mixer .................................................................................... 215
   B.8 Modeling the Combustion Chamber .............................................................................. 217
   B.9 Modeling the Compound Alternator ............................................................................. 219
C. PLANAR SOFC MODELING .................................................................................................. 222
   C.1 One Dimensional Model ................................................................................................ 222
   C.2 Two Dimensional Model ............................................................................................... 229
1. LIST OF FIGURES

Fig. 5.1.1  Block diagram of a SOFC PCS block diagram showing the SOFCs, the PES, and the BOPS. 20
Fig. 5.1.2  Axial division of TSOFC. 22
Fig. 5.1.3  a) Validation of model at 3 atm pressure. 24
b) Validation of model at 15 atm pressure. 24
Fig. 5.1.4  Illustration of fuel stream transient dynamics. 25
Fig. 5.1.5  Individual fuel element locations at the time of the electrical change (Lagrangian approach). 25
Fig. 5.1.6  Correlation between temporal and spatial discretizations. 26
Fig. 5.1.7  a) Variation of current with dimensionless time. 27
b) Variation of power with dimensionless time. 27
Fig. 5.1.8  Axial profiles of hydrogen partial pressure as functions of time. 28
Fig. 5.1.9  Increase in fuel utilization during electrical transient episode. 29
Fig. 5.1.10 Current and fuel utilization transients during transient episode. 30
Fig. 5.1.11 Illustration of SWPC TSOFC response to a galvanostatic control. 31
Fig. 5.1.12 Duality of cell potential drop due to polarization curve and fuel depletion effects. 32
Fig. 5.1.13 Impact of initial fuel utilization upon fractional voltage drop due to “polarization curve” effect. 32
Fig. 5.1.14 One-dimensional homogenous slab model for PSOFC providing discretizations involving finite-
difference method. Temperature, current, and molar-flow rates of air and fuel are calculated
each time for n = 1, ..., N. 33
Fig. 5.1.15 Temperature profile of the 1-D discrete model. 35
Fig. 5.1.16 Spatial homogenous model for the PSOFC providing two-dimensional discretizations involving
finite-difference method. 36
Fig. 5.1.17  a) Spatial temperature profiles for 1D and 2D models 39
b) Current flux outputs for 1D and 2D fuel cell models 39
Fig. 5.1.18 Architecture of a typical PES for the residential PCS. 41
Fig. 5.1.19 The four topologies used for studying the impact of power-electronics on the SOFC stack, (a) represents line-commutated topology, (b) represents self-commutated topology, (c) represents transformer-isolated DC-AC converter topology, (d) represents transformer-isolated DC-DC topology. 44
Fig. 5.1.20 a) Steady state input current characteristics for the line-commutated CSI topology. 45
b) Frequency domain characteristics for the line-commutated CSI topology. 45
Fig. 5.1.21 a) Steady state input current characteristics for the self-commutated PWM VSI topology 46
b) Frequency domain characteristics for the self-commutated PWM VSI topology. 46
Fig. 5.1.22 a) Steady state input current characteristics for the high-frequency transformer-isolated
cycloconverter topology 46
b) Frequency domain characteristics for the high-frequency transformer-isolated cycloconverter
topology. 46
Fig. 5.1.23 a) Steady state input current characteristics for the high frequency transformer isolated Ćuk-VSI
topology. 47
b) Frequency domain characteristics for the high frequency transformer isolated Ćuk-VSI topology. 47
Fig. 5.1.24 Implementation of the PES model using SimPowerSystem toolbox in Simulink. 47
Fig. 5.1.25 Super-configuration of the proposed SOFC based power system established prior to the
parametric study and optimization process. 48
Fig. 5.1.26  Compact heat exchanger section.
Fig. 5.1.27  Compact heat exchanger spatial discretization.
Fig. 5.1.28  Transient behavior of the coupled model’s rotational speed.
Fig. 5.1.29  Transient behavior of the coupled model’s compressor outlet mass flow rate.
Fig. 5.1.30  Schematic of the reduced order BOPS model.
Fig. 5.1.31  Specific load profiles for the reduced order model.
Fig. 5.1.32  Comparison of non-optimized and optimized transient responses of the reformate flow out of the BOPS to the SOFC anode.
Fig. 5.1.33  Load profile used for the comparison of non-optimized and optimized transient responses of the reformate flow out of the BOPS to the SOFC anode.
Fig. 5.1.34  Comparison of non-optimized and optimized transient responses of the reformate flow out of the reduced order BOPS code.
Fig. 5.1.35  Implementation of a unified model for a SOFC power-conditioning system using multi-software platform.
Fig. 5.1.36  The modeling framework for a comprehensive PSOFC based PCS modeling framework.
Fig. 5.1.37  Interfacing steps for gPROMS to Simulink.
Fig. 5.1.38  a) Comprehensive model block diagram.
Fig. 5.1.39  b) Reduced order model with lumped harmonic load replacing the PES.
Fig. 5.1.40  a) Comprehensive model block diagram.
Fig. 5.1.41  b) Reduced order model with lumped harmonic load replacing the DC-AC converter.
Fig. 5.1.42  a) Switching model of a DC-DC boost converter.
Fig. 5.1.43  b) Switch-average model of the DC-DC boost converter.
Fig. 5.1.44  a) Accuracy of the averaged boost converter model.
Fig. 5.1.45  b) Block diagram of reduced order modeling framework PSOFC PCS implemented in MATLAB/Simulink.
Fig. 5.1.46  Variations of load current due to the load transient.
Fig. 5.1.47  Current transient (10 A to 65 A) which results in a sudden drop in the PSOFC stack output voltage.
Fig. 5.1.48  Sudden surge in the hydrogen utilization due to the load transient.
Fig. 5.1.49  PSOFC stack conversion efficiency vs. fuel utilization.
Fig. 5.1.50  Spatial temperature distribution in °C before and after the load transient.
Fig. 5.1.51  Spatial temperature gradient before and after the load transient.
Fig. 5.1.52  Thermal analysis of the effects of load transients on the SOFC stack.
Fig. 5.1.53  Temperature variation of the elastic moduli of the sample LSM cathodes.
Fig. 5.1.54  Schematic of a PSOFC based residential power conditioning system.
Fig. 5.1.55  Voltage-current (V-I) characteristics of AC loads at different power factors.
Fig. 5.1.56  Reactive-power circulation due to a non-unity-power-factor load.
Fig. 5.1.57  a) Current distortion due to a rectifier load.
Fig. 5.1.58  b) Fourier analysis of the distorted current.
Fig. 5.1.59  Power-electronics induced high- and low-frequency ripples in the fuel cell current.
Fig. 5.1.60  Effect of low frequency ripple on the performance and efficiency of the stack.
Fig. 5.2.1  a) Block diagram of the proposed PCS.
Fig. 5.2.2  b) Schematic of the proposed PCS.
Fig. 5.2.3  a) Zero ripple inductor (an ideal transformer) with an external inductor and a filter capacitor.
Fig. 5.2.4  b) Transformer model showing the leakage inductances (L1, L2), magnetizing inductance.
Fig. 5.2.5  c) Ideal transformer model with an external trimming inductor connected to the secondary.
Fig. 5.2.6  Variation of load current due to the load transient.
Fig. 5.2.7  Current transient (10 A to 65 A) which results in a sudden drop in the PSOFC stack output voltage.
Fig. 5.2.8  Sudden surge in the hydrogen utilization due to the load transient.
Fig. 5.2.9  PSOFC stack conversion efficiency vs. fuel utilization.
Fig. 5.2.10  Spatial temperature distribution in °C before and after the load transient.
Fig. 5.2.11  Spatial temperature gradient before and after the load transient.
Fig. 5.2.12  Thermal analysis of the effects of load transients on the SOFC stack.
Fig. 5.2.13  Temperature variation of the elastic moduli of the sample LSM cathodes.
Fig. 5.2.14  Schematic of a PSOFC based residential power conditioning system.
Fig. 5.2.15  Voltage-current (V-I) characteristics of AC loads at different power factors.
Fig. 5.3.3  a) Schematic diagrams for coupled-inductor structure which reduces the HF current ripple  
   b) The half-bridge active filter which reduces low frequency ripple current of the fuel cell stack  
   c) The schematic of the ZRF  

Fig. 5.3.4  a) Proposed high-frequency inverter.  
   b) Conventional high-frequency inverter.  

Fig. 5.3.5  a) Schematic of the AC-AC converter topology for single- and three-phase applications.  
   b) Sine-wave-modulated PWM control of phase a of the AC-AC converter  
   c) Timing chart showing the scheme for the gating pulses for switches Q1 and Q2.  

Fig. 5.3.6  Current is reduced to zero from a positive value when the load current freewheels (Q1, Q3 and  
   Q5 are simultaneously turned on).  

Fig. 5.3.7  a) Schematic of the proposed experimental PCS.  
   b) Current-mode control scheme for the ZRBC.  
   c) Control scheme for the overall DC-AC converter.  

Fig. 5.3.8  Experimental prototype of the proposed PCS.  
Fig. 5.3.9  SOFC stack, components and installation photos.  
Fig. 5.3.10  25-cell stack initial V-I characteristics.  
Fig. 5.3.11  Initial 800 hours of stack operation, predominantly in RFC mode.  
Fig. 5.3.12  Experimental setup of the 25 cell PSOFC stack with the PES.  
Fig. 5.3.13  Setup for the stack characterization.  
Fig. 5.3.14  Setup to study the effect of the ripple on the stack.  
Fig. 5.3.15  Setup for measuring the stack impedance.  
Fig. 5.3.16  Connection diagram for the stack impedance measurement.  
Fig. 5.3.17  PES prototype for long-term ripple study.  
Fig. 5.3.18  PES prototype for the long-term load-transient study.  
Fig. 5.3.19  Expanded segment of load profile data on 12/08/2005.  
Fig. 5.4.1  Comprehensive hierarchical controller architecture for the fuel cell based power system.  
Fig. 5.4.2  Topology of multi-converter based hybrid power management system.  
Fig. 5.4.3  Theoretical efficiency of the 5 kW stack with fuel utilization at various flow rates (moles sec⁻¹).  
Fig. 5.4.4  Optimal fuel utilization tracking based controller architecture for the fuel cell based power  
   system.  
Fig. 5.4.5  Multi-level control system configuration.  
Fig. 5.4.6  Electrical energy use for peak cooling day in Atlanta, Georgia on 07/11.  
Fig. 5.4.7  Electrical energy use for peak heating day in Atlanta, Georgia on 01/12.  
Fig. 5.4.8  Approximated electric load profile based on a peak cooling and a peak heating day in Atlanta,  
   Georgia.  
Fig. 5.4.9  Subsystems (including controllers) and subsystem coupling functions.  
Fig. 5.4.10  System coupling functions  
Fig. 6.1.1  Steady-state I-V characteristics comparison of the planar SOFC stack  
Fig. 6.1.2  a) Effect of load current transient (2.2 A to 12 A) on the voltage of the stack model.  
   b) The experimental validation of its effect on the planar stack, scope channel 1 (10 V /div) and  
   channel 4 (2 A/div) measures the stack voltage and current respectively.  
Fig. 6.1.3  Validation of the effect of load transient (no load (NL) – full load (FL) – no load (NL)) on the  
   planar SOFC stack temperature.  
Fig. 6.1.4  Validation of the effect of multiple load transient (NL-FL-NL) on the planar SOFC stack  
   temperature  
Fig. 6.1.5  a) Effect of 40 percent current ripple on the stack voltage of the model.  

5/6/2006
b) Experimental validation of the ripple effect on planar SOFC stack, scope channels A and D show the stack voltage and current respectively.

Fig. 6.2.1 Comparison of long-term ASR degradation due to low-frequency ripple, constant current and load transient.

Fig. 6.2.2 a) The drop in the output power of the PSOFC due to ASR degradation caused by load transient. b) The drop in the output power of the PSOFC due to ASR degradation caused by ripple.

Fig. 6.3.1 Effect of severity of the load transient on the fuel (hydrogen) utilization and mean stack temperature.

Fig. 6.3.2 Effect of the duration of load transient on the increase in the mean stack temperature.

Fig. 6.3.3 Residual stress at different interfaces before the load transient.

Fig. 6.3.4 Residual stress (in MPa) at different interfaces in PSOFC after the load transients.

Fig. 6.3.5 Risk of rupture intensities at the interface of electrode with cathode after the load transients.

Fig. 6.3.6 Estimated stack reliability with probability of failure of a cell.

Fig. 6.3.7 Effect of power factor of the load on the magnitude of stack current ripple.

Fig. 6.3.8 Effect of power factor of load on the increase in the mean temperature of the stack.

Fig. 6.3.9 Effect of THD on the stack current ripple.

Fig. 6.3.10 Effect of THD on the increase in the mean temperature of the stack.

Fig. 6.3.11 Effect of low frequency ripple on operable fuel utilization.

Fig. 6.3.12 Effect of low frequency ripple on achievable efficiency of the stack.

Fig. 6.3.13 Effect of low-frequency ripple on stack temperature.

Fig. 6.4.1 Response of the battery current due to the load transient and flow adjustment.

Fig. 6.4.2 Response of the bus voltage and fuel utilization to a sudden load transient which is followed by the flow adjustment of BOPS for a fixed fuel utilization of 0.78.

Fig. 6.4.3 Efficiency of the stack before and after the load transient.

Fig. 6.4.4 Fuel utilization variation due to change in the fuel flow rate after the load transient.

Fig. 6.4.5 Multi-converter system efficiency as compared to a single 5 kW converter and power sharing using five converter modules.

Fig. 6.5.1 SOFC system phase I/Phase II reduced super-configuration established at the end of Phase I for purposes of dynamic synthesis/design optimization in Phase II.

Fig. 6.5.2 FPS purchase cost breakdown (based on a production volume of 200,000 units per year).

Fig. 6.5.3 WRAS purchase cost breakdown (based on a production volume of 200,000 units per year).

Fig. 6.5.4 SOFC system total cost breakdown (based on a production volume of 200,000 units per year).

Fig. 6.5.5 Steam generator start-up temporal and spatial thermal responses on the water side.

Fig. 6.5.6 Steam generator start-up comparison of thermal responses on the water side.

Fig. 6.5.7 Steam-methane reformer start-up dynamic response for low pre-heating.

Fig. 6.5.8 Steam methane reformer wall temperature start-up response for high pre-heating.

Fig. 6.5.9 Compact heat exchanger III start-up thermal time response comparison between pre-heating and no pre-heating.

Fig. 6.5.10 Compact heat exchanger III 2D spatial temperature distribution at steady state for the cold-side stream.

Fig. 6.5.11 Reformate tank pressure (state variable) optimum dynamic response.

Fig. 6.5.12 Steam-methane reformer optimum inlet methane mass flow (control variable).

Fig. 6.5.13 Air tank pressure (state variable) optimum dynamic response.

Fig. 6.5.14 Steam-methane reformer gas exit temperature (state variable) optimum dynamic response.

Fig. 6.5.15 3D depiction of the steam-methane reformer optimum hot gases inlet temperature (control variable) dynamic response.

Fig. 6.5.16 Anode and cathode inlet temperature optimum dynamic behavior.

Fig. 6.5.17 Methane conversion optimum dynamic response.
Fig. 6.5.18  3D depiction of the methane conversion optimum dynamic response.
Fig. 6.5.19  Stack hydrogen requirements and BOPS optimum hydrogen supply (part of the reformate mass flow which is a state variable) from the reformate tank.
Fig. 6.5.20  Fuel tank pressure transient with PID controller for decreasing changes in load demand starting from full load.
Fig. 6.5.21  Methane conversion transient with PID controller for decreasing changes in load demand starting from full load.
Fig. 6.5.22  FPS, SS, and SOFC system optimum dynamic efficiency profile.
Fig. 6.5.23  FPS and SOFC system optimum dynamic efficiency profiles at each of the two drastic load changes (at 1 hr and at 24 hr).
Fig. 6.5.24  Reformer reference temperature effect on system efficiency.
Fig. 6.5.25  Effects of variations in steam-methane reformer size on system dynamics.
Fig. 6.5.26  Effect of variation in steam-methane reformer size on cost rate.
Fig. 6.5.27  Effect of variation in steam-methane reformer size on cost rate at 1 hr and 24 hr.
Fig. 6.5.28  Zoom-in at 24 hr of the effects of variation in steam-methane reformer size on cost.
Fig. 6.5.29  Effect of variation in heat exchanger II size on system dynamics.
Fig. 6.6.1  a) Coupled inductor performance results showing input current split between the DC and the AC windings for an optimum value of external inductance.
              b) Experimentally-observed input ripple-current variation in the DC winding with variation in external inductance.
Fig. 6.6.2  Input current ripple reduction with APF (Ch3: 20 A/div, 10 ms/div and Ch4: 20 A/div, 10 ms/div).
Fig. 6.6.3  a) Measured efficiency for the proposed PCS and its subsystem
              b) Combined efficiency of stack and PCS for various fuel cell ripple current.
Fig. 6.6.4  a) Illustration of the HF inverter operation: showing gating pulse for HF inverter switches.
              b) Transformer primary voltage and current waveforms of the HF inverter.
Fig. 6.6.5  a) Parametric plot showing the percentage ZVS achievable versus load current for different values of leakage inductances
              b) Transformer efficiency versus output power for various values of leakage inductances.
Fig. 6.6.6  a) Two different winding arrangements for a 5 kW, 25 kHz isolation transformer fabricated using P-49925-UC, ferrite core. Primary and secondary windings on the same leg using a AWG 10 solid copper wire. The leakage inductance was measure to be 1.2 µH.
              b) Primary and secondary windings distributed over the entire length of the core using a two strand AWG 14 copper wire. The leakage inductance was measure to be 450 nH.
2. LIST OF TABLES

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>5.1.1</td>
<td>Baseline conditions used in the transient case study.</td>
<td>28</td>
</tr>
<tr>
<td>5.1.2</td>
<td>Input data for the reformer simulation.</td>
<td>51</td>
</tr>
<tr>
<td>5.1.3</td>
<td>Geometric model of the steam generator.</td>
<td>53</td>
</tr>
<tr>
<td>5.1.4</td>
<td>Reduction in computational overhead and accuracy comparison.</td>
<td>67</td>
</tr>
<tr>
<td>5.3.1</td>
<td>Key power-stage component listing for the designed PES.</td>
<td>90</td>
</tr>
<tr>
<td>5.3.2</td>
<td>Stack specifications for the experimental validation.</td>
<td>94</td>
</tr>
<tr>
<td>5.3.3</td>
<td>Geometric model of the steam generator.</td>
<td>95</td>
</tr>
<tr>
<td>5.4.1</td>
<td>Test condition of the validation experiment.</td>
<td>95</td>
</tr>
<tr>
<td>5.4.2</td>
<td>Control and state variables pairing.</td>
<td>110</td>
</tr>
<tr>
<td>5.4.3</td>
<td>Coupling function definition.</td>
<td>116</td>
</tr>
<tr>
<td>5.4.4</td>
<td>SOFC decision and principal dependent optimization variables and constraints.</td>
<td>118</td>
</tr>
<tr>
<td>5.4.5</td>
<td>FPS synthesis/design decision variables and constraints.</td>
<td>119</td>
</tr>
<tr>
<td>5.4.6</td>
<td>FPS operational decision variables and constraints.</td>
<td>120</td>
</tr>
<tr>
<td>6.1</td>
<td>WRAS decision and principal dependent optimization variables and constraints.</td>
<td>121</td>
</tr>
<tr>
<td>6.2</td>
<td>Optimum cost of the total SOFC system and subsystem for the first and the final iteration of the DILGO approach.</td>
<td>143</td>
</tr>
<tr>
<td>6.3</td>
<td>WRAS, and SOFCS optimum capital and operational cost.</td>
<td>145</td>
</tr>
<tr>
<td>6.4</td>
<td>Effects of variation in steam-methane reformer size on life cycle costs.</td>
<td>160</td>
</tr>
<tr>
<td>6.5</td>
<td>Effects of variation in heat exchanger II size on life cycle costs.</td>
<td>162</td>
</tr>
</tbody>
</table>
3. INTRODUCTION

Renewable energy sources (such as fuel cell) are expected to provide 15% of the world energy demand in the near future (International Energy Agency Report, Ellis et al. 2001, Raissi 1997). Solid-oxide fuel cells (SOFCs) are expected to play a significant role in helping to meet the demands of energy quality and reliability of distributed power generation. SOFCs have become an irresistible competitor in distributed generation due to their insurmountable advantages like high energy efficiency, near zero emissions, ease of installation, silent operation, and fewer moving parts and higher power quality. However, certain challenges remain before SOFCs can be applied to real-world applications. These challenges include the issues of reliability and lifetime of the SOFCs. For SOFCs to be used commercially, it is essential that SOFC technology be demonstrated to achieve long life (longer than 40,000 hours for stationary applications and longer than 5000 hours for transportation applications).

Development of high-performance and durable solid-oxide fuel cells (SOFCs) and a SOFC power-generating system requires knowledge of the feedback effects from the power-conditioning electronics and from application-electrical-power circuits that may pass through or excite the power-electronics subsystem (PES)\(^1\). It is thus important to develop analytical models and methodologies to investigate the effects of the feedback from the PES and the application loads on the reliability and performance of SOFC systems for stationary and mobile applications. The behavior of a PES has a direct impact on the stack performance and the lifetime of the SOFC\(^2\) (Gemmen, 2001; Hartvigsen, 2002; Mazumder et al., 2003, Acharya et al., 2003). For example, a DC-DC converter will impose its own time-varying load on the fuel cell, apart from that due to variations in the application loads and other effects from DC-AC and DC-DC converters the stack may be subjected to a time varying load. If the peak-current levels from these loads are high, it can lead to a low-reactant condition within the SOFC. As such, there is a need for analytical models and methodologies, which can be incorporated into a system tool to investigate the issues of safe load-fluctuation and effective load-following, and explore how to manage each of SOFC subsystem’s response optimally\(^3\). Furthermore, such an analytical tool could also help determine how much current and voltage ripples a SOFC can acceptably withstand, how does the slow-(line) and fast-(switching) scale ripple (Mazumder et al., 2001a) affect the performance and operating life of the SOFC stack, and how should the power electronics be designed and operated to mitigate these problems.

\(^{1}\) SOFC power-generating systems may provide direct or alternating current (AC or DC) to satisfy application specific power needs. The current, voltage, and power quality are controlled by electronic power conditioning systems. Generally, voltage regulators, DC-DC converters, and chopper circuits are used to control and adjust the fuel cell DC output voltage to a useful value. Inverters are used to convert this DC voltage to a useful AC voltage for stationary applications.

\(^{2}\) NETL guidelines specify SOFC operating lifetime as > 40,000 hours for stationary applications and > 5000 hours for mobile applications.

\(^{3}\) For example, by matching the optimal power-electronics subsystem to a particular SOFC system and application, such a system tool provides a designer with sufficient knowledge of both system and subsystem topologies. Additionally, subsystem and component response times are known to enable her or him to make the most judicious, as opposed to the most conservative choice of components.
Filters are typically specified to reduce ripple current to "perceived" low risk levels. However, the larger the filter size, the higher would be the cost of the PES. An energy buffering device can be used to mitigate the effect of the load transients. However, the larger the size/capacity of the buffering device higher would be the cost. Therefore, understanding of the electrical impact of the PES on SOFCs allows the optimization and design of more cost-effective and reliable power electronics and energy buffering device for SOFC based system.

Thus, there is a need to develop analytical tools and investigative methodologies to address the issues outlined earlier, and design and development of cost-effective, reliable, and optimal PESs. However, any such attempt to resolve the electrical impacts of PES on SOFC would be incomplete unless one utilizes a comprehensive analysis, which takes into account the interactions of SOFC, PES, balance-of-plant subsystem (BOPS), and application loads as a whole. SOFCs respond quickly to changes in load, because of rapid electrochemistry. This is not true, however, for the thermal, mechanical, and chemical BOPS components and particularly for the fuel-processing subsystem, where load-following time constants are typically several orders of magnitude higher. Differences in response times between the electrochemical/electrical and thermal/mechanical/chemical subsystems of the overall SOFC system can lead to undesirable effects, given significant variations in load.

SOFC manufacturers, traditionally model the PES as constant impedance, while manufacturers of PES model the SOFC as stiff voltage sources for their analysis. Both these approaches yield inaccurate results. To overcome the lack of comprehensive analytical tools to model SOFC based systems, manufacturers of SOFC (utility) PES have so far implemented conservative (and expensive) schemes for managing stack response to application load variations (i.e., controls tactics for delayed load-following to allow for balance-of-plant response, expensive inductor filtering, etc.). SOFC systems are thus less practical from an applications and cost standpoint. Therefore, to comprehensively analyze these multiple-scale effects, analytical models are needed to perform system and component engineering studies to evaluate how an entire integrated fuel cell system works, to optimize designs, and to determine the best design approach to achieve the highest performance at least-cost. Finally, accurate dynamic modeling is critical to employing well thought-out and optimized control schemes, which respond reliably to operating conditions across an entire load profile and are applicable to a wide variety of SOFCs and system configurations.

One of the biggest problems to the comprehensive simulation is the issue of multiple-time scales associated with the vastly different response times of SOFC and BOPS dynamics as compared to that of the PES. While the PES time scale is in microsecond, the response times of SOFC and BOPS is in seconds (if not in minutes); the minimum ratio is a staggering million. Even though, the switching models are the real representatives of the power converters, the models suffer from the disadvantage of being discontinuous because of their switching. With the switching frequency in the order of tens of kilohertz, the discontinuous system has to be solved at their boundary of discontinuity in each cycle, which renders the model computationally expensive. Therefore, a reduced order modeling approach is needed to model the system without any loss in the accuracy of the responses as compared to the comprehensive system model.
The system model need to be validated experimentally in the steady state and their response should be validated during transients so that, the model will be useful while conducting the study of the interaction analyses among various subsystem models.

The SOFC PCS is subjected to several electrical feedbacks induced due to the variation and quality of the load, and the architecture of the PES. The load induced feedbacks include a) the load transient, which occurs due to a sudden variation in the load power demand, b) load power factor, which states the reactive power demand by the load, and c) load harmonic distortion, also called total harmonic distortion (THD), governed by the harmonic content in the current drawn by the load. Similarly, the PES introduces low-(line) and high-(switching) frequency ripple. Therefore, a study to identify the electrical feedbacks which may potentially degrade the performance and reliability of the SOFCS is needed.

Achenbach (1995) and Hartvigsen et al. (1993) have demonstrated preliminary results on the impacts of linear electrical load impedance and their change on the dynamics of a SOFC. Acharya et al. (2003, 2004) have demonstrated effects on the performance and durability of a SOFC (TSOFC) stack. Gemmen (2001) had estimated the degrading effects of electrical loads and inverter current ripple on the performance of proton-exchange membrane (PEM) fuel cells. To avoid the deteriorating effects of any such feedbacks of the PES and the AL, on SOFCS, one needs to quantify their degrading impacts. Therefore, a study on the impacts of these feedbacks on the performance and durability of the SOFCS with parametric variation of the feedbacks needs to be conducted.

The durability and reliability of SOFCs depend not only on their electrochemical performance, but also on the ability of their components to withstand mechanical stresses that arise during its operation. When a PSOFCS is subjected to a sudden increase in the load, current density in the cell increases leading to an increase in the temperature. Any non-uniform increase in the temperature inside the cell leads to non uniform thermal expansion inside the cell. For a planar cell with strict binding among each cell components, a slight mismatch in thermal expansion coefficient among the cell components can cause severe residual stress, which may degrade the performance and durability of the planar cell [Montross et. al, 2002, and Yakabe et. al 2001]. Therefore, it is imperative to investigate the effect of the load transient on the mechanical properties of the PSOFC.

The parametric study of these electrical feedbacks can only predict the short-term degrading impacts on the PSOFCS. However, for the PSOFC PCS to meet the lifetime specifications, a long term study needs to be conducted which can predict the deteriorating impact of some of the effects in the long term. Since it is impossible to conduct long-term (order of 1000 hours) study of the large-scale simulation model of the PSOFC PCS, this study needs be conducted experimentally.

Since the power-electronics system (PES), connected to the fuel cell stack usually draws a current, which has a low-frequency ripple (e.g., 120 Hz for single- and two-phase systems) and a high-frequency (HF) switching ripple, the hydrogen utilization and fuel cell efficiency varies over the nominal DC operating point of the stack. Thus, to ensure energy-efficient operation of the fuel cell stack, the output current ripple of the fuel cell stack should be minimized. In
(Gemmen, 2001) it is suggested that, to mitigate the effects of the low-frequency (< 400 Hz) current ripple on the durability of the fuel cell, the magnitude of the ripple should be minimized. It is shown that, the 120-Hz ripple current of the power conditioner can contribute to a reduction in the available output power of the fuel cell stack and increased distortion of the terminal voltage. Therefore, a PES need to be designed which will eliminate any such ripple current on the SOFCS. While improving the energy density of the fuel cell is necessary, it is also important to reduce the losses of the PCS to deliver the power of the fuel cell stack efficiently to the load.

The slow response time of the BOPS mechanical system as compared to the fuel cell electrochemistry and the power electronics system has been a major concern for fuel cell system designers. Several works are in progress to enhance the response time of the BOPS. However, it is practically impossible to match the response time of the fuel cells, which is in the order of milliseconds. To avoid the low reactant condition, arisen due to the load transient, and aggravated by the slow response time of the BOPS, the SOFC need to operate at a flow rate that is capable of handling the rated load current. However, at lower loads the fuel utilization and hence the efficiency of the fuel cell stack goes down drastically. This reduces the efficiency of the fuel cell based power system and hence increases the unit cost of power. So energy buffering devices like a battery, which would provide the additional energy immediately to the load during the load transient, is needed in conjunction with the fuel cell stack. To optimize the size and response of the battery while eliminating the degrading impacts of the load transient on the stack, a control strategy needs to be developed which would control the energy flow between the energy generator (fuel cell stack) and the energy buffering device (battery).
4. EXECUTIVE SUMMARY

Motivation and Problem Statement: Development of high-performance and durable solid-oxide fuel cells (SOFCs) and a SOFC power-generating system requires knowledge of the feedback effects from the power-conditioning electronics and from application-electrical-power circuits that may pass through or excite the power-electronics subsystem (PES). Therefore, it is important to develop analytical models and methodologies, which can be used to investigate and mitigate the effects of the electrical feedbacks from the PES and the application loads (ALs) on the reliability and performance of SOFC systems for stationary and non-stationary applications. However, any such attempt to resolve the electrical impacts of the PES on the SOFC would be incomplete unless one utilizes a comprehensive analysis, which takes into account the interactions of SOFC, PES, balance-of-plant system (BOPS), and ALs as a whole. SOFCs respond quickly to changes in load and exhibit high part- and full-load efficiencies due to its rapid electrochemistry, which is not true for the thermal and mechanical time constants of the BOPS, where load-following time constants are, typically, several orders of magnitude higher. This dichotomy can affect the lifetime and durability of the SOFCs and limit the applicability of SOFC systems for load-varying stationary and transportation applications. Furthermore, without validated analytical models and investigative design and optimization methodologies, realizations of cost-effective, reliable, and optimal PESs (and power-management controls), in particular, and SOFC systems, in general, are difficult. On the whole, the research effort can lead to a) cost-constrained optimal PES design for high-performance SOFCs and high energy efficiency and power density, b) effective SOFC power-system design, analyses, and optimization, and c) controllers and modulation schemes for mitigation of electrical impacts and wider-stability margin and enhanced system efficiency.

Technical Approaches: As outlined above, the SOFC-energy-system project comprises mainly four elements: i) component (SOFC, PES and AL, and BOPS) and system modeling (comprehensive and reduced-order), ii) analyses of electrical-feedback effects and their impacts on SOFC, iii) BOPS parametric optimization, and iv) load- and ripple-mitigation power-management control and topologies for stationary applications.

Component Modeling: In phase 1, a transient tubular SOFC (TSOFC) model was developed (and implemented in Visual Fortran) using Lagrangian approach and validated while in phase 2, a 2D and a 1D spatio-temporal model of the planar SOFC (PSOFC) has been successfully developed, implemented (in Matlab) and validated (under steady-state and transient conditions) for characterizing the performance of a multi-kW SOFC power module subject to electrical stimuli. Next, using switching and averaged models (for higher accuracy of switching-ripple dynamics and reduced computation time, respectively), we have developed in a low-cost platform (Simulink and SimPowerSystems), a simple but flexible mechanism to simulate line-transformer-isolated or high-frequency-transformer based multi- or single-stage PES models. The simulation results have been validated using previously published results on application-related PES topologies and in-house experiments. These topologies have different current-ripple characteristics and hence, allow a detailed analysis of the effect of PES on the SOFC reliability and performance. Basic application-load models have also been developed towards electrical characterization. Finally, a comprehensive mathematical model of the BOPS consisting of a set of nonlinear infinite-dimensional equations, which describe the mass and associated energy
flows in each of the lines of the subsystems is developed based on the chemical reactions inside each reactor and on the laws of conservation of mass and energy for each component in the subsystem.

**System Modeling:** Subsequent to the development of a phase-1 multi-software SOFC system model (comprising SaberDesigner, Visual Fortran, iSight, and gPROMS), in phase 2, a low-cost and almost-all-Simulink (BOPS is implemented in gPROMS but integrated to Simulink via gOSimulink) comprehensive numerical modeling framework for PSOFC-based stationary energy system and vehicular APU (for PNNL) has been developed. The power-conditioning system (PCS) model comprises the comprehensive transient models of PSOFC, BOPS, PES, and AL and can be used for resolving the interactions among PSOFC, BOPS, PES, and AL, control design and system optimization, and fuel-cell durability studies. The PCS model has several key properties including the following: i) it can predict simultaneously predict spatial as well as temporal dynamics; ii) it has two levels of abstraction: comprehensive (for detailed dynamics) and reduced-order (for fast simulation); and iii) the fast-simulation model can be implemented completely in Simulink/Matlab environment, thereby significantly reducing the cost as well as time. We compared the computational overhead and accuracy of the fast-simulation and comprehensive models and the show significant savings in time obtained using the former without compromising accuracy adversely.

**Analyses of Electrical-feedback Effects and their Impacts on SOFC:** A detailed study is conducted on the electrical-feedback effects (including load transients, current ripple variations due to load power factor and inverter operation, and load harmonic distortions) that have an impact on the electrochemistry and the thermal properties of the SOFC, thereby affecting the performance and reliability of the cells. Subsequently, detailed experimentation is carried out to validate the simulation data on interaction analyses. Using this validated model, parametric analyses on the impacts of transience, power factor, and distortion of the application load as well as low-frequency current ripple is conducted. The study clearly establishes that sizing of a SOFC system needs to take into account ripple magnitude and input-filter design simultaneously. The impact of load transience on electrically-induced thermal cycling is not as significant as thermal cycling, but the frequency of repetition and load magnitude needs to be paid close attention as electrical transients have significantly more occurrence. Finally, using a uniquely designed experimental methodology, we explore the long-term impact of current ripple and repetitive load transient has any additional impact on SOFC area-specific resistance (ASR) and corresponding effective loss of stack power as compared to the case when the stack is subjected only to a dc current; for both cases, the average current is kept the same.

**BOPS Parametric Optimization:** To determine the optimal synthesis/design and dynamic operation of the SOFC system, a parametric system optimization is conducted. This requires the optimal synthesis/design and dynamic operation of each of the BOPS subsystems to be carried out in an integrated fashion, leading to establishment of a feasible system super-configuration which provides high efficiency and reliability. Based on this super-configuration, detailed dynamic models for each component where developed and then coupled in order to generate a system level dynamic model. Using the system level dynamic model, parametric studies were done in order to determine system behavior for various combinations of system-level parameters and components locations and dimensions. The results of the parametric studies were used to determine the most promising subset of this super-configuration i.e., reduced super configuration
based on system response, fuel consumption, capital cost, operational constraints, etc. During phase 2, the resulting reduced super-configuration was subjected to a large scale synthesis/design optimization while taking into account its effects on system operation, i.e., on the dynamic response of the system. The parametric studies showed this configuration to provide adequate fuel efficiency.

**Load- and Ripple-mitigating Power-management Control and Topology:** Based on the electrical-feedback analyses, a novel patent-pending topological power-management controlling strategy and architecture for a SOFC PCS (including battery-buffering unit) to improve steady-state energy efficiency of the PES (almost flat efficiency across the power range as compared to progressively drooping efficiencies as in conventional case) and hence the PCS (by optimizing the fuel utilization in the stack in the steady-state) is developed at University of Illinois. Further, using a multi-loop feedback, the control also integrates to a battery-buffer control to mitigate the effect of the load transient on the SOFCS (e.g., fuel utilization). A new methodology has also been developed to systematically relinquish the control of the battery (after transience phases out) at a rate governed by the control bandwidth of the BOPS.

Based on these analyses, (and using partial supports from DOE SECA and California Energy Commission), University of Illinois has developed a novel low-cost, zero-ripple, energy-efficient, and high-power-density PES, which can meet SECA price target of $40/kW in volume production and enhances the durability of a SOFCS. The proposed PES achieves i) over 92.1% peak efficiency at 5 kW for single-phase output; ii) practical elimination of the low- and high-frequency ripple currents drawn from the SOFCS without using any bulky input filter, thereby optimizing stack sizing and significantly enhancing the life and energy efficiency of the SOFCS; and iii) 50% reduction in voltage stresses for the intermediate inverter, which leads to higher reliability. The proposed patent-pending topology addresses several key SECA industry issues for PES including cost, SOFC sizing, performance, and reliability, and energy efficiency.

**Key Achievements:** Outlined below are the significant achievements of this SECA project:

1. Developing a low-cost, flexible, scalable, and multi-resolution SOFC-energy-system simulation platform for analyzing the dynamics of SOFC, BOPS, PES, and AL, and their interactions. This inexpensive software can be used by the SECA as well as SOFC energy industries for designing robust electronics, optimal control, system optimization by using it both as a supplementary/complementary tool;

2. Clearly establishing what effects different classes of electrical feedbacks have on SOFC performance and reliability followed by experimental validation;

3. Develop a patent-pending novel topological power-management control scheme (whose application is independent of basic converter topology) which can a) ensure an-almost flat energy efficiency across the power range (which increases the overall SOFC PCS energy efficiency) and b) eliminate the need for battery power conditioner (that saves system cost, weight, and volume) for SOFC load-transient mitigation;

4. A novel (patent-pending) ripple-mitigating inverter that a) meets DOE SECA’s cost and efficiency targets for PES in volume production, b) enables SOFC optimal stack sizing, energy efficiency, and reliability, and is scalable for higher power;
5. Productive Management: A unique facet of this project was to effectively bring together a group of multi-disciplinary experts to work on a set of focused applied-research problems which are of significant importance to SECA and SOFC industries and solve it in a timely-fashion. The multi-tier collaboration among University of Illinois, Ceramatec, Virginia Tech, and Georgia Tech also extended to coordination with PNNL and ORNL regarding modeling, interaction-analyses, and validation efforts, transfer of codes to PNNL, and engagement with Cummins Power Generation regarding transfer of experimentally-validated and simulation data regarding model- development efforts. As a further reachout to this effort, software codes will be made available for all other SECA industries.

6. Quality and High-visibility Publications


7. **Dr. Mazumder organized a high-visibility fuel-cell power management session in 2003** at the IEEE Industrial Electronics Conference (IECON), which is one of the most prestigious conferences in the world and attended by experts from USA and the rest of the world. The invited papers were presented by General Electric, Oakridge National Laboratory (ORNL), Plug Power, and University of Illinois.

8. **Student Placements:**
   
i. Dr. Diego Rancruel (advisor Prof. Michael von Spakovsky) is working for GE Power Systems since 2005.

   ii. Dr. Rajni K. Burra (advisor Prof. Sudip K. Mazumder) is working for GE Corporate Research since February 2006.
5. MODELING, ANALYSIS AND EXPERIMENTAL VALIDATIONS

5.1 COMPONENT AND SYSTEM MODELING

SOFC electrochemical and thermal-transport-phenomena have been investigated and are used to characterize the stack behavior under load-varying conditions. The resulting algorithms and code integrates with power-electronics and system model codes to simulate “real world” changes in current and voltage ripples, load following, start up/shut down, etc. This allows the study of fuel cell reliability and performance over a domain of transient conditions, which are typical of the distributed generation and mobile power markets targeted within SECA. Ultimately, the goal is to resolve design approaches that enable SOFCs to be tolerant to variations in load in a cost-effective and efficient way. Towards this end, this project develops and integrates dynamic models of each of these subsystems (i.e. power-electronics subsystem, SOFCS, and balance-of-plant) into a comprehensive analytical tool, which is further used through sensitivity parametric studies and/or dynamic optimization to create a variety of control strategies for stationary and transportation applications.

Fig. 5.1.1: Block diagram of a SOFC PCS block diagram showing the SOFCS, the PES, and the BOPS.

SOFC-based PCS (as shown in Fig. 5.1.1) consists of three principal subsystems: (a) the SOFCS, (b) the BOPS, and (c) the PES. The chemical reactions responsible for producing electricity take place in the fuel cell stack. The BOPS acts as a fuel processor and converts
hydrocarbon-based fuel to hydrogen. It is also responsible for maintaining the temperature of the fuel/air supply and their flow rates. The PES is responsible for processing the SOFCS output to useful voltage/current levels. The subsystem modeling was divided among our team of investigators, who have proven theoretical and practical expertise in the component- and system-level modeling, interaction analysis, and optimization of these types of distributed and vehicular subsystems and systems, that is,

(a) **SOFC Stack**: Ceramatec Inc. and Georgia Tech.
(b) **Power Electronics**: University of Illinois and Synopsys Inc.
(c) **Balance of Plant**: Virginia Tech.
(d) **System Integration**: University of Illinois, Ceramatec and Virginia Tech.

The following subsections describe in detail the approach to model each of the subsystems. Section 5.1.1 describes the SOFCS subsystem (SOFCSS) modeling approaches to characterize SOFCS behavior under load-varying conditions. The model was integrated with the PES model (described in Section 5.1.2) to simulate SOFC current and voltage dynamics. The detailed BOPS model is then described in Section 5.1.3. The modeling framework for integrating the system model has been described in Section 5.1.4. A detailed investigation of interactions among various subsystems is conducted based on the developed integrated system model in the following section.

### 5.1.1 SOFC Stack Subsystem (SOFCSS) Model

In earlier phase of the project, the primary focus had been to realize and establish a validated SOFCS model. In order to leverage the extensive demonstration, field data, and design insights, a tubular SOFC (TSOFC) stack had been chosen as the test bed technology. An electrochemical transient model of the tubular design has been developed using Lagrangian approach, and is validated with the existing stacks. However, in Phase II, the main focus of the modeling work has been to develop a comprehensive spatio-temporal model of planar SOFCS, which is the key design route within the SECA infrastructure and a key initiative of the Department of Energy (DOE).

A number of investigators (Yentekakis et. al), (Erdle et. al), (Ferguson, 1991), (Hartvigsen et. al, 1993), (Hendriksen, 1994) and (Ferguson et. al, 1996) have developed and published results of solid oxide fuel cell (SOFC) models over the years. Such models employ a diverse range of approaches to quantify the state and transport of the various forms of mater and energy within the fuel cell. Each approach is chosen to address the questions at hand. Some may incorporate a high degree of spatial resolution, providing detailed feedback to a designer striving to optimize heat and current flux pathways within the stack. Others may focus on providing a detailed thermal stress state in an effort to improve the structural reliability of the stack. Still others, most concerned with numerically probing the SOFC in order to optimize power and efficiency, may homogenize the geometry concerned only with the overall effect of temperature, reactant and potential distributions, but doing so over the entire stack domain rather than on a small unit cell defined by regions of geometric symmetry. A recent trend, driven by the mass marketing of computational fluid dynamics (CFD) codes views the problem from a Navier-Stokes centric position, providing detailed spatial resolution of the velocity and pressure distributions of the reactant flows. And, as fuel cells emerge from the traditional domain of the electrochemist, there
are a number of models that endeavor to apply a high fidelity polarization model so as to capture the most subtle inflections in the current-voltage characteristic.

Because there is such a wide range of physical results being sought by modeling, there is a correspondingly wide range of numerical methodologies (closed form parametric, finite element (FEA/FEM), control volume, etc.), and computational platforms (spreadsheet, problem specific user generated code, and commercial CDF and finite element codes) being used in SOFC modeling. Each with its own merits and utility in addressing specific questions related to SOFC design and operation. Similarly, it is not possible, practical or even desirable to create a single SOFC model encompassing the full range of physical phenomena, time scales and level of resolution required to address all the issues pertaining to SOFC systems. Modeling an SOFC from the unique perspective of its interaction with the power electronics introduces new issues which are not effectively handled by existing models, and which derive no benefit from the baggage of high spatial resolution models. Also, as power electronic systems (PES) are traditionally analyzed in different computational environments than SOFC systems, an SOFC model developed specifically for integration in a PES was needed.

5.1.1.1 TSOFC Model

The designed tubular SOFC (TSOFC) design (Haynes and Wepfer, 2000) is based on fundamental electrochemistry (as opposed to curve fit correlations and “black box” simplifications). The attempt to simulate the TSOFCs was an extension of the work of Bessette (1994) and Kanamura et al. (1989).

![Fig. 5.1.2: Axial division of TSOFC.](image)

This model uses “slice technique” to compute the system dynamics. This technique, as illustrated in Fig. 5.1.2, divides the cell into a preset number of subdivisions (or slices). Mass and energy balances for fuel oxidation are made on each slice in an axial march. Each slice has an equilibrium voltage (i.e., Nernst potential), depending on constituent partial pressures at the slice:

\[
E = \frac{1}{nF} \left[ -\Delta G^\circ_{\text{steam, }1000^\circ C} - R_n T \ln \frac{P_{H_2O}}{P_{H_2}P_{O_2}^{1/2}} \right]
\]  

(5.1.1)
The equilibrium voltage represents the largest possible potential difference, from a thermodynamic standpoint. The actual cell voltage is a common value among the slices and is dictated as an operating parameter. It is less than the equilibrium potential due to electrochemical irreversibility.

Fuel cells cause ions and valence electrons to complete a circuit; hence, current is produced. Any finite rate process, however, also generates irreversibility. In the case of fuel cells, these irreversibilities manifest as polarizations or losses in potential difference. The three types of polarization are activation, concentration and ohmic. Fuel cell reactions require certain "activation energy" in order for them to occur. The activation energy, which depends on how ions are transferred and the rate at which they are transferred, must be subtracted from the energy theoretically available (i.e., the Nernst potential). Fortunately, the high operating temperature of present TSOFCs promotes fast reaction kinetics, and activation polarization may be considered small (Minh and Takahashi, 1995), (Maskalick, 1989). Reactants are transported from their respective (i.e., fuel and air) streams to the fuel cell; thus, mass transfer irreversibility, or concentration polarization, occurs. Bagotsky (1993) gives the following relation for quantifying concentration polarization.

\[ \Delta V_{\text{polarization,conc}} = \frac{RT}{nF} \sum \ln \left( \Pi_{\text{reactant}} \left[ 1 - \frac{i}{i_{\text{ij}}} \right]^{3} \right) \]

The most significant loss is that due to ohmic resistance to current flow:

\[ \Delta V_{\text{polarization,ohmic}} = iR_{\text{eff}} \]

The effective resistance of the TSOFC was developed from consideration of the "transmission line" model (Nisancioglu, 1989). The following electrochemical governing equation thus resulted:

\[ \Delta V_{\text{polarization,total}} = E_{\text{slice}} - V_{\text{operate}} \]

The first term is the sum of the concentration and ohmic losses and is current dependent. Once the current was converged upon for a given slice, constituent mole fractions and partial pressures for the next slice were calculated. These calculations were based on the stoichiometric relationship between current and reaction constituents (hydrogen, oxygen and steam), as well as shift reaction equilibrium (carbon monoxide combining with steam to form hydrogen and carbon dioxide). A detailed discussion of the material balances may be seen in Haynes (1999). The power generated in each slice is given by:

\[ \text{Power}_{\text{slice}} = i_{\text{slice}} \times V_{\text{operate}} \]

Successive slices are "marched" through until the current and power distributions for the entire cell are known. The total current and power are then accumulations of the slice values. As alluded to, the operating voltage must be lower than the lowest equilibrium potential, which occurs at the last slice due to reactant use. The model was applied to the recent generation, one and one-half meter electro active TSOFC design, and there was good agreement between model and experiment, as shown below.

\[ \text{as the ratio of charge transfer to ohmic resistances (i.e., effectively a Wagner number (Prentice, 1991)) lower with design advancement, activation polarization can be characterized either via the Butler-Volmer relations or simplifications thereof (i.e., “ohmic” activation resistances or Tafel relations).} \]
Fig. 5.1.3 is a sample of model and experiment agreement across a domain of pressure ratios. The model transitions from small over predictions of current to slight under predictions as operating voltage increases. This is attributable to error in calculating the polarization. Actual concentration polarization phenomena have minor impact at low current densities (higher voltages) and are critical at high current densities (lower voltages). As more experimental data is released and modeling theory is developed, the polarization terms will be refined. Predictions are, however, consistently within 3%-5% of the experimental values. A foundational steady state model enabled the development of transient simulation capabilities.

![Comparison of Model and Experiment](a) 3 atm pressure.  
![Comparison of Model and Experiment](b) 15 atm pressure.

**Fig. 5.1.3:** Validation of model at (a) 3 atm pressure and (b) 15 atm pressure.

**Electrical Transient Response Model (Lagrangian Approach)**

Although electrochemical transient responses are fast in comparison to thermal-hydraulic transients, finite electrical transient effects still arise due to changes in constituent concentrations. Fig. 5.1.4 is a schematic of the hydrogen concentration profile along the fuel cell. The solid curve concentration profile corresponds to the cell’s initial steady state. At “t = 0”", the operating voltage idealistically decreases (i.e., cell potential behaves as a perfect step function) to accommodate an increase in load demand. The reactants supply, however, is predicated upon the prescribed fuel utilization and initial current. In accordance with Faraday’s Law, there is a decline in reactant concentrations when the load increases. This decrease continues until a new electrical steady state is reached (at t=T). Transient analyses are facilitated by focusing attention on individual fluid elements as they travel along the cell; this method is called a Lagrangian approach.
**Fig. 5.1.4:** Illustration of fuel stream transient dynamics.

Fig. 5.1.5 illustrates the Lagrangian approach. Consider an idealistic step change (e.g., decrease) in cell potential. During the cells’ transient response to load change, each fuel element approaches the cell with the same inlet characteristics, approximating invariant reactants supply\(^5\) (e.g., load fluctuating scenarios). The exit properties of each fluid element, however, depend upon its location at the time of the load hike, \(t=0^+\). Element 2 of Fig. 5.1.5, in the given example of a sudden decrease in cell potential, will have greater reactant depletion than element 1. This is because element 2 has longer exposure to electro-active area at the lower operating voltage. The electrical transient episode ensues until each fluid element approaching the cell again experiences an identical change in constituents. This occurs when element 3 reaches the end of the cell (note element 3 is at the beginning of the cell when the cell potential decreases). After element 3, every subsequent fluid element (e.g., element 4) enters at the new operating voltage; these elements then experience the same reaction phenomena. The time of the electrical episode is thus nearly the length of the cell divided by the fuel velocity in this idealized, yet physically pertinent, scenario. Note that this streamlined computational approach has two major assumptions with respect to the fuel stream which are now discussed.

**Fig. 5.1.5:** Individual fuel element locations at the time of the electrical change (Lagrangian approach).

\(^5\) Depending upon fuel flowrate, the timeframe of the electrical transients is a fraction of a second. Note that fuel processors have response times on the orders of seconds (e.g., partial oxidation/authothermal units) and minutes (e.g., steam reformers).
The first assumption is that the fuel stream effects dominate those of the oxidant stream. Note that the oxidant stream is not considered in the transient analysis. Typically oxidant is supplied in large excess quantities for thermal management of the cell. A key result is that changes in current will not have nearly the impact upon oxidant utilization as they will the fuel utilization. In fact, as will be shown, the reactant utilization effect of changes in load is a dominant factor in resolving the SOFC response; so a mitigated change in oxidant utilization due to the capacity of the oxidant stream precludes the computational burden required for simultaneously characterizing both fuel and oxidant streams (which will flow at differing velocities, further compounding difficulties). Additionally, electrode transient effects are not quantified; specifically within the anode. The given test case tubular design is cathode-supported and has relatively thin anodes, hence minimizing the need for analyzing transient chemical/electrochemical behavior within a porous medium. At an extreme, a zero-thickness anode would have no capacitive effects upon the transient system. The team, however, realizes that such capacitive effects may occur with pertinence within the other prevalent designs such as anode-supported SOFCs. The given approach and the transient electrode characterization spearheaded by (Gemmen et al., 2003) can thus complement each other, and again a collaboration within the SECA Infrastructure is motivated.

The fluid elements involved in the transient episodes were computationally “tracked.” This was done via two-dimensional arrays containing field variable information (i.e., axial position and time). The Lagrangian basis is that a fluid element occupies a certain location at a given time.

\[ \eta_{\text{element, fluid}} = \eta(\bar{x}, t) \]  

(5.1.6)

where the symbol \( \eta \) represents the properties of the fluid element in question (e.g., constituent partial pressures). The electrical power produced along the cell depends upon these properties. In accord with the Lagrangian methodology, the axial discretization (i.e., slice length) is compliant with the flows’ velocity and the temporal discretization (i.e., desired simulation time step) of the cell. The following equation and Fig. illustrate principle.

\[ \Delta \bar{x} = \bar{v} \Delta t \]  

(5.1.7)

Fig. 5.1.6: Correlation between temporal and spatial discretizations.

The following relation results.

\[ \eta_{\text{fluid, element}}(t + \Delta t) = \eta(\bar{x} + \Delta \bar{x}, t + \Delta t) \]  

(5.1.8)
The quasi-steady state electrochemistry assumption is incorporated, meaning that electrochemical phenomena occur as if at steady state, at the given instant. This is primarily based upon the large exchange current densities that SOFCs often engender. The Reynolds Transport Theorem is then utilized.

\[
\hat{n}_{j,\text{intermed}}(\bar{x} + \Delta \bar{x}, t + \Delta t) = \hat{n}_{j,\text{entering, slice}}(\bar{x}, t) + \Delta \hat{n}_j(\bar{x}, t) \quad (5.1.9)
\]

The "j" subscript represents hydrogen, oxygen and steam, and (5.1.9) accounts for the temporal change in constituents due to electrochemical oxidations.

\[
\hat{n}_k(\bar{x} + \Delta \bar{x}, t + \Delta t) = \hat{n}_{k,\text{intermed}}(\bar{x} + \Delta \bar{x}, t + \Delta t) + \hat{n}_{k,\text{shift, change}}(\bar{x}, t) \quad (5.1.10)
\]

**Fig. 5.1.7:** Variation of (a) current and (b) power with dimensionless time.
The subscript “$k$” represents hydrogen, steam, carbon monoxide and carbon dioxide. Equation (5.1.10) accounts for the temporal change in constituents due to the shift reaction, which was modeled via equilibrium chemistry due to the hot fuel stream and nickel catalyst within the anode. These temporal expressions of mass conservation enabled the transient electrochemical model to “march out” in time.

**Load-following Initial Analysis/Case Study: Idealized Potentiostatic-control Step Change**

A number of the settings are a compilation of test conditions reported by the Department of Energy.

<table>
<thead>
<tr>
<th>Table 5.1.1: Baseline conditions used in the transient case study.</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Pressure (atm)</strong></td>
</tr>
<tr>
<td><strong>Stoichiometric number</strong></td>
</tr>
<tr>
<td><strong>Fuel utilization (%)</strong></td>
</tr>
<tr>
<td><strong>Operating voltage (Volts)</strong></td>
</tr>
<tr>
<td><strong>Inlet methane mole fraction</strong></td>
</tr>
<tr>
<td><strong>Inlet hydrogen mole fraction</strong></td>
</tr>
<tr>
<td><strong>Inlet carbon monoxide mole fraction</strong></td>
</tr>
<tr>
<td><strong>Inlet steam mole fraction</strong></td>
</tr>
<tr>
<td><strong>Inlet carbon dioxide mole fraction</strong></td>
</tr>
</tbody>
</table>

An idealistic 0.1 V decrease (to 0.5V) occurs at “$t = 0^+$”. Besides fuel utilization (discussed shortly) and corresponding NOS, all other baseline conditions remain fixed (including reactants supply rate). The voltage drop event corresponds to the spikes shown in Fig. 5.1.7. The percentage increase in power is not as great as that of the increase in current density. Although current density increases, it was simultaneous with a voltage decrease. The result is a dampened rise in power.

**Fig. 5.1.8:** Axial profiles of hydrogen partial pressure as functions of time.
Subsequent to these initial spikes current and power decreases. Over half of the gain in current is lost, and the final power output is less than its initial value. These undesired effects stem from the decreased reactant concentrations along the cell. An explanation follows.

Fig. 5.1.8 shows the decrease in hydrogen partial pressures throughout the time period (T) of the electrical response. The initial increase in current, shown in Fig. 5.1.8 consumes an excess of the fuel stream’s hydrogen content. An effect-and-counter-effect then develops between current generation and fuel utilization.

![Graph showing Increase in Fuel Utilization As a Function of Dimensionless Time](image)

**Fig. 5.1.9:** Increase in fuel utilization during electrical transient episode.

Fig. 5.1.9 illustrates the rise in fuel utilization during the transient episode. The additional invariant fuel supply results in an increase in fuel utilization. The increase in fuel utilization, in turn, promotes current reduction, because reactant depletion issues (e.g., concentration polarization, smaller Nernst potentials) become more pronounced. The effects of each upon the other cause current and fuel utilization to change accordingly until current electrochemically “matches” the original reactants supply rate and the new operating voltage. Fuel utilization then reaches a terminal value, and changes in electricity cease; this is neglecting second order effects of diminutive temperature rise during the timescale of electrical transients.

The current reduction here causes the power to fall below its initial value, because the decrease in operating voltage supersedes the net increase in current. An attempt at rapidly increasing the power output of a cell stack, via independent load response, may actually lead to a rapid decrease in power generation; additionally, too large an increase in current may lead to dangerously high fuel utilizations (e.g., greater than 95%). As will be shown, however, appropriate process settings facilitate using this rapid response controls scheme.
Fig. 5.1.10: Current and fuel utilization transients during transient episode.

Fig. 5.1.10 illustrates the trends in current density and fuel utilization caused by an idealized step decrease in cell potential. The additional current density and invariant fuel supply results in an *increase* in fuel utilization. The increase in fuel utilization, in turn, promotes current *reduction*, because reactant depletion issues (e.g., concentration polarization, smaller Nernst potentials) become more pronounced. The effects of each, upon the other cause current density and fuel utilization to change accordingly until current density electrochemically “matches” the original and invariant reactants supply rates and the new operating voltage. Fuel utilization then reaches a terminal value, and changes in electricity cease; this is neglecting second order effects of diminutive temperature rise during the timescale of *electrical* transients and, again, porous media capacitive transients within the thin TSOFC anode of the present case study.

The current density reduction here causes the power to fall below its initial value, because the decrease in operating voltage supersedes the *net* increase in current density. An attempt at rapidly increasing the power output of a cell stack, via independent load response, may actually lead to a rapid decrease in power generation; additionally, too large an increase in current may lead to dangerously high fuel utilizations (e.g., greater than 95%). It is thus imperative that simulations well-characterize the viable domains for timely and effective cell response to load variation.
Response Characteristics to Load Current Variation

The potentiostatic methodology, wherein load-following was presumed to occur with change in cell potential as the stimulus is not the actual means of PES (current demand) control, but this pilot approach was used for various reasons. First, it enabled the establishment of a fundamental, yet viable, time constant (i.e., the quotient of fuel flow passage length divided by fuel velocity) that can be used to help characterize the transients associated with electrical stimuli (especially if it is clearly resolved that electrode transients occur relatively fast). Secondly, cell potential is a more suitable fuel cell control condition, regarding simulation, than is current demand, because an established cell potential allows for a dirichlet boundary condition to be imposed. This is as opposed to a current (density) wherein this Neumann boundary condition will invariably have non-uniformities. This isopotential modeling approach inherent within the potentiostatic transient methodology was thus incorporated as a “kernel” algorithm of the enhanced model, wherein variation in current demand (as opposed to cell potential) was the stimulus to allow for PES design studies.

Again the PES systems integration emphasis required the model accommodate Fig. 5.1.11 illustrates a sudden increase in current demand at time $t=0^+$, for three different scenarios of initial fuel utilization for a Siemens Westinghouse TSOFC. Voltage decreases correspondingly in two stages. The first decline is a sharp decrease corresponding to a sudden movement along the right of the polarization curve (i.e., toward increasing current density). This is modeled to occur fairly instantaneously due to the fast nature of electrochemical transients. The additional, more gradual, decrease in cell potential is the accumulated effect of reactant depletion. Fig. 5.1.12 further illustrates this phenomenon.

![Fig. 5.1.11: Illustration of SWPC TSOFC response to a galvanostatic control.](image-url)
Graphical movement from state 1 to state 2 (i.e., the “polarization curve” effect) corresponds to the initial spike in cell potential. This path is constrained to occur along the initial condition, lower fuel utilization polarization curve; subsequently, the reactant depletion effect causes a vertical decline to state 3 (i.e., the “reactant depletion/accumulation” effect), which corresponds to the final steady state point for the same current but higher fuel utilization. Referring again to Fig. 5.1.12, it is noted that there are staged decreases in cell potential, as a result of progressive reactant depletion and the requirement to maintain the new current demand. The transient episode is thus multiples of the time constant (here denoted as $\tau$), since the point of steady state attainment is that wherein each fuel parcel enters the cell electroactive area and “sees” a fairly stable cell potential. One then denotes that a potentiostatic step change, as opposed to a galvanostatic step change, control capability results in shorter electrical transients. Notice that larger initial fuel utilizations prolong the relative transient due to enhanced fuel depletion effects. This is further illustrated in the following figure.

**Fig. 5.1.13:** Impact of initial fuel utilization upon fractional voltage drop due to “polarization curve” effect.
The larger the initial fuel utilization, the more prevalent the reactant depletion effects that manifest via lowered Nernst potentials and limiting current densities; hence, the “reactant depletion/accumulation” effect of hikes in current is substantially more influential. As illustrated in Fig. 5.1.13, the larger the initial fuel utilization, the smaller the “polarization curve” effect in comparison to the “reactant depletion/accumulation” effect. Regarding current ripple, the amplitudes and periodicities thus far tested can cause rapid oscillations along the polarization curve, without substantial realization of reactant depletion/accumulation effects. This is graphically shown in the PES studies discussed within this report.

Note that this capability to characterize SOFC response to step changes in current demand has enabled the simulation of any arbitrary load variation (e.g., fluctuation and following). This is done by using the principle of superposition, wherein any current profile can be temporally discretized as a successive number of step changes, and keeping “track”, of reactants parcels (ref. above commentary) throughout the entire time domain. This feature utility has been the heart of the integrated application’s ability to resolve SOFC subsystem response to PES dynamics.

5.1.1.2 PSOFC Model

A larger emphasis of the SECA program has been the planar design of the SOFC due to its high efficiency, modularity and fuel flexibility. To this end, PSOFCS models have been developed based on the first principle which would enable integration of the model with the PES and the BOPS models. At first, a 1-D discrete model has been developed in a low cost MATLAB/ Simulink platform which discretizes the planar cell along its length.

For accurate prediction of the effects of system interactions on the PSOFC, spatial variation of different parameters is to be considered. Therefore, a two dimensional PSOFC model has been developed, based on discretization in both directions.

**One-dimensional Discrete PSOFC Model**

The mathematical model of the 1-D planar cell was designed to accept required system inputs (reactant stream flow rates, compositions, and temperatures, cell geometric parameters, and cell current) and return the corresponding outlet conditions.

![Fig. 5.1.14: One-dimensional homogenous slab model for PSOFC providing discretizations involving finite-difference method. Temperature, current, and molar-flow rates of air and fuel are calculated each time for n = 1, .., N.](image)

The cell temperature (T) in the 1D model, as shown in Fig. 5.1.14, is computed from the time-dependent solution of the energy balance equation of each of the discrete slab:
\[ \rho C_p \frac{\partial T}{\partial t} - k \frac{\partial^2 T}{\partial x^2} = Q \]  

(5.1.11)

where \( C_p \) is the combined specific heat at constant pressure, \( \rho \) is the mass density of the control volume and \( Q \) represents the sum of the resistive heating and the heat generated by the electrochemical and shift reactions taking place within the slab,

\[ Q = \left( \frac{V_{in} - V_{op}}{l} \right) j_i + (-\Delta H_{shift}) \]  

(5.1.12)

where \( V_{op} \) is the operating voltage, \( j_i \) is the current density, \( l \) is the cell thickness, \( \Delta H_{shift} \) is the enthalpy of the shift reaction in the control volume(slab) and \( V_{in} \) is the thermal neutral voltage, given as:

\[ V_{in} = -\frac{\Delta H}{nF} \]  

(5.1.13)

where, \( \Delta H \) is the enthalpy of the main reaction, \( n \) is the molar flow rate of the fuel. To approximate the second-order partial-differential equation, a finite-difference method by central differences (Constantinides et al, 1999) is used.

\[ \frac{\partial^2 T}{\partial x^2} \approx \frac{1}{\Delta x^2} \left[ T_{n+1,t} - 2T_{n,t} + T_{n-1,t} \right] \]  

(5.1.14)

By approximating \( \frac{\partial T}{\partial t} \) as a simple forward difference and substituting \( [(T_{j+1}-T_j)/\Delta t] \) for \( \frac{\partial T}{\partial t} \), substituting (5.1.12) into (5.1.11), and marching the solution through time yields the Euler’s explicit-integration scheme for the determination the discrete temperature variation.

The expression for temperature becomes

\[ T_{n,t+1} = T_{n,t} + \frac{\kappa \Delta t}{\rho C_p \Delta x^2} (T_{n+1,t} - 2T_{n,t} + T_{n-1,t}) + \frac{\Delta t}{\rho C_p} Q. \]  

(5.1.15)

Given the temperature distribution along the fuel cell at time=0, Equation 5.15 is used to advance the solution in time for each successive time step. Fig. 5.1.15 shows the temperature profile of the discrete model with time. These temperature solutions are then used to solve for the other variables that are not described by a partial differential equation (5.1.11).

Boundary conditions are set such that the temperature at the inlet of the cell is equal to the inlet streams temperature, and at the outlet, the cell is radiating to an environment with a fixed temperature. For example, the stack enclosure temperature can be set to 5 degrees less than the inlet temperature \( (T_\infty = T_{in}-5) \).
Based on the temperature profile obtained using Equation 5.1.15, the Nernst or reversible potential, current density, heat generation, updated flow rates and re-equilibration of the shift reaction, are then calculated at each of the nodal points representing a stream-wise position in the stack. In the course of each of the iteration, the assumed operating voltage is used to determine the current density in each of the control volumes throughout the cell using

\[ j_n = \frac{E_n - V_{op}}{ASR_n} \]  

(5.1.16)

where ASR<sub>n</sub> is the local temperature-dependent area-specific resistance and E<sub>n</sub> is the Nernst potential which is defined as

\[ E_n = -\frac{\Delta G}{nF} \]  

(5.1.17)

\( \Delta G \) is the change in the Gibb’s free energy. The current density as in (5.16) is then summed to compute the total cell current:

\[ I = \sum_{n=1}^{steps} \frac{(E_n - V_{op})(ASR_n)}{nF} \]  

(5.1.18)

The local current-density values are used to determine the change in stream composition based on the electro-chemical reaction in each control volume. The fuel exit-composition of each control volume is equilibrated with respect to the shift reaction before entering the downstream control volume.

In order to enable the specification of the SOFC current and compute an operating voltage, an iterative secant root finding method is employed which varies the assumed operating voltage until the computed total current result matches the specified input current.
**Two-dimensional PSOFC Model**

For accurate prediction of the effects of system interactions on the PSOFC, one needs to analyze the PSOFC internal parametric variations. Because a transient model of the PSOFC cannot predict the spatial dynamics, a spatio-temporal electro-thermo-chemical model of the PSOFC (in Simulink), is developed which provides spatial discretizations of the cell. This model is designed to accept required system inputs (reactant stream flow rates, compositions, and temperatures, cell geometric parameters, and cell current) and computes the corresponding spatial properties of the fuel cell.

The model represents cross-flow geometry for the fuel and air streams as shown in Fig. 5.1.16. A single 10cm x 10cm cross-flow SOFC was discretized using a 30 x 30 control volume grid, with each control volume approximated as having homogenous properties throughout. The outer 1 cm perimeter is treated as electrochemically inactive seal area, leaving a 64 cm² active cell area. Radiation boundaries are applied to each exit stream boundary, while both reactant inlet faces are treated as adiabatic (insulated), but open (mass inflow) boundaries. The primary transient variable ‘temperature’ is integrated through time using the Euler explicit method, giving a system of equations of the form: $[T_{t+1}] = [A][T_t] + [B]$.  

The vector $T$ is of rank 900 (30 x 30). If the full matrix $[A]$ were stored, it would have nearly one million entries, of which less than 4500 would be non-zero. Therefore, a sparse storage pointer reference scheme is used such that $[A]$ and a pointer reference array are dimensioned [900, 5] resulting in a near 100 fold reduction in memory requirements and operation count.

![Spatial homogenous model for the PSOFC providing two-dimensional discretizations involving finite-difference method.](image)

**Fig. 5.1.16**: Spatial homogenous model for the PSOFC providing two-dimensional discretizations involving finite-difference method.
Such efficiencies are important to achieve the extremely short iteration times required when coupled to the PES model.

The air and fuel flows are each modeled as 24 independent parallel 1-D channels, in the same way that the flows were treated in the 1-D model. The electrochemical model also follows directly from the 1-D model, again assuming an isopotential condition across the surface of the anode and cathode. The resulting model will compute the temporal evolution of temperature, composition, and resulting current density distributions on the 30 x 30 grid. The overall voltage/current operating point corresponding to the current PES state will be passed back to the PES model.

The cell temperature (T) in the two-dimensional (x and y) model, as shown in Fig. 5.1.16, is computed from the time-dependent solution of the following equation:

\[
\rho C_p \frac{\partial T}{\partial t} - k \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) = Q
\]

(5.1.19)

\[
Q = \left( \frac{V_{in} - V_{op}}{1} \right) j_i + \left( -\Delta H_{\text{shift}} \right)
\]

(5.1.20)

\[
V_{in} = -\frac{\Delta H}{nF}
\]

(5.1.21)

where \(V_{in}\) is the thermal neutral voltage, \(V_{op}\) is the operating voltage, \(j_i\) is the current density, \(\rho\) is the mass density of the control volume, \(C_p\) is the combined specific heat at constant pressure, \(l\) is the cell thickness, \(\Delta H_{\text{shift}}\) is the enthalpy of the shift reaction in the control volume, \(\Delta H\) is the enthalpy of the main reaction, \(n\) is the molar flow rate of the fuel and \(k\) is the thermal conductivity of the fuel cell. To approximate the second-order partial-differential equation, a finite-difference method using central differences is used:

\[
\frac{\partial T^2}{\partial x^2} \approx \frac{1}{\Delta x^2} \left[ T_{m+1,n,t} - 2T_{m,n,t} + T_{m-1,n,t} \right]
\]

(5.1.22a)

\[
\frac{\partial T^2}{\partial y^2} \approx \frac{1}{\Delta y^2} \left[ T_{m,n+1,t} - 2T_{m,n,t} + T_{m,n-1,t} \right].
\]

(5.1.22b)

By approximating \(\frac{\partial T}{\partial t}\) as a simple forward difference and substituting \([\left(T_{j+1} - T_j\right)/\Delta t]\) for \(\frac{\partial T}{\partial t}\), substituting (5.1.20) into (5.1.19), and marching the solution through time yields the Euler’s explicit-integration scheme for the determination the spatial temperature variation. With the step size \(\Delta x = \Delta y\), the expression for temperature becomes

\[
T_{m,n,t+1} = T_{m,n,t} + \frac{k\Delta t}{\rho C_p \Delta x^2} \left( T_{m-1,n,t} + T_{m,n-1,t} + T_{m,n+1,t} + T_{m+1,n,t} - 4T_{m,n,t} \right) + \frac{\Delta t}{\rho C_p} Q.
\]

(5.1.23)

Fig. 5.1.17(a) shows the spatial temperature distribution in the planar cell. In the course of each of the iteration, the assumed operating voltage is used to determine the current density in each of the control volumes throughout the cell using

\[
ji_{m,n} = \frac{(En_{m,n} - V_{op})}{\text{ASR}_{m,n}},
\]

(5.1.24)

where \(\text{ASR}_{m,n}\) is the local temperature-dependent area-specific resistance and \(En_{m,n}\) is the Nernst potential which is defined as
\[ E_{n,m} = -\frac{\Delta G}{nF}, \]  

(5.1.25)

\( \Delta G \) is the change in the Gibb’s free energy. The current density as in (5.24) is then summed to compute the total cell current:

\[ I = \sum_{m=1}^{\text{steps}} \sum_{n=1}^{\text{steps}} \Delta x_n \Delta y_n (E_{n,m} - V_{op})/(\text{ASR}_{m,n}) \]  

(5.1.26)

The local current-density values are used to determine the change in stream composition based on the electro-chemical reaction in each control volume. The fuel exit-composition of each control volume is equilibrated with respect to the shift reaction before entering the downstream control volume. These local current-flux values are used to determine the change in stream composition based on the reaction in each control volume:

\[ \text{H}_2 + \frac{1}{2} \text{O}_2 \rightarrow \text{H}_2\text{O}. \]  

(5.1.27)

The fuel exit-composition of each control volume is equilibrated with respect to the shift reaction before entering the downstream control volume. Equation (11) is used to adjust the compositions to enforce the shift equilibrium constraint at the entrance to each control volume:

\[ K_p = e^{-\Delta G_o / R T} = \frac{(p_{CO_2} + \omega) \cdot (p_{H_2} + \omega)}{(p_{CO} - \omega) \cdot (p_{H_2O} - \omega)} \]  

(5.1.28)

where \( \Delta G_o \) is a temperature-dependent variable, \( p_{CO_2}, p_{H_2}, p_{CO}, \) and \( p_{H_2O} \) are the partial pressures of CO\(_2\), H\(_2\), CO, and H\(_2\)O, respectively, \( K_p \) is the constant of equilibrium, \( R \) is the universal gas constant, and \( \omega \) is adjust in the gas compositions due to the shift reaction.

Results of comparison for the temperature, current density are shown in Fig. 5.1.17 below. It is possible to show the results along the entire length of the 1D model over a period of time; however, the 2D model only allows a snapshot of the fuel cell surface for a single point of time.
Fig. 5.1.17: (a) Outputs for 1D and 2D fuel cell models. Spatial temperature profile and (b) Current flux outputs for 1D and 2D fuel cell models

5.1.2 PES Model

The voltage of the SOFCS varies with current drawn by the load, decreasing significantly at higher load currents. Therefore, a PES is needed to process the raw output power from the stack and provide power to the load at constant DC or AC voltage. Typically, the PES include multiple interconnected power converters (typically a DC-DC converter followed by a DC-AC converter for stationary applications and DC-DC converter for mobile applications). The switching scheme in such power converters can be based on pulse-width modulation (PWM), resonant, quasi-resonant, soft-switched, or line-commutated. Furthermore, the topological structures of these converters can be vastly different from each other. As such, the mathematical models of the PES may include discontinuous differential equations, discrete differential equations, functional differential equations, digital automata, impulsive differential and non-smooth differential
equations, ordinary and even partial differential equations. In addition, these models include system-level constraints.

The traditional approach to modeling such systems using averaged models (Middlebrook et al., 1977 a, b) is inadequate and in many cases, results based on them yield inaccurate results (Lee, 1990). These averaged models completely neglect the impact of switching frequency and hence can not predict the dynamics on fast scale. Instability in standalone or integrated converter can occur on a slow as well as on a fast scale (Mazumder et al., 2001a). Secondly, even the slow-scale averaged model may have more than one equilibrium solution or more than one stable orbit. A linearized small-signal analysis ignores the presence of these other solutions. Therefore, a small-signal analysis can not predict anything about the domain of attraction of the nominal solution or orbit. If two of the solutions are stable, then the system will have two operating points, one of which is the nominal solution. This possibility is completely ignored in linearized average models. Consequently, small-signal averaged model can not predict the post-instability dynamics.

To model a PES, one needs a unified modeling framework, which can handle any type of dynamical system\(^6\) with varying levels of detail. Such a unified framework is an indexed collection of dynamical systems along with a map for transitions among them. A transition occurs whenever the state satisfies certain conditions, given by its membership in a specified subset of the state space. Hence, the entire system can be thought of as a sequential patching together of dynamical systems with initial and final states and with the transitions performing a reset to a generally different initial state of a generally different dynamical system whenever a final state is reached. Formally, the unified model \(U_{\text{model}} = (P, C_{\text{CDS}}, C_{\text{ATM}}, C_{\text{AJTM}}, C_{\text{DDC}}, C_{\text{CJS}}, C_{\text{CJDM}})\) is a dynamical system with the following elements: \(P\) is the set of discrete states; \(C_{\text{CDS}} = \{C_{\text{CDS}_p}\}_{p \in P}\) is the collection of continuous dynamical systems, where each \(C_{\text{CDS}_p} = (Y_p, S_p, T_p, U_p)\) is a dynamical system with continuous state spaces \((Y_p)\) and dynamics \((T_p)\) and as well as a set of continuous controls \((U_p)\); \(C_{\text{ATM}} = \{C_{\text{ATM}_p}\}_{p \in P}\), where \(C_{\text{ATM}_p} \subset Y_p\) for each \(p \in P\) is the collection of autonomous (state-dependent) transition sets; \(C_{\text{AJTM}} = \{C_{\text{AJTM}_p}\}_{p \in P}\) is the collection of autonomous jump-transition maps; \(C_{\text{DDC}} = \{C_{\text{DDC}_p}\}_{p \in P}\), is the collection of discrete dynamics and controls; \(C_{\text{CJS}} = \{C_{\text{CJS}_p}\}_{p \in P}\), where \(C_{\text{CJS}_p} \subset Y_p\) is the collection of controlled jump sets; \(C_{\text{CJDM}} = \{C_{\text{CJDM}_p}\}_{p \in P}\) is the collection of jump destination maps (Mazumder, 2001c).

Illustration

To illustrate the modeling of the PES, let us consider the architecture as in Fig. 5.1.18. The model consists of a DC-DC (boost) converter to step-up the PSOFC output voltage to a higher

\(^6\) A dynamical system is defined as a system \(\Sigma = (Y, S, T)\), where \(Y\) is an arbitrary topological space in the state space of \(\Sigma\). The transition semi-group \(S\) is a topological semi-group with identity and \(T\) is an extended transition map \(T: Y \times S \rightarrow Y\) is a continuous function satisfying the identity and semi-group properties.
intermediate DC bus voltage. A DC-AC converter (inverter) is further used to convert the output of the DC-DC boost converter, to feed the AC load. For this purpose, a pulse-width-modulated voltage source inverter (VSI) is used, due to its simpler control scheme. The high frequency harmonic content of the output of the VSI is eliminated by the output filter.

The PES is a piecewise linear (PWL) systems, whose state-space equations can be expressed as

$$\dot{x}(t) = A_i x(t) + B_i u(t) + C_i v(t)$$

where \( x(t) \in \mathbb{R}^n \) are the states of the system, \( u(t) \in \mathbb{R}^m \) and \( v(t) \in \mathbb{R}^p \) represent the inputs and the outputs of the system, respectively. The matrices \( A_i, B_i \) and \( C_i \) describe the dynamics of the state-space model for the \( i \)th switching state of the system. The sequence and the duration of the switching states are governed by the closed loop controller of the system.

As an illustration, the DC-DC boost converter as in Fig. 5.1.18 can be modeled using (5.1.29) as

$$\dot{x}_1 = A_1 x_1 + B_1 u_1 + C_1 v_1$$

where, \( x_1 \) represents the state vector, given as \([i_L \ v_C]^{T}\) and \( u_1 \) is the input vector of the system, given as \([V_{stk} \ 0]^{T}\) and \( v_1 \) is the output vector \([0 \ i_{bus}]^{T}\). When the switch \( S \) of the boost converter is turned ON, the energy content in the inductor \( L \) increases and the system of Equation (5.1.30) becomes:

$$\dot{x}_1 = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} x_1 + \begin{bmatrix} -1/L \\ 0 \end{bmatrix} u_1 + \begin{bmatrix} 0 \\ -1/C \end{bmatrix} v_1.$$  (5.1.31a)

And when the switch \( S \) is turned OFF, the stored energy in the inductor is transferred to the output capacitor \( C \) of the converter through the diode \( D \) and Equation (5.1.30) becomes:

$$\dot{x}_1 = \begin{bmatrix} 0 & -1/L \\ 1/C & 0 \end{bmatrix} x_1 + \begin{bmatrix} 1/L \\ 0 \end{bmatrix} u_1 + \begin{bmatrix} 0 \\ -1/C \end{bmatrix} v_1.$$  (5.1.31b)

Therefore, the DC-DC boost converter can be completely described as

$$\dot{x}_1 = \begin{bmatrix} 0 & -\bar{s}/L \\ \bar{s}/C & 0 \end{bmatrix} x_1 + \begin{bmatrix} 1/L \\ 0 \end{bmatrix} u_1 + \begin{bmatrix} 0 \\ -1/C \end{bmatrix} v_1.$$  (5.1.32)

where the switching function \( s (\bar{s} = NOT(s)) \) represents the turn ON and turn OFF states of the switch \( S \). The switching function is determined to obtain the required bus voltage.
Similarly the VSI, as shown in Fig. 5.1.18, can be modeled as in (5.1.29)
\[
\dot{x}_2 = A_2 x_2 + B_2 u_2 + C_2 v_2
\]  
(5.1.33)
where, \(x_2\) represents the state vector, given as \([i_{bus} v_{out}]^T\) and \(u_2\) is the input vector of the system of equation and is given as \([v_c 0]^T\) and \(v_2\) is the output vector \([0 i_{load}]^T\).

The switch pairs SW1-SW3 and SW2-SW4 switch in complement with a very small time delay between the switching of SW1 (SW3) and SW2 (SW4). When the switch pair SW1-SW3 turned ON, (5.1.33) becomes
\[
\dot{x}_2 = \begin{bmatrix}
0 & -1/L_f & 0 \\
1/C_f & 0 & -1/C_f \\
\end{bmatrix} x_2 + \begin{bmatrix}
1/L_f \\
0 \\
\end{bmatrix} u_2 + \begin{bmatrix}
0 \\
-1/C_f \\
\end{bmatrix} v_2.
\]  
(5.1.34a)

When the switch pair SW2-SW4 turned ON, the system of equation (13) becomes
\[
\dot{x}_2 = \begin{bmatrix}
0 & 1/L_f & 0 \\
-1/C_f & 0 & -1/C_f \\
\end{bmatrix} x_2 + \begin{bmatrix}
1/L_f \\
0 \\
\end{bmatrix} u_2 + \begin{bmatrix}
0 \\
-1/C_f \\
\end{bmatrix} v_2.
\]  
(5.1.34b)

The overall VSI can be described as
\[
\dot{x}_2 = \begin{bmatrix}
0 & (-s_a + s_b)/L_f & 0 \\
(s_a - s_b)/C_f & 0 & -1/C_f \\
\end{bmatrix} x_2 + \begin{bmatrix}
1/L_f \\
0 \\
\end{bmatrix} u_2 + \begin{bmatrix}
0 \\
-1/C_f \\
\end{bmatrix} v_2
\]  
(5.1.35)

The switching function \(s\) of the VSI is given as \(s = [s_a s_b]\), where \(s_a\) represent the ON state of the SW1-SW3 pair and \(s_b\) represents the ON state of the SW2-SW4 pair. The ON time of \(s_a\) and \(s_b\) are generated by a sinusoidally modulated switching sequence to obtain an averaged sine wave AC at the output of the VSI. Combining (5.1.32) and (5.1.35), the complete PES system can be expressed as:-
\[
\dot{X} = \begin{bmatrix}
0 & -\bar{s}/L & 0 & 0 \\
\bar{s}/C & 0 & -1/C & 0 \\
0 & 1/L_f & 0 & (-s_a + s_b)/L_f \\
0 & 0 & (s_a - s_b)/C_f & 0 \\
\end{bmatrix} X + \begin{bmatrix}
1/L \\
0 \\
0 \\
-1/C_f \\
\end{bmatrix} U + \begin{bmatrix}
0 \\
0 \\
0 \\
-1/C_f \\
\end{bmatrix} V
\]  
(16)

where \(X = [i_L v_C i_{bus} v_{out}]^T\) is the state vector, \(U\) is the input vector of the system, given as \([V_{stk} 0 0 0]^T\) and \(V\) is the output vector, given as \([0 0 0 i_{load}]^T\).

5.1.2.1 Environment for PES Model Development

In earlier phase of the project, the focus of PES modeling was to identify and compare the architecture of the PES in the stationary applications. To attain this objective, Saber Designer simulation platform was used. Among the commercially available simulators, Saber Designer has the most extensive (over 30000) library of mathematical computer models in power-electronics components and systems, electromechanical-energy conversion, hydraulics, thermal, magnetic, control systems, and signal processing. The SOFC model developed in FORTRAN was incorporated in the Saber PES model using dynamic link libraries (.DLL) and a MAST template.
One of the issues identified in the prior phase of the project is the difficulty in integration of the subsystem models. Again, the increasing demand of reduction of the cost for the simulation platforms lead us to identify a cheaper simulation platform, which would not only provide avenue for implementation of the PES model, but also would ease the integration with other subsystem models without multiple interfaces. For the lower cost and easier integration of the SOFC PCS subsystem models, MATLAB/Simulink has been identified as the suitable platform.

SimPowerSystems extends Simulink with tools for modeling and simulating basic electrical circuits and detailed electrical power systems. These tools allow modeling the generation, transmission, distribution, and consumption of electrical power, as well as its conversion into mechanical power. This is well suited to the development of complex, self-contained power systems, such as those in automobiles, and power utility applications.

5.1.2.2 PES Topologies

For the study, three PES topologies were selected for SOFC stationary power applications. The specifications of the PES for SOFC power conditioning were,

Output voltage: ~120 V (phase voltage)
Output power: 5 kW
Input: 72 V SOFC stack.

As illustrated in Figs. 5.1.19(a)-(d), the PES topologies essentially consist of a DC-DC stage to step up the voltage from 72 V to a value suitable for power conversion in the next stage. The DC-DC converter uses a PWM controller to control its switching. The PWM controller consists of a three-pole, two-zero voltage mode compensator and a PI current controller.

Fig. 5.1.19(a) shows the traditionally used thyristor-based line commutated current-source inverter (CSI) topology (El-Tamaly et al., 2000, Naik et al., 1995). The switches in the three legs switch at 60 Hz with a 120° shift between the three phases. Fig. 5.1.18(b) shows the commonly used self-commutated PWM voltage-source inverter (VSI) (Konishi et al., 1998). The switching frequency is determined by the PWM controller circuitry. And Fig. 5.1.19(c) shows the high-frequency-transformer-isolated cycloconverter topology (Kawabata et al., 1990). This topology is similar to the topology in Fig. 5.1.19(b), except for the presence of the high-frequency transformer between the DC-AC and the AC-AC stages. The advantage of using such a topology is that the bulky line transformers, used for isolation, is replaced by a much smaller high-frequency transformer. However, such a topology uses an extra stage for AC-AC conversion. Fig. 5.1.19d shows the topology with transformer isolation in the DC-DC stage, leading to reduction in the number of stages and the number of switching elements.

PES input current depends on both the application loads as well as its switching mechanism. Filters are used to reject the high frequency harmonic components to a large extent but the low frequency ripple cannot be eliminated unless large bulky filters are used. Since the different PES topologies considered in this study have different switching schemes and high frequency rejection mechanisms, the harmonic content of input current for the three cases are vastly different. Therefore each PES will impose different stresses on the SOFCs, and an in-depth understanding of the effect of the fast- and slow-scale ripple (Mazumder, Nayfeh, and
Boroyevich, 2001(a)-(d) is necessary to propose any reliability solution. Figs. 5.1.20 - 5.1.23 show the steady state input current and their corresponding frequency domain spectrum respectively for the topologies of Figs. 5.1.19(a) - (d). The line-commutated topology imposes a current ripple at the line-frequency and its lower order harmonics, while the topologies in (b) and (c) impose a high-frequency (switching) and a low-frequency (line) current ripple on the SOFC.
Fig. 5.1.19: The four topologies used for studying the impact of power-electronics on the SOFCS, (a) represents line-commutated topology, (b) represents self-commutated topology, (c) represents transformer-isolated DC-AC converter topology, (d) represents transformer-isolated DC-DC topology.

Fig. 5.1.20: Steady state (a) input current characteristics and (b) frequency domain characteristics for the line-commutated CSI topology of Fig. 5.1.19(a).
Fig. 5.1.21: Steady state (a) input current characteristics and (b) frequency domain characteristics for the self-commutated PWM VSI topology of Fig. 5.1.19(b).

Fig. 5.1.22: Steady state (a) input current characteristics and (b) frequency domain characteristics for the high-frequency transformer-isolated cycloconverter topology of Fig. 5.1.19(c).
Fig. 5.1.23: Steady state (a) input current characteristics and (b) frequency domain characteristics for the high frequency transformer isolated Ćuk-VSI topology of Fig. 5.1.19(d).

Fig. 5.1.24: Implementation of the PES model using SimPowerSystem toolbox in Simulink.

In the later phase of the project, the PES models are ported into a low-cost Simulink platform. Fig. 5.1.24 shows the implemented circuit model of the residential PES topology using SimPowerSystem toolbox.

5.1.3 BOPS Modeling

PES response to changes in electrical loads depends on the response of the SS, which in turn depends on the BOPS response. Thus, steady and transient models of the BOPS must also be taken into account for accurate analysis of the overall FCS. During Phase I of the project, the
main objective was to establish a feasible system super-configuration which provides both high efficiency and reliability. Based on this super-configuration, detailed dynamic models for each component were developed and then coupled in order to generate a system level dynamic model. Using the system level dynamic model, parametric studies were done in order to determine system behavior for various combinations of system-level parameters and components locations and dimensions. The results of the parametric studies were used to determine the most promising subset of this super-configuration i.e. reduced super configuration based on system response, fuel consumption, capital cost, operational constraints, etc. Fig. 5.1.25 shows the proposed SOFC based auxiliary power unit reduced super-configuration. During Phase II, the resulting reduced super-configuration was subjected to a large scale synthesis/design optimization while taking into account its effects on system operation, i.e. on the dynamic response of the system.

The BOPS consists of a fuel-processing subsystem (FPS) to convert natural gas to a hydrogen-rich reformate gas and a thermal management and power recovery subsystem to maintain fuel and oxidant temperatures and pressures at prescribed levels for the SOFCs and provide energy for the fuel reforming. The models developed for these subsystems can be used to analyze the thermodynamic, kinetic, and geometric characteristics of FCSs and their components at full and part loads.

**Fig. 5.1.25:** Super-configuration of the proposed SOFC based power system established prior to the parametric study and optimization process.
5.1.3.1 Fuel Processing Subsystem (FPS)

The main objective of the FPS is to convert the natural gas to the hydrogen-rich reformate gas that will provide the hydrogen fuel required for the operation of the SOFCS. The FPS configuration (see Fig. 5.1.25) shows that the necessary amount of fuel feed, consisting primarily of methane, is taken from a pressurized storage tank. For stationary applications, the fuel may be supplied by either a pressurized tank or a commercial line. Regardless of the fuel supply system, the operational pressure in the reactor is never higher than 3 bars. After entering the system, a fraction of the fuel is supplied to the reforming line while the remaining fuel is used for combustion. The methane flowing down the reforming line is preheated by passing it through a compact, plate-fin type heat exchanger (HX III) and is then mixed with steam produced in a steam generator (C) in a reformer mixer (H) before entering the steam-methane reformer (A). The energy needed to drive the endothermic reforming reaction in the reformer is provided by the combustion gases leaving the combustor (B). The reformate gases coming out of the reformer are stored in a tank (FT), which then acts as an energy buffer between the BOPS and the SS. This permits rapid supply of fuel to the SS when the stack demand is larger than the reformer production rate. One of the most important features of the proposed configuration is the recirculation of the anode products into the reformer mixer. The reactants coming out of the anode are rich in water vapor, which reduces the amount of new vapor required from the steam generator. This in turn yields a smaller steam generator and a smaller water tank (G).

5.1.3.2 Thermal Management Subsystem (TMS) and Work Recovery and Air Supply Subsystem (WRAS)

The combustion mixture, supplied to the combustor (B), consists of air taken from the air tank, a percentage of the hydrogen-depleted anode exhaust gas, and methane that bypasses the reforming line. Burning the residual hydrogen in the stack tail gas translates into a decreased consumption of additional methane in the burner and, therefore, to increased efficiency of the configuration. Furthermore, using air bleed from the stack introduces additional increments in efficiency by eliminating the compression stage. However, air coming from the stack is rich in nitrogen, the amount depending on stack requirements. Therefore, using it depends on whether or not its heat capacity is enough to meet the thermal management needs. After providing the required thermal energy for the endothermic reforming reaction, the combustion gases are split into three streams, the first preheats the methane (HXIII), the second is passed through the steam generator where it supplies the necessary energy for producing the steam consumed in the reforming process, and the third is used to preheat the air flowing into the stack (HX IV). The mass flow of hot gases through these components is controlled by the methane and steam water exit temperature from the HX III and steam generator. Finally, the combustion gas streams are mixed together before being expanded (E) and exhausted to the atmosphere.

In the BOPS and the SS, the temperatures of a number of critical components (particularly the SOFCS and the pre-reformer of the FPS) have to be carefully controlled, and the flow and utilization of energy from several sources within the configuration have to be managed efficiently in order to achieve high overall efficiencies. Therefore, the TMS plays a significant role in the operation of the FCS. Its major functions include maintaining the stack operating temperature in the appropriate range, bringing the hydrogen-rich reformate gas and compressed air to the desired anode inlet conditions before exiting the FPS and the WRAS, respectively, and
controlling the steam reformer operational conditions and the generation of the steam required for the FPS. A number of high performance heat exchangers are used within the configuration in order to meet these objectives. Furthermore, since the SOFC operates at a high temperature, high-grade waste energy is used to precondition the streams coming into the stack. The stream coming out of the cathode is still rich in oxygen. Therefore, most of it is sent to the combustor mixer and a fraction of it is sent to the expander. The exit temperature of the reformate gases and the rate of conversion at the reformer are controlled by the temperature and mass flow of hot gases. For fast response, a bigger mass flow of air is required than that provided by the cathode. This extra air is taken from the air tank. In addition, energy recovery by flowing the mixed combustion gas streams mentioned above through an expander is used to offset some of the parasitic power requirements. The work generated by the gas mixture is used to drive the air compressor, which in turn compresses the air to be stored in the air tank and then used in the stack and the combustor. For many operating conditions, the work produced by the expander does not quite match the work required by the compressor. This additional work is supplied by an electric motor which takes power from the SS/PES.

5.1.3.3 BOPS Model Description

The mathematical model of the BOPS consists of a set of equations for component and subsystem mass and energy conservation, kinetic behavior, and geometry. Descriptions of the modeling approaches used for the principal components follow.

**Modeling of the steam methane reformer**

A number of simplifying assumptions are introduced to facilitate the modeling of the SMR reactor. These are the following:

- A single reactor tube is analyzed. Thus, all the tubes in the reactor behave independently of one another.
- Reforming and combustion gases behave ideally in all section of the reactor.
- The gas flow pattern through the channels is assumed to be plug flow.
- All reactions are considered to be the kinetically controlled. The rate expressions consider equilibrium.
- A uniform temperature exists throughout each catalyst particle.
- No carbon deposition is allowed in the SMR reactor.
- Axial dispersion and radial gradients are negligible.
- The outside shell wall is adiabatic.

For the kinetic modeling, the rate equation developed by Bodroy et al. (1964) and Keiski et al. (1993) were selected to represent the demethanation and water gas shift reaction rates, respectively. The reformate gas side energy balance includes the gas sensible heat exchange, reaction enthalpies, heat exchange with the hotter tube-wall, heat exchange with the catalyst particles, and an accumulation or storage term. Mazumder et al. (2003) presents a detailed explanation of the reformer kinetic model along with the energy balances of the reactor wall and the hot-side gases. Table 5.1.2 shows input parameter information for the reformer model.
Table 5.1.2: Input data for the reformer simulation.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Packing density in the reformer</td>
<td>1281.48 (kg/m³)</td>
</tr>
<tr>
<td>Heat capacity of the catalyst</td>
<td>1.026 (kJ/kg-K)</td>
</tr>
<tr>
<td>Specific surface area of the catalyst</td>
<td>669.29 (m²/m³)</td>
</tr>
<tr>
<td>Arrhenius demethanation activation energy</td>
<td>83736 (J/mol)</td>
</tr>
<tr>
<td>Arrhenius demethanation frequency factor</td>
<td>0.0987 (kmol/kg h)</td>
</tr>
<tr>
<td>Steam to methane ratio</td>
<td>3.2</td>
</tr>
<tr>
<td>Number of finite difference sections in the reformer</td>
<td>20</td>
</tr>
</tbody>
</table>

**Modeling of the compact heat exchangers:**

The heat exchangers used in the BOPS configuration are all plate-fin type, compact heat exchangers with a single-pass, cross-flow arrangement. Their modeling details are presented in Mazumder et al. (2003). The heat transfer and pressure drop models used are based on the work of Shah (1981) and Kays and London (1998). A dynamic energy balance and empirical correlations for the heat transfer coefficients are applied in order to relate the geometric models of the heat exchangers to the thermodynamic ones. The expression for the heat exchanger effectiveness is obtained from Incropera and DeWitt (1990) and is valid for single-pass, cross-flow arrangements with both fluids unmixed. Since the fluid is a gas, its thermal capacitance is assumed to be small compared to the wall. In our research, a numerical approach was applied to solve the transient thermal response of the compact heat exchangers. In order to guarantee adequate accuracy, two-dimensional, spatial discretization was employed as well (Figs. 5.1.26 and 5.1.27).

![Compact heat exchanger section](image)

**Fig. 5.1.26: Compact heat exchanger section.**

**Modeling of the steam generator:**

The steam generator consists of an economizer, an evaporator, and a superheater. These three integrated component parts were modeled as a counter-flow, shell-and-tube heat exchanger with a single-pass shell and one tube pass. Since the same type of shell-and-tube heat exchanger is
taken into account to describe the economizer, evaporator, and superheater geometries, the geometric models developed are identical. The necessary equations are obtained from Kakaç and Liu (1998) and are the appropriate ones for this particular shell-and-tube configuration. The geometric model of the steam generator is presented in Table 5.1.3. The economizer, evaporator, and superheater dynamic models are formulated similarly. In general, the steam generator is discretized spatially into n sections. For each section (index i), a dynamic energy balance for the tubing is formulated. These energy balances are similar to the ones presented for the compact heat exchangers.

**Modeling of the hydrogen and air tanks:**

Thermodynamic models are developed by applying dynamic mass and energy balances to the fuel and air tanks in order to determine the required inlet and exit mass flows. Creation of robust and detailed thermodynamic models of these components is complemented by geometric models, which are widely applicable and can be used to simulate the buffering requirements at both full and part loads. The final dimensions of the tanks are found by simulating the biggest possible disturbance under the most demanding condition, taking into account the power demand profile and final operating conditions, and by finally computing the fuel demand during the transient. The mass flow output of the tanks is determined by the stack hydrogen and air requirements, which in turn are defined by the load conditions and load controller. The tank’s output is regulated according to the demand using servo valves, which are operated by an electric signal. The mass flow input is determined by the reference pressure in the tanks. The reference pressure is a parameter required by the control system and is a product of the system optimization. For the hydrogen tank the inlet mass flow comes from the steam methane reformer, which in turn is feed by a high pressure methane tank. The methane output from this high pressure tank is regulated.
again by a servo valve and depends, as mentioned above on the hydrogen tank pressure. For the air tank, the inlet mass flow comes from the screw air compressor, whose mass flow output is determined by regulating the compressor speed. The required compressor work input is supply by the expander and the electrical motor.

<table>
<thead>
<tr>
<th>Fixed Parameter Description</th>
<th>Value</th>
<th>Fixed Parameter Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tube wall thickness (mm)</td>
<td>1.5</td>
<td>Tube count calculation constant</td>
<td>0.93</td>
</tr>
<tr>
<td>Number of passes</td>
<td>1</td>
<td>Tube layout constant</td>
<td>1</td>
</tr>
</tbody>
</table>

**Table 5.1.3:** Geometric model of the steam generator (Kakaç and Liu, 1998).

<table>
<thead>
<tr>
<th>Variable Description</th>
<th>Model Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tube inner diameter</td>
<td>Assigned value</td>
</tr>
<tr>
<td>Number of tubes</td>
<td>Assigned value</td>
</tr>
<tr>
<td>Length</td>
<td>Assigned value</td>
</tr>
<tr>
<td>Tube outer diameter</td>
<td>( d_{so} = d_{so} + 2t_w )</td>
</tr>
<tr>
<td>Pitch</td>
<td>( P_{T}^{so} = 1.25d_{so} )</td>
</tr>
<tr>
<td>Shell diameter</td>
<td>( D_{s}^{so} = 0.637 \frac{CL}{CTP} \sqrt{\frac{\pi n_{tubes}^{so} (P_{T}^{so})^2}{P_{T}^{so}}} )</td>
</tr>
<tr>
<td>Baffle spacing</td>
<td>( B = 0.6D_{s}^{so} )</td>
</tr>
</tbody>
</table>

**Modeling of the air compressors, the expander and the motor:**

The WRAS is a small but important part of the whole fuel cell system. The compressor is driven by an expander, which is fed with hot gases from the FPS and air from the stack cathode. An electric motor is used to supply additional power to the compressor in case the power extracted from the expander is not enough to run the compressor.

It has become very evident through research that the performance and overall efficiency of a fuel cell system is very dependent on the air management subsystem. Unfortunately, no off-the-shelf compressor/expander/motor technologies are available that simultaneously meet the entire unique air supply requirements of fuel cell systems (efficiency, performance, cost, pressure-flow, size and weight). Due to this, a great deal of information from various literature sources and internet homepages were evaluated in order to produce the model needed. Compressor, expander and motor maps that describe component behavior as a function of inlet and outlet pressures, mass flow rate, rotor speed and inlet temperature were developed based on Larminie and Dicks (2003). The compressor map for a general screw compressor is also the basis for the expander map. Kovacevic (2003) was used in the design of the screw compressor in order to determine its dimensions from which moment of inertia and speed could be determined. Although screw compressors are expensive to manufacture, they have important advantages that lead to the choice of that type of compressor. For one, hand screw compressors provide the oil-free output required by the fuel cell system and provide an extended range of pressure ratios. In addition,
they operate at a high efficiency over a wide range of flow rates. The governing equations for the compressor and expander were deduced from Bianchi, Peretto and Spina (1998) as well as from the technical report of The Boeing Company (1977). Equations for modeling the motor were taken from Palm (1986). While motor specifications were taken from the homepage of Minarik Drives & Control (2004). After studying the available literature, it was decided to use a DC motor for running the compressor.

For the dynamic analysis of a compressor or fan, the pressure and mass flow are state variables. Assuming that the inlet temperature is known, performance maps can then be used to calculate the rotational speed and efficiency as well as the output temperature and work input. Heat transfer from the fluid in a compressor to the impeller and casing is a complex phenomenon, particularly during start-up transients. Heat flows from the fluid to the casing to the ambient as well as from the fluid to the impeller to the casing to the ambient through the bearings, seals, and shaft. The thermal capacitance of the casing, impeller, and inlet duct can be approximated by a single thermal mode at a particular temperature. A similar approach is used for the expander.

The work required by the compressor is determined from a mechanical energy balance. The shaft component is used to compute the turbo-machinery rotational speed based on input values of turbine power output and compressor power input.

The compressor, expander and motor are coupled to each other through the same shaft and, therefore, the rotational speed of all the three components must be the same due to the rigidity of the shaft. Thus, the rotational speed N acts as a coupling constraint variable on the coupled unit. The implication of this constraint is that under transient conditions, for example, when the inlet mass flow rate requirement is increased for the compressor, the rotational speed and the power requirement must be varied and correspondingly the rotational speed of the motor and the expander are changed. This is done by the control system which adjusts the voltage of the motor instantaneously resulting in the desired conditions.

As an illustration of the behavior of the complete compressor-expander-motor unit, the dynamic behavior of the rotational speed N for a step change in motor inlet voltage is shown in Fig. 5.1.28. After a step change in speed of about 70 rpm the unit again reaches steady state conditions after 40 sec. Similarly, the dynamic behavior of the compressor mass flow rate can be seen in Fig. 5.1.29.
5.1.3.4 Reduced Order Model

A reduced order model of the BOPS is needed to be used with the PES in real time simulations. The reduced order model of the BOPS was generated for 7 different load profiles specified by the UIC and by VT (Fig. 5.1.31 The 7 specific load profiles for the reduced order model. The detailed optimized BOPS/SS code, which consists of three distinct codes, one for each of the three subsystems comprising the BOPS/SS, i.e. the FPS (fuel processing subsystem), the WRAS (work recovery and air supply subsystem), and the SS (stack subsystem), was run for
various load profiles specified by UIC and by VT was run to generate data points. The data points for every input and output variable of the BOPS was then exported from gPROMS into a text file for the 7 load profiles. The text file was then imported into MATLAB and a linear correlation between each data point made to be able to get the data for every instance of time.

**Fig. 5.1.30:** Schematic of the reduced order BOPS model.

The reduced order model based on the detailed optimized BOPS/SS code as shown in Fig. 5.1.30 was used by UIC to do a real time simulation and worked well for that application. A comparison of the non-optimized BOPS/SS code and the optimized code response to the 7 specific load profiles was also made, both directly from gProms and also with the reduced order BOPS model. The comparison is illustrated in Fig. 5.1.32 below for the load profile shown in Fig. 5.1.31. What is obvious from Fig. 5.1.33 is that the optimal control architecture developed simultaneously with the optimal BOPS/SS synthesis, design, and operation does much better in more effectively meeting the demands of fuel to the stack and shows significantly greater stability in doing so. The non-optimized control architecture was developed using a traditional design approach (including no large-scale optimization) and as is traditionally done was developed independently of the synthesis/design and operation of the BOPS/SS configuration and components. The procedure which we developed and used for optimizing the BOPS/SS, on the other hand, avoided both of these traditional design approach drawbacks since the synthesis/design and operational/control were developed (and, in fact, optimized) simultaneously.
Fig. 5.1.31: Specific load profiles for the reduced order model.
Figure 5.1.32: Comparison of non-optimized and optimized transient responses of the reformate flow out of the BOPS to the SOFC anode.
Figure 5.1.33: Load profile used for the comparison of non-optimized and optimized transient responses of the reformate flow out of the BOPS to the SOFC anode shown in Fig. 5.1.32.

The results based on the reduced order BOPS model are seen in Fig. 5.1.34. When comparing Fig. 5.1.34 with the output from gProms, it is clear that the results from the reduced order model give good comparison.

Figure 5.1.34: Comparison of non-optimized and optimized transient responses of the reformate flow out of the reduced order BOPS code.
5.1.4 Comprehensive System Modeling

The problem of integrated-system design/operational optimization for variable loads and/or environmental conditions is complex and difficult to solve. It represents a mixed integer and non-linear programming (MINLP) problem for which no general solution has been found. This is further complicated by the need to examine a large number of alternate synthesizes, designs, and operational-control strategies at each level of the problem. SOFCs respond quickly to changes in load, because of their rapid electrochemistry. The PES also responds quickly to changes in application load or other variations. This is however not true for the thermal, mechanical, and chemical BOPS components and particularly for the fuel-processing subsystem, where load-following time constants are typically several orders of magnitude higher.

Differences in response times between the electrochemical/electrical and thermal/mechanical and chemical subsystems of the overall SOFC system significantly increase the computational complexity. For example, the load following time constants of the BOPS are typically of the order of seconds, while that of the SOFC and the PES is in microseconds. Hence the number of iterations of the PES/SOFC model has to be of the order of millions to get any meaningful results. Such complex simulations are extremely cumbersome on commercially available computational facilities (as specified by DOE). Hence there is a need to develop efficient simulation techniques to model such systems. This section first describes the comprehensive system model and then goes on to describe the reduced order models that are developed for efficient and less cumbersome calculations.

5.1.4.1 Comprehensive System Model and Methodology on Multi-software Platform

Such a methodology enables the use of software/package that is most suited to model any given subsystemTo study the electrical interaction of SOFC, PES, BOPS, and the application loads as a whole, a multi-software platform as shown in Fig. 5.1.35 were implemented using *iSIGHT*\(^7\). While the *Visual-Fortran* code (SOFC) is embedded in the *Saber Designer* (PES and application load) using *dynamic link library (DLLs)*, modules developed in the *gPROMS*\(^8\) (BOPS) environment was integrated with *Saber Designer* using *iSIGHT* software (Mazumder et al., 2003). The PES model supplies input power data to the BOPS model through the *iSIGHT* software.

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\(^7\) iSight is a software developed and distributed by Engineous Software Inc. iSIGHT integrates simulation codes and provides engineering intelligence to drive the investigation of design alternatives. iSIGHT frees engineers from doing countless iterative routines at the keyboard, leaving more time to create innovative ideas and gain competitive position.

\(^8\) gPROMS is an equation-based system (i.e. based on first principles) which analyzes the relationships governing a process (chemical, thermal, mechanical, electrochemical, and electrical) and then performs a dynamic or steady-state simulation, optimization or parameter estimation. The powerful modeling language and a robust and fast-solution technology provides a framework, which has a high degree of success in both synthesis/design and operational modeling, simulation, and optimization of complex and dynamic fuel cell based total-energy systems. Thus, a general model for the balance-of-plant in the gPROMS environment requires modifying or adding to the existing thermodynamic, kinetic, geometric, and cost models, which have been integrated with the PES and SOFCSS modules.
interface. The BOPS model then calculates the SOFCS parameters (like fuel-flow rate and temperatures) and supplies this data to the SOFC model, using *iSIGHT* and *DLLs*. This integration of multiple software platforms enable us to use the most powerful software tools used to model each of the SOFC subsystems.

For SOFC cell-level analysis, an additional finite-element (FE) simulating package *TOPAZ/FEMLAB*\(^9\) was used in addition to the above multi-software platform. Initially a long-term simulation is conducted using the analytical models of SOFC, BOPS, PES, and application load. Once a steady-state is reached, the equilibrium values of the SOFC current and voltages are fed to the FE model of the SOFC (the parameters of this model is the same as that of the analytical SOFC model) along with boundary conditions to obtain the spatial resolution of cell current-density and temperature distributions.

With such tools for dynamic simulation and modeling, it is possible to conduct parametric studies and optimizations to determine control strategies (for stationary and/or transportation auxiliary power load profiles) and their effects on the efficiency, power density, fuel utilization and conversion, system response and configuration, and component design of SOFC systems.

**Fig. 5.1.35:** Implementation of a unified model for a SOFC power-conditioning system using multi-software platform.

\(^9\) FEMLAB supplies highly sought-after new technology for the modeling and simulation of physics in all science and engineering fields. Its main attribute is the ease with which modeling can be performed and its unlimited multiphysics capabilities, in 1D, 2D and 3D - the perfect way to apply state-of-the-art numerical analysis to your expertise in modeling.
5.1.4.2 Low-cost System Modeling Framework

The powerful multi-software modeling platform discussed in the previous subsection, is developed in the proven platforms for each of the subsystem models. Therefore, it was relatively simple to design the overall PCS. However, this introduces the following limitations: i) relatively expensive overall software platform, ii) high computational overhead due to the need for data exchange via the iSIGHT software interface and due to the high order of the overall comprehensive PCS model (e.g., order of the BOPS model greater than 450) and the significant variation in scales among the PES switching model and the BOPS and TSOFC models, iv) no spatial data of the TSOFC is obtainable without freezing the time, and v) the modeling framework does not provide any avenue for RTS of the PCS.

To alleviate these limitations, a numerical modeling framework for PSOFC PCS is developed. The framework can provide spatial (up to two dimensions) as well as temporal data simultaneously. It has the ability to work with comprehensive transient models of PSOFC, BOPS, PES, and AL, if one needs to focus on details, or with reduced-order models, for fast computation and RTS and integration with bigger vehicular-system model. Finally, because the system model is developed primarily in Simulink/Matlab environment, the software cost is minimal as compared to the previous attempt.

Fig. 5.1.36: The modeling framework for a comprehensive PSOFC based PCS modeling framework.

Fig. 5.1.36 shows the new comprehensive modeling framework. The system models comprise PSOFC, BOPS, PES, and AL. This comprehensive model requires two low-cost softwares for implementation (Simulink/Matlab including SimPowerSystem and gPROMS including gO:Simulink).

The BOPS (modeled in gPROMS) output is interfaced to the MATLAB/Simulink through gO:Simulink interfacing software. Similarly the output of the planar stack and control signal input is sent from the Simulink using the gO:Simulink. Fig. 5.1.37 illustrates the ease of interfacing the existing gPROMS model with the Simulink.
The planar SOFC mathematical spatio-temporal model is embedded into Simulink using the MATLAB embedded function block. This function block takes the fuel and air output from the fuel processor (in the BOPS) and the current drawn from the stack by the PES model and provides the output voltage to the PES Simulink model.

5.1.4.3 Modeling Approaches to Resolve Effect of Multiple Time Scales

Differences in response times between the electrochemical/electrical and thermal/mechanical/chemical subsystems of the overall SOFC system imply that real-time simulations have to be performed in order to obtain meaningful results. However real-time simulations using the comprehensive model are extremely cumbersome and time consuming. Hence more efficient simulation techniques are needed for studying the system interactions.

Two Step Approach

Since the PES model comprises of a number of switching functions, their real-time simulation using the comprehensive model (as discussed in Section 5.1.2) is extremely tedious. In order to reduce the complexity of the simulation, a two-step approach was taken. In the first step, simulations on different PES topologies were performed using Saber Designer with an ideal voltage source as the input. The harmonic content (obtained using Fourier transforms) and the profile of the PES input current were estimated. In the second step, the PES is replaced by a

---

10 The switching functions are determined by the state-variables of the system at each time instant. A transition in the switching function occurs whenever the state-variables satisfy certain conditions.
lumped load (with similar harmonic content and profile as estimated in the first step) in the comprehensive simulation platform as shown in Fig. 5.1.38. While developing the lumped load,

**Fig. 5.1.38:** (a) Comprehensive model block diagram; (b) reduced order model with lumped harmonic load replacing the PES.

it was ensured that all the harmonics were present and the magnitudes matched, so that the stresses imposed by the lumped load on the SOFC is similar to that imposed by the PES. The process of the lumped load development was purely iterative. The reduced order model was then used to investigate the effect of the PES dynamics on the SOFC's life and performance. This model substantially reduces the simulation times and at the same time can model the power electronic system to a good degree of accuracy.

**Fig. 5.1.39:** (a) Comprehensive model block diagram; (b) reduced order model with lumped harmonic load replacing the DC-AC converter.

In order to study the effect of SOFC variations on PES network transients and dynamics, a second reduced order model, as shown in Fig. 5.1.39, is implemented. Here the SOFC is assumed to be a time varying voltage source, where the output voltage varies with the PES input current. Since the time scales for the PES dynamics are comparatively much smaller, the BOPS model was neglected for this reduced order study. For obtaining primary results, the investigation was limited to the DC-DC boost converter, with the DC-AC stage replaced by a lumped harmonic load, which is obtained following a similar procedure as outlined earlier in this section.
Reduced-order Modeling Approach

The switching models are the real representatives of the power converters. Fig. 5.1.40a shows the switching model of a DC-DC boost converter. However, the models suffer from the disadvantage of being discontinuous because of their switching. With the switching frequency in the order of tens of kilohertz, the discontinuous system has to be solved at their boundary of discontinuity in each cycle, which renders the model computationally expensive. Therefore, to increase the speed of the PCS simulation, we need to avoid the discontinuity, thereby reducing the sampling rate and bring it as close as possible to that required by the PSOFC and BOPS models without significantly compromising the accuracy.

As such, we adopted an averaged-modeling technique (Lee, 1990) to analyze the behavior of the PES without significant computational overhead. Fig. 5.1.40b shows the averaged model of the DC-DC boost converter in equivalent-circuit form (Lee, 1990). One can notice that unlike the switching models, the averaged models do not have any discontinuous elements. Further, the averaged (circuit) models enable the usage of built-in circuit modules in Simulink. We note that, an averaged model ideally provides the averaged dynamics of the PES and as such it transforms the PES model from a discontinuous to a smooth form. Fig. 5.1.41 shows the accuracy of the average model to that of the switching model of a boost converter. The accuracy of the averaged model typically varies with the switching frequency, with higher accuracy for higher operating frequency.

Fig. 5.1.40: a) Switching model and b) switch-average model of the DC-DC boost converter.
To reduce the complexity of the BOPS model we took polynomial approximation approach. To realize the polynomial-approximation model, first, we subjected the BOPS model to different sets of load transients and steady-state electrical feedbacks and stored the transient responses of all the output BOPS parameters (such as temperature, air and fuel flow rates, and air and fuel compositions), which are used to interface the BOPS model to the PSOFC model, in a database. Subsequently, we applied multi-order (starting from linear to seventh-order) polynomial approximations on each set of these data to obtain the closest approximation that provides optimal compromise between speed of simulation and accuracy with regard to the data obtained using the comprehensive model.

Table 5.1.4, shows the percentage improvement in simulation time obtained using the reduced-order models of the PSOFC, PES, and BOPS. The simulation time is based on 10 seconds of individual subsystems of the PSOFC PCS simulation on a two-processor Intel Xeon PC, with each processor operating at 2 GHz. A significant improvement is obtained using the PES averaged model because the averaged model transforms the problem from analyzing a discontinuous-nonlinear differential equation (where an accurate determination of the switching transients is necessary leading to high computational overhead) to analyzing a smooth differential equation. Importantly, since the switching frequencies of the converters are high, the dynamics of the PES obtained using the average models are close to that obtained using the corresponding switching model. The polynomial approximation of the comprehensive BOPS model yields significant savings in time without compromising accuracy. This is true for the PSOFC one-dimensional model as well.

![Graph showing comparison between Average Model and Switching Model](image)

**Fig. 5.1.41:** Accuracy of the averaged boost converter model.
Table 5.1.4: Improvement in computational overhead and comparison of accuracy.

<table>
<thead>
<tr>
<th>Subsystems</th>
<th>Models being compared</th>
<th>Simulation time</th>
<th>Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>PES</td>
<td>Averaged model vs switching model</td>
<td>0.00945</td>
<td>1.12%</td>
</tr>
<tr>
<td>BOPS</td>
<td>$7^{th}$ order polynomial fit vs comprehensive model</td>
<td>0.3787</td>
<td>2.89%</td>
</tr>
<tr>
<td></td>
<td>$5^{th}$ order polynomial fit vs comprehensive model</td>
<td>0.2745</td>
<td>3.29%</td>
</tr>
<tr>
<td></td>
<td>$3^{rd}$ order polynomial fit vs comprehensive model</td>
<td>0.217</td>
<td>9.40%</td>
</tr>
<tr>
<td></td>
<td>Linear fit vs comprehensive model</td>
<td>0.1617</td>
<td>13%</td>
</tr>
<tr>
<td>PSOFC</td>
<td>One-dimensional vs two-dimensional model</td>
<td>0.4285</td>
<td>5.21%</td>
</tr>
</tbody>
</table>

Fig 5.1.42 shows the reduced-order system model for the PSOFC based PCS modeled in MATLAB/Simulink platform. This consists of averaged PES model; best curve fit BOPS model and the one-dimensional planar stack model. Since the complete system is implemented in Simulink, it enables real-time simulation using Real-Time Workshop toolbox in MATLAB/Simulink.

5.2 System-Interaction Analysis

5.2.1 Effects of PES and AL on SOFC Stack

The factors that effect the stack lifetime and durability include operating temperature, thermal cycling of SOFCS material, mechanical pressure fluctuations. Effect of these factors on the material properties of SOFC has been reported earlier (Virkar et al., Huang et al., Hsiao et al. and Travis et al.). These studies on SOFCS reliability have primarily focused on investigating the effect of material properties and electro-kinetics of the chemical reactions on the operating life and performance. However, there is a need to study the impact of the electrically-induced feedback effects (induced due to the PES and the ALs) on the PSOFC performance.
However the effects of the PES dynamics on the performance of SOFCS has not been investigated in great detail. Recently, Gemmen et al. attempted to estimate the effects of electrical loads and inverter ripple on the durability and performance of proton-exchange membrane (PEM) fuel cells using a simple first order model for the PES. Achenbach (1995) and Hartvigsen et al. (1993) have demonstrated preliminary results on the impacts of linear electrical load impedance and their change on the dynamics of a SOFC. As part of our project, we study the effect of PES dynamics (the models have been described in section 5.1.2.2) on the SOFCS performance. Our focus in this study has been to investigate the system level interactions between the various subsystems of the SOFC based system, specifically to study the effect of application load and PES on SOFC performance and durability.

5.2.1.1 Effects of AL

One of the most commonly observed load-induced feedbacks is the load-transient, which is attributed to sudden variation in the power demand of the load or its sudden isolation from the fuel cell stack. Other important feedback effects are the power factor of the load and its harmonic distortion, both of which are indicative of the quality of the load.

Effects of Load-transients

Fig. 5.2.1 shows the load current transients due to variations in the power demands of the load. Because PSOFC (like other fuel cells) is not a stiff voltage source, its voltage level decreases with an increase in the current drawn from it. This is due to an increase in the polarization loss at a higher current density. For the PSOFC, operation below a minimum voltage should be avoided because the mass-transport limitations of the electrochemical reaction can cause the anode of the cell to be re-oxidized. This degrades the cell performance and ultimately shortens the life of the stack. Hence, load transients, which may drop the voltage of the PSOFC below this minimum voltage, can degrade the performance and durability of the stack.

SOFC hydrogen utilization is directly proportional to the current drawn by the PES (Khandkar et al., 1998) and can be defined as

\[ U = \frac{I}{nF} \]  

(5.2.1)

where \( n \) is the hydrogen flow rate, which is determined by the BOPS and \( nF \) is the charge flow between the anode and the cathode. Hence, the hydrogen utilization closely follows the PES input current, and increases significantly at higher load currents.
Fig. 5.2.1: Variation of load current due to the load transient.

We analyze the effects of load transient on the performance and durability of the PSOFCS. Fig. 5.2.2 shows the drop in the output voltage of the stack, due to the load transient. Because the response time of the BOPS is significantly lower than that of the PES/PSOFCS, the input fuel-flow rates of the stack will not change soon after the load-transient. This leads to sudden increase in fuel utilization inside the PSOFCS so as to attain a new electrochemical steady state.

Fig. 5.2.3 shows that, hydrogen (fuel) utilization increases very sharply immediately after the load transient, and decreases at a slower rate in pace with the increase in the fuel supply by the BOPS. The peak in the hydrogen utilization is attributed to the period of inactivity of the BOPS. As shown in Fig. 5.2.4, the stack efficiency and hence the system efficiency increases with an increase in the fuel utilization in the stack. And to maximize the efficiency of the stack, it should operate at fixed high fuel utilization. However, the load transient increases the fuel utilization sharply, and this may lead to a low reactant condition in the stack, thereby degrading the stack performance.
Fig. 5.2.2: Current transient (10 A to 65 A) which results in a sudden drop in the PSOFCS output voltage.

Fig. 5.2.3: Sudden surge in the hydrogen utilization due to the load transient.
An increase in the heat rate (because of increased rate of the exothermic reaction) and almost no change in flow rates in the stack (until the BOPS flow rates adjust to the increased demand of fuel and air), increases the fuel cell temperature with time. However, the thermal time constant of the stack being much larger than that of the SOFC electrochemistry/PES time constant, the increase in the cell temperature just after the load transient is minimal, and the mean temperature increases to a higher thermal steady state value after approximately 600 seconds.

For the finite-element stress analysis of the effect of this load transient, the spatial distribution of temperature inside the cell and the spatial temperature gradient inside the cell is obtained before and after the load transient. Fig. 5.2.5 shows the spatial temperature distribution before and after the rated load transient. Because the developed thermal stress is dependent upon the temperature gradient, we obtain corresponding temperature gradients as shown in Fig. 5.2.6.
Mechanical reliability and durability of SOFCs as any other material are determined by the stress distribution in, and the stochastic distribution of strengths of, their components. The stress distribution is a complex function of several parameters, including geometry of the SOFC, temperature distribution and external mechanical stress. The residual stresses induced due to mismatch in the thermo-elastic properties of SOFC components during its operation, largely affects the durability and reliability of the SOFC. The determination of this residual stress distribution in SOFC materials and components typically requires the use of computational tools (e.g., computational fluid dynamics and finite-element stress analyses), which in turn requires knowledge of physical and mechanical properties of the materials and the components at various temperature.
Fig. 5.2.7 show the steps involved in thermal analysis of the effect of the load transient. The first step in the analysis involves determining the elastic properties of the electrodes and the electrolyte at various temperatures using a resonant ultrasound spectrometer (RUS). The elastic properties for the Ni/YSZ anode and the YSZ electrolyte are determined by Radovic et. al, (2004 a and b) respectively. For the LSM cathode, the elastic properties at different temperatures are experimentally determined and as shown in Fig. 5.2.8.

Fig. 5.2.7: Thermal analysis of the effects of load transients on the SOFCS.

Fig. 5.2.8: Temperature variation of the elastic moduli of the sample LSM cathodes.
Due to thermal expansion mismatch among the components and non-uniform temperature gradient in the SOFC due to a load transient, the components of the SOFC are subjected to biaxial stress at the interface between them. This stress is determined using finite element stress analyses. To estimate the residual stresses at the interfaces between the electrodes and the electrolyte, zero residual stress temperature at the interfaces needs to be obtained. The PSOFC zero residual stress temperature, which depends on the processing routine of the planar cell, is obtained by X-ray diffraction at various temperatures (Lara-Curzio, 2004) and found to be about 900 °C.

Using the residual stresses induced at various interfaces, the risk of rupture intensities is obtained. And the probability of failure is obtained.

**Fig. 5.2.9:** Schematic of a PSOFC based residential power conditioning system.

**Effect of Load Power Factor**

For a passive AC load, load power factor (which can vary between 0 and 1), as illustrated in Fig. 5.2.10, represents the phase difference between the voltage across a load and the current drawn by it. When the load is resistive, it draws only active power from the source and hence, the power factor is unity. However, at non-unity power factors, an AC load draws both reactive and active powers from the source. The reactive power ($P_{\text{reactive}}(t)$), as shown in Fig. 5.2.11, circulates in the circuit. To support $P_{\text{reactive}}(t)$, additional reactive current is drawn from the source apart from the active current (which feeds active power to the load). Therefore, the current drawn by the reactive load increases with an increase in the reactive power demand by the load.

The current drawn by the inverter from the output of the DC-DC converter, as shown in Fig. 5.2.9 can be written using small signal analysis as

$$i_{\text{bus}} = \left( i_{\text{load}} + C_f \frac{dv_f}{dt} \right) d_{\text{vsi}}$$  \hspace{1cm} (5.2.2)

where $d_{\text{vsi}}$ is the duty ratio of the inverter switches assuming small signal approximation and can be defined as $d_{\text{vsi}} = d_m \sin \omega t$, $\omega$ is the frequency of the reference voltage for the inverter.
Fig. 5.2.10: Voltage-current (V-I) characteristics of AC loads at different power factors.

Fig. 5.2.11: Reactive-power circulation due to a non-unity-power-factor load.
Assuming no phase delay of the output voltage of the inverter with respect to the reference voltage, \( v_f \) can be written as \( V_m \sin \omega t \). Then assuming stiff bus voltage, equation (5.2.2) becomes

\[
i_{bus} = (i_{load} + \omega V_m C_f \cos \omega t) d_m \sin \omega t
\]  
(5.2.3)

**Case A.**

For a resistive load, \( i_{load} = I_m \sin \omega t \), and Equation (5.2.3) becomes

\[
i_{bus} = (I_m \sin \omega t + wV_m C_f \cos \omega t) d_m \sin \omega t
\]

\[
= \frac{I_m d_m}{2} (1 - \cos(2\omega t)) + \frac{\omega V_m C_f d_m}{2} \sin(2\omega t)
\]

The filter capacitance being very small, the second term in equation (5.2.8) is negligible as compared to the first term. The approximate expression for the bus current becomes,

\[
i_{bus} = \frac{I_m d_m}{2} (1 - \cos 2\omega t)
\]  
(5.2.5)

**Case B**

For a reactive load with power factor, \( pf = \cos \phi \), \( i_{load} = I_m / \sin (\omega t + \phi) \). Now for same active power as in Case A,

\[
\frac{V_m I_m}{2} = \frac{V_m I_m'}{2} \cos \phi \Rightarrow I_m = \frac{I_m}{\cos \phi}
\]  
(5.2.6)

Now, (5.2.3) becomes

\[
i_{bus}(t) = \left( \frac{I_m}{\cos \phi} \sin(\omega t + \phi) + \omega V_m C_f \cos \omega t \right) d_m \sin \omega t
\]

\[
= \frac{I_m d_m}{2} \left( 1 - \frac{\cos(2\omega t + \phi)}{\cos \phi} \right) + \frac{wV_m C_f d_m}{2} \sin 2\omega t
\]

(5.2.7)

Using the same approximation as in (5.2.5), the expression for the bus current becomes,

\[
i_{bus}(t) = \frac{I_m d_m}{2} (1 - A \cos(2\omega t + \phi))
\]

(5.2.8)

where \( A = 1/ (\cos \phi) > 1 \) for all \( \phi \neq 0 \). At the output of the boost converter, assuming constant duty ratio, \( D \), of the boost converter in the steady state,

\[
i_{bus}(t) = (1 - D)i_{FC}(t) - i_C(t)
\]  
(5.2.9)

Assuming a fraction \( \delta \) of the ripple in the bus current flows in the bus capacitor \( C \),

\[
i_C(t) = \frac{I_m d_m}{2} (1 - \delta)A \cos(2\omega t + \phi)
\]

(5.2.10)

To allow stiff voltage approximation, the size of the capacitance should be chosen such that, the ripple in the bus voltage is less than 5 percent. That is,

\[
|\Delta V_{bus}(t)| = \left| \frac{I_m d_m}{C} \frac{(1 - \delta)A}{2} \int \cos(2\omega t + \phi) dt \right| = \left| \frac{I_m d_m}{4 \omega C} (1 - \delta)A \right| < 0.05 \times \frac{V_m}{d_m}
\]

(5.2.11)

Now,

\[
(1 - D)i_{FC}(t) = \frac{I_m d_m}{2} (1 - \delta A \cos(2\omega t + \phi))
\]  
(5.2.12)
\[ i_{FC}(t) = \frac{I_m d_m}{2(1-D)}(1 - \delta \cos(2\omega t + \phi - \theta)) \]  \hspace{1cm} (5.2.13)

Since, \( i_{FC}(t) = I_{FC} + \hat{i}_{FC}(t) \), where \( I_{FC} \) is the mean stack current and \( \hat{i}_{FC}(t) \) is the ripple component of the stack current. Now the fraction of the ripple in the stack current is given by,

\[ \hat{i}_{FC}(t) = \frac{\delta}{I_{FC}} \cos(2\omega t + \phi - \theta) \]  \hspace{1cm} (5.2.14)

Equation (5.2.14) states that the amplitude of the ripple in the stack current increases with an increase in \(|\phi|\). Hence the ripple current increases with decrease in the load power factor. This ripple further depends on the output capacitance connected across the DC bus.

**Effect of THD**

Total harmonic distortion signifies the harmonic content in an AC quantity, and is defined as the ratio of sum of powers of all harmonic frequency components in a signal above the fundamental frequency to the power of the fundamental frequency component. An AC-DC rectifier load is a typical example of the load which induces harmonic distortion to the AC current at the output of the inverter (Refer Fig. 5.2.9). As shown in Fig. 5.2.12a, current drawn from the inverter, \( i(t) \), is distorted. The harmonic analysis of the distorted current, as shown in Fig. 5.2.12b, reveals the presence of the significant odd-order harmonics that decreases with increase in the frequency.

The current drawn by the inverter from the output of the DC-DC converter, as shown in Fig. 5.2.9 can be written using small signal analysis as

\[ i_{bus} = \left(i_{load} + C_r \frac{dv_r}{dt}\right) dv_{si} \]  \hspace{1cm} (5.2.15)

where \( dv_{si} \) is the duty ratio of the inverter switches assuming small signal approximation and can be defined as \( dv_{si} = d_m \sin \omega t \), \( \omega \) is the frequency of the reference voltage for the inverter. Assuming no phase delay of the output voltage of the inverter with respect to the reference voltage, \( v_f \) can be written as \( V_m \sin \omega t \). Then assuming stiff bus voltage, equation (5.2.15) becomes

\[ i_{bus} = (i_{load} + \omega V_m C_r \cos \omega t) d_m \sin \omega t \]  \hspace{1cm} (5.2.16)

Let us consider that the load current contains higher order harmonics (odd order specifically since AC current), then the load current can be explained as

\[ i_{h,load}(t) = \sum I_{mk} \sin(k\omega t + \phi_k) \]  \hspace{1cm} (5.2.17)

Using (5.2.21) the current drawn by the inverter can be written as:

\[ i_{bus}(t) = \frac{d_m}{2} \sum_{k=1,3,5,..} I_{mk} \left[ \cos((k-1)\omega t + \phi_k) - \cos((k+1)\omega t + \phi_k) \right] + \omega V_m C_r \sin(2\omega t) \]  \hspace{1cm} (5.2.18)

The filter capacitance being very small, the second term in (5.2.18) is negligible as compared to the first term for finite load current. Assuming the real power drawn by the harmonic load to be the same as that of a resistive load drawing current with amplitude \( I_m \), then \( I_m = I_{ml1} \cos \phi_1 \). Rewriting (5.2.18) in terms of the fundamental current, \( I_{ml1} \).
\[ i_{\text{bus}}(t) = \frac{I_m d_m}{2} \sum_{k=1,3,5...} c_k \left[ \cos((k-1)\omega t + \phi_k) - \cos((k+1)\omega t + \phi_k) \right] \]

\[ = \frac{I_m d_m}{2} \left[ \cos \phi_1 - \left( \cos(2\omega t + \phi_1) - \sum_{k=3,5...} c_k \{ \cos((k-1)\omega t + \phi_k) - \cos((k+1)\omega t + \phi_k) \} \right) \right] \]

\[ = \frac{I_m d_m}{2} \left[ 1 - \frac{1}{\cos \phi_1} \left( \cos(2\omega t + \phi_1) - \sum_{k=3,5...} c_k \{ \cos((k-1)\omega t + \phi_k) - \cos((k+1)\omega t + \phi_k) \} \right) \right] \]

where \( c_k = I_{mk} / I_{m1} \) and \( \phi_k \) is described by,

\[ \phi_k = \cos^{-1} \left( \frac{\cos \phi_1}{\sqrt{k^2 (1 + \cos^2 \phi_1) - \cos^2 \phi_1}} \right) \]  

(5.2.20)

Simplifying (5.2.20), we obtain

\[ i_{\text{bus}}(t) = \frac{I_m d_m}{2} \left[ 1 - A \sum_{j=2,4,6...} (c_{j-1} \cos(j\omega t + \phi_{j-1}) - c_{j+1} \cos(j\omega t + \phi_{j+1})) \right] \]

(5.2.21)

where \( A = 1/\cos(\phi_1) \), \( \alpha_j \) and \( \psi_j \) are given as

\[ \alpha_j = \sqrt{c_{j-1}^2 + c_{j+1}^2 - 2c_{j-1}c_{j+1} \cos(\phi_{j+1} - \phi_{j-1})} \]

\[ \psi_j = \tan^{-1} \left( \frac{c_{j-1} \sin \phi_{j-1} - c_{j+1} \sin \phi_{j+1}}{c_{j-1} \cos \phi_{j-1} - c_{j+1} \cos \phi_{j+1}} \right) j = 2, 4, 6........ \]

At the output of the boost converter, assuming constant duty ratio, \( D \), of the boost converter in the steady state,

\[ i_{\text{bus}}(t) = (1-D)i_{FC}(t) - i_C(t) \]  

(5.2.23)

Assuming a fraction of the ripple in the bus current is absorbed in the bus capacitor \( C \),

\[ i_C(t) = \frac{I_m d_m A}{2} \sum_{j=2,4,...} (1-\delta_j) \alpha_j \cos(j\omega t + \psi_j) \quad \text{where} \quad \delta_j = \frac{2\delta_j}{j} \quad \text{for} \quad j = 2, 4, 6, .... \]

(5.2.24)

To allow stiff voltage approximation, the size of the capacitance should be chosen such that, the ripple in the bus voltage is less than 5 percent. That is,

\[ |\Delta V_{\text{bus}}(t)| = \left| \frac{1}{C} \frac{I_m d_m A}{2} \sum_{j=2,4,...} (1-\delta_j) \alpha_j \int \cos(j\omega t + \psi_j) dt \right| \]

\[ = \frac{I_m d_m A}{2\omega C} \sum_{j=2,4,...} \frac{(1-\delta_j)}{j} \alpha_j \cos(j\omega t + \psi_j) < 0.05 \times \frac{V_m}{d_m} \]

(5.2.25)

Now,

\[ (1-D)i_{FC}(t) = \frac{I_m d_m}{2} \left[ 1 - A \sum_{j=2,4,...} \delta_j \alpha_j \cos(j\omega t + \psi_j) \right] \]  

(5.2.26)
Fig. 5.2.12: a) Current distortion due to a rectifier load, b) Fourier analysis of the distorted current.
\[
i_{\text{FC}}(t) = \frac{I_{\text{m}}d_{\text{m}}}{2(1-D)} \left( 1 - 2A\delta \sum_{j=2,4,6...}^{j} \frac{\alpha_j}{j} \cos(j\omega t + \psi_j) \right)
\]  
(5.2.27)

Since, \(i_{\text{FC}}(t) = I_{\text{FC}} + \hat{i}_{\text{FC}}(t)\), where \(I_{\text{FC}}\) is the mean stack current and \(\hat{i}_{\text{FC}}(t)\) is the ripple component of the stack current. Now the fraction of the ripple in the stack current is given by,

\[
\frac{\hat{i}_{\text{FC}}(t)}{I_{\text{FC}}} = \frac{\delta}{\cos \phi_1} \sum_{j=2,4,6...}^{j} a_j \cos(j\omega t + \psi_j)
\]  
where \(a_j = \frac{2\alpha_j}{j}\), \(j = 2, 4, 6, \ldots\)  
(5.2.28)

Equation (5.2.28) states that the amplitude of the ripple in the stack current increases with an increase in \(|\phi_1|\). Again this ripple is dependent on \(\alpha_j\) and \(\psi_j\) (5.2.22), which depend on the fraction of the harmonic components \(c_j\) and their frequencies, \(j\omega\).

Now let us consider the harmonic current consists of third and fifth harmonics.

**Case I**

Let us assume, \(c_3 = 0.2, c_5 = 0.11\) and \(\phi_1 = 0.4\). Then \(\phi_3 = 0.903\) and \(\phi_5 = 1.13\) radians and THD = 0.228.

From (5.2.22) \(\alpha_2 = 0.8304, \psi_2 = 0.284, \alpha_4 = 0.096, \psi_4 = 0.642, \alpha_6 = 0.11, \psi_6 = 1.13\). Using the following values the fraction of the ripple in the bus current is found to be 0.995 to that of the mean bus current. With \(\delta = 0.2\), and the ripple in stack current is 0.193.

**Case II**

Let us assume, \(c_3 = 0.5, c_5 = 0.24\) and \(\phi_1 = 0.4\). Then \(\phi_3 = 0.903\) and \(\phi_5 = 1.13\) radians and THD = 0.554.

From (5.2.22) \(\alpha_2 = 0.611, \psi_2 = -0.005, \alpha_4 = 0.272, \psi_4 = 0.703, \alpha_6 = 0.24, \psi_6 = 1.13\). Using these values, with \(\delta = 0.2\) and using (5.2.28), the fraction of the ripple in the stack current is 0.188.

From above two cases we observe, the ripple in the stack current decreases with an increase in the THD for a particular power factor of the fundamental current \(\cos \phi_1\). The above analysis concludes that the magnitude of the ripple in the current drawn from the bus, \(i_{\text{bus}}(t)\), and therefore in the current drawn from the PSOFCS, \(i_{\text{FC}}(t)\), are dependent both on the power factor of the fundamental load current and the fractions of harmonic contents in the load.

5.2.1.2 Effects of PES

Most commonly observed effect of PES are the ripples. These ripples could be classified into two categories based on their frequency; a) low frequency ripple and b) high frequency ripple. Fig. 5.2.13 illustrates typical ripple current in the SOFCS.

**Low-frequency ripple**

A single-phase fuel cell DC-AC converter (also known as inverter as shown in Fig. 5.2.9) for stationary application feeds an AC load at line frequency, which is 60 Hz in USA and 50 Hz in Europe. The AC current drawn by the load from the inverter introduces ripple in the current drawn from the fuel cell. This low-frequency ripple current (with a frequency that is twice that of the line frequency) increases with an increase in the load current. Fig. 5.2.13 illustrates the low-frequency ripple in the PSOFCS-stack (PSOFCS) current. This ripple current is also dependent on the power factor and load distortion discussed in 5.2.1.1. Because the electrochemical time constant of the PSOFCS is less than the time period of the ripple, the low-frequency ripple
current may potentially affect the electrochemical properties of the stack, such as the fuel utilization in the stack and the current density. To draw maximum power from the stack and hence to achieve very high efficiency, the stack must be operated at a particular current level as shown in Fig. 5.2.14. However, due to the presence of low frequency ripple in the stack current, the operating mean stack current has to be decreased, to avoid zero reactant condition, as illustrated in Fig. 5.2.14. This decrease in the mean stack current decreases the stack fuel utilization.

**Fig. 5.2.13:** Power-electronics induced high- and low-frequency ripples in the fuel cell current.

**Fig. 5.2.14:** Effect of low frequency ripple on the performance and efficiency of the stack.
High-frequency ripple

High-frequency ripple usually refers to the switching ripple of the PES and is typically over 10 kHz. It has an impact on the electrochemical impedance and efficiency of the PSOFC. However, because the time period of the high-frequency ripple is much smaller compared to the electrochemical time constant of the planar fuel cell, it may have negligible impact on the performance of the planar cell.

5.3 EXPERIMENTAL WORK

5.3.1 Experimental Prototype Design of the Ripple Eliminating PES

The proposed power-electronics system (PES) is shown in Fig. 5.3.1 has the following power-stage sub-systems: (A) zero-ripple boost converter, (B) high-frequency (HF) inverter, and (C) an AC-AC converter.

5.3.1.1 Zero-ripple Boost Converter (ZRBC)

Fig. 5.3.1 (a) shows the schematic of the proposed ZRBC, which steps up the voltage of a fuel cell stack. Unlike a conventional boost converter, because the ZRBC eliminates the switching ripple of the source current, it enhances the durability and life of the fuel cell or photovoltaic module.

The main feature of the ZRBC is the zero-ripple inductor, which is a very tightly coupled (k = 1) ideal transformer. The transformer the primary winding comprises N1 turns and has a self-inductance L1 and secondary winding comprises N2 turns and has a self-inductance L2. Fig. 5.3.2 explains the concept of the zero ripple inductor starting with a non-ideal transformer (k < 1) (Fig. 5.3.2b). The currents I_in and I_out are AC currents and voltages V_in and V_o are input and output voltages, respectively. In practice k < 1 and the secondary winding will have fewer turns than the primary winding. The ripple gain is zero for an ideal zero ripple inductor, but in practice a very small ripple is there. Typically the voltage across the capacitor C_f is same as the input voltage with a small voltage ripple because of ripple current. The secondary winding carries the ripple current and the primary winding carries the DC current. For a tightly coupled transformer (k = 1) L_ext is adjusted to vary the current ripple.

The ZRBC is a standard non-isolated boost converter, in which the conventional inductor is replaced with a zero-ripple filter (ZRF). The ZRF (as shown in Fig. Fig. 5.3.3(c)) is viewed as a
combination of a coupled inductor (shown in Fig. 5.3.3(a)) and a half-bridge active-power filter (APF) (shown in Fig. 5.3.3(b)). Such a hybrid structure serves the dual purpose of reducing the high and the low-frequency current ripples. The coupled inductor minimizes the HF ripple from the fuel cell current \( (I_{FC} + i_{2HF} = i_{1HF}) \) while the APF minimizes the low-frequency ripple current of the fuel cell current \( (I_{FC} + I_{acLF} = I_{inLF}) \). Symbol \( I_{FC} \) is the DC current supplied by the fuel cell,

**Fig. 5.3.1:** (a) Block diagram and (b) schematic of the proposed PES. The shaded block in (b) illustrates the extension of the proposed PES to a three-phase output system.

\( i_{2HF} \) is the HF AC current supplied by the capacitor C (in Fig. 5.3.3(a)) or equivalently, a series combination of identical capacitors \( C_1 \) and \( C_2 \) (in Fig. 5.3.3(c)), and \( I_{acLF} \) is the low frequency AC current supplied by the APF storage reactor \( L_r \). For effective reduction of the HF current from the fuel cell output, the values of the capacitors \( C_1 \) and \( C_2 \) should be large and series inductance small. However, the series combination should be small enough to provide a high impedance path to the low frequency current \( I_{acLF} \).
5.3.1.2 High Frequency (HF) Inverter

The proposed high-frequency inverter (Fig. 5.3.4(a)) has 4 switches (S1-S4) just like the conventional high-frequency inverter. However, unlike the conventional HF inverter, as shown in Fig. 5.3.4(b), the switches are arranged in a multilevel topology leading to a 50% lower voltage stress on the power devices and reduced switching losses. The proposed inverter has a high-frequency transformer (N = 1) with a center-tapped secondary. Turn-on and turn-off of switches S1 and S2 and S3 and S4 are complementary. During first half of the switching cycle, S1 and S2 are turned on (while S3 and S4 are turned off) allowing the current to ramp up in the primary of the transformer and flow through capacitor C1. In the second half, current flows through capacitor C2, transformer primary, S3 and S4 and hence, the current is negative. During the off state, the voltage across the switch is equal to half the input voltage and hence, switches with a voltage rating of $V_{in}/2$ could be used. This also leads to lower switching losses. The zero-current in the transformer primary is due to the freewheeling current in the AC-AC converter switches and the load.
However, when the grid fails, the control system changes mode from voltage-mode control to current-mode control.

12 For a grid-connected system, this voltage-mode controls work as long as the grid is available. However, when the grid fails, the control system changes mode from voltage-mode control to current-mode control.
Fig. 5.3.4: (a) Proposed and (b) conventional high-frequency inverters. The proposed HF inverter reduces voltage stress of the power devices by 50%, which also leads to lower switching losses.
Fig. 5.3.5: (a) Schematic of the AC-AC converter topology for single- and three-phase applications; (b) sine-wave-modulated PWM control of phase a of the AC-AC converter; and (c) timing chart showing the scheme for the gating pulses for switches Q1 and Q2.

Zero-current Switching
When the AC-AC converter outputs a nonzero voltage, the load current is supplied from the inverter through the high-frequency transformer. When the output voltage of the AC-AC converter is zero, the load current freewheels in the converter. This results in a zero-current condition in the secondary of the transformer, and consequently, a zero-current condition in the primary winding of the transformer. Thus, inverter switches S1 and S2 and S3 and S4 can, respectively, be turned off/on and on/off under zero-current-switching conditions, leading to reduction in switching losses and increase in the efficiency. Fig. 5.3.6 shows that zero-current switching (Q1, Q3 and Q5 are simultaneously turned on).
Fig. 5.3.6: Current is reduced to zero from a positive value when the load current freewheels (Q1, Q3 and Q5 are simultaneously turned on).

The final schematic of the proposed PCS is shown in Fig. 5.3.6. A working prototype (Fig. 5.3.7) is developed for the following specifications: (a) nominal SOFCS voltage: 70 V, (b) output voltage: ~ 110 V, signal phase, 60 Hz (c) output power: 5 kW (d) switching frequency of DC-DC converter: 20 kHz (e) switching frequency of DC-AC converter: 20 kHz. Table 5.3.1 lists the key power stage components. The results of the prototype is discussed in the Section 6.
Fig. 5.3.7: (a) Schematic of the proposed experimental PCS. (b) Current-mode control scheme for the ZRBC. (c) Control scheme for the overall DC-AC converter.
Fig. 5.3.8: Experimental prototype of the proposed PCS.

Table 5.3.1: Key power-stage component listing for the designed PES.

<table>
<thead>
<tr>
<th>Designator</th>
<th>Manufacturer</th>
<th>Part Number</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>S, Q1-Q4</td>
<td>IXYS</td>
<td>IXFX55N50</td>
<td>500 V, 55 A, 80 mΩ</td>
</tr>
<tr>
<td>S1-S4</td>
<td>IXYS</td>
<td>IXFX120N20</td>
<td>200 V, 120 A, 17 mΩ</td>
</tr>
<tr>
<td>D</td>
<td>Infineon Technologies</td>
<td>SDT12S60, SiC Schottky</td>
<td>600 V 12 A</td>
</tr>
<tr>
<td>Coupled Inductor</td>
<td>Magnetics Inc.</td>
<td>58867-A2 (μ=60) High-flux Toroidal</td>
<td>500 μH @FL, 700-750 μH @NL, N1 = 73, N2 = 15</td>
</tr>
<tr>
<td>HF Transformer</td>
<td>Magnetics Inc.</td>
<td>P-49925-UC, Ferrite Core</td>
<td>Np = 34, Ns = 80</td>
</tr>
<tr>
<td>HF inverter Controller IC</td>
<td>Texas Instruments</td>
<td>UCC3875</td>
<td>Phase Shift Controller</td>
</tr>
<tr>
<td>HS</td>
<td>Aavid Thermalloy</td>
<td>60095</td>
<td>1.90 °C/W, W= 4.12”, H=1.75”, Area= 36.8 sq.in</td>
</tr>
</tbody>
</table>
5.3.2 Experimental Stack Prototype

5.3.2.1 Stack Construction

Stack 25UIC437 was constructed for testing of stack impedance, interaction of stack and PES, SOFC temporal model validation, and load profile testing. The cells are 10 x10 cm with a 64 cm² active electrode area.

The electrolyte is produced at Ceramatec by tape casting and sintering of commercially available Scandia Stabilized Zirconia powder. The thickness is approximately 180 μm. The electrodes with proprietary compositions and are synthesized at Ceramatec and applied by screen printing and sintering operations. The interconnects are fabricated using a ferrite stainless alloy which is treated using a process developed by Ceramatec over the past 15 years.

The stack was installed in a test stand equipped with the needed reactant feed measurement, control and preheat systems, as shown in Fig. 5.3.9. A thin gauge thermocouple was installed near the center of the stack by insertion into an interconnect channel on the air exhaust face of the stack. Voltage tap leads were similarly provided every 5 cells. Voltages (overall stack and 5 cell groups), current, temperatures (air inlet plenum which acted as the furnace controller value measurement, furnace enclosure, and stack core) were measured and recorded using a custom developed Lab-View application. Steam generation for electrolysis mode was by means of saturation of a hydrogen/nitrogen fuel stream in a controlled temperature water bubbler. Photographs of cell and interconnect components, a similar 22 cell stack (tested in RFC mode at INL in July), and its installation in the test fixture are shown in Fig. 5.3.9.

The initial performance is shown in an I-V sweep from electrolysis through open circuit to fuel cell mode in Fig. 5.3.10. The area specific resistance (ASR) in RFC mode was 1.3 ohm-cm² at an average core temperature of 815°C. The fuel cell mode ASR was lower (1.0 ohm-cm² ) due to the higher operating temperature resulting from fuel cell operation and limited cooling air flow in a test station originally designed for 10 cell stacks. Note the smooth and continuous transition from one mode to the other about the open circuit (zero current) point indicating the reversibility of the SOFC/RFC device.

The stack was subjected to a power electronics/impedance test to validate the effect of PES and AL on the stack, as described in Section 5.3.3 during the period of 15th to 20th of August 2005. In the intervening time, until the load profile hardware was available, the stack was operated in RFC mode as shown in Fig. 5.3.11 as a hot standby mode giving an indication of degradation.
Fig. 5.3.9: SOFCS, components and installation photos.

**SECA Power Electronics Stack Test**

- **846°C Stack Core**
  - 49.4% Steam Utilization
  - \( y = -1.313x + 0.942 \)
  - \( R^2 = 1.000 \)

- **896°C Stack Core**
  - 72.4% Utilization
  - \( y = -1.045x + 0.933 \)
  - \( R^2 = 0.993 \)

**Fig. 5.3.10:** 25-cell stack initial V-I characteristics.
Fig. 5.3.11: Initial 800 hours of stack operation, predominantly in RFC mode.

The full load profile history graph is shown in Fig. 5.3.10. (hours 1005-1490 as of 17 Oct.2005). In the middle of the interval shown in Fig.5.3.10, there were two upset conditions. First, the computer running the data system controlling the load cycle locked up, leaving the stack in 16V regulation mode. The data recording system then failed altogether.

During this data blackout period, which happened over a weekend, the hydrogen tank cluster ran out due to a failure of the local industrial gas vendor to refill the tanks as requested and routinely done. Once the problems were discovered and corrected the following Monday morning, stack load profile operation resumed. A peak performance offset of a little over 0.5A resulted from this upset. The damage to this stack from operation over the weekend without hydrogen was minimal. Every other SOFC test underway at the time in the Ceramatec SOFC laboratories suffered greater damage as measured by cell performance, with the exception of a cell being operated on CO/CO₂, which was of course unaffected. In another tests for this project, which is described later, four stacks of 5 cells under constant resistance loading suffered a 50% performance drop from the event.

5.3.3 Validation of PES Feedbacks on PSOFCS

To prove the accuracy of the PSOFCS PCS modeling works, and to validate the effects of electrical feedbacks on PSOFCS, the PES was connected to the stack. The stack consists of 25 planar cells in series. In the stack, all the planar cells are mounted in a single manifold. The cross-flow arrangement for the reactants is done. Each cell has an electro-active area of 64 cm². Temperatures of the reactants (fuel and air) are maintained at 802 °C (1075 K). The detail
specifications and test conditions of the stack are described in Table 5.3.2. Fig. 5.3.12 shows the photograph of the test setup.

**Fig. 5.3.12:** Experimental setup of the 25 cell PSOFCS with the PES.

**Table 5.3.2(a):** Stack specifications for the experimental validation

<table>
<thead>
<tr>
<th>Specification</th>
<th>Value</th>
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<tbody>
<tr>
<td>Number of cells in the stack</td>
<td>25</td>
</tr>
<tr>
<td>Cell electro-active area</td>
<td>64 cm²</td>
</tr>
<tr>
<td>Stack Open circuit voltage (Voc)</td>
<td>23.75 V</td>
</tr>
<tr>
<td>Area specific resistance (ASR)</td>
<td>1.291 ohm.cm²</td>
</tr>
<tr>
<td>Fuel composition [H₂: H₂O: N₂]</td>
<td>[0.461 : 0.462: 0.077]</td>
</tr>
<tr>
<td>H₂ flow rate</td>
<td>9.54 slpm</td>
</tr>
<tr>
<td>N₂ flow rate</td>
<td>1.6 slpm</td>
</tr>
<tr>
<td>Air flow rate</td>
<td>38.2 slpm</td>
</tr>
<tr>
<td>Air inlet temperature</td>
<td>800 °C</td>
</tr>
<tr>
<td>Stack core temperature</td>
<td>816 °C</td>
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Table 5.3.2(b): PES specifications for the experimental validation.

<table>
<thead>
<tr>
<th>Boost Converter</th>
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<tbody>
<tr>
<td>Inductance (L)</td>
</tr>
<tr>
<td>Output Capacitance (C)</td>
</tr>
<tr>
<td>Bus Voltage</td>
</tr>
</tbody>
</table>

Table 5.3.2(c): Test condition of the validation experiment.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
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<tbody>
<tr>
<td>Ambient pressure</td>
<td>0.859 atm</td>
</tr>
<tr>
<td>Water vapor pressure</td>
<td>0.397 atm</td>
</tr>
<tr>
<td>at 76.7°C</td>
<td></td>
</tr>
</tbody>
</table>

5.3.3.1 Characterization of the PSOFC Stack

Fig. 5.3.13 shows the setup for the characterization of the stack. The DC electronic load is varied in steps to draw different amount of current from the stack. The voltages of the stack at different current levels are noted using the LeCroy Oscilloscope.

![Fig. 5.3.13: Setup for the stack characterization and load transient study.]

5.3.3.2 Study of Load Transient

Fig. 5.3.13 shows the setup to study the effect of the load-transient on the stack. The DC electronic load is used to vary the load so that the current drawn from the stack varies from 2.2 A to 12 A. For multiple load transient, the electronic load is programmed to vary between two specified loads after a particular time interval.

5.3.3.3 Low-frequency Ripple Study

Fig. 5.3.14 shows the setup to study the effect of the ripple on the stack. The PES consists of a bidirectional boost converter. The switch of the converter is modulated using a biased sine wave reference at 60 Hz, generated using the signal generator. To observe various percentage of the ripple in the current, the bias and the amplitude of the sine wave is varied.

5.3.3.4 Stack Impedance Measurement

The setup to measure the impedance of the stack is given in Fig. 5.3.15. The network analyzer provides output from its source terminal, which is swept across the range of the frequencies. A coupling capacitor is connected, as shown in Fig. 5.3.16, to eliminate the DC which may interfere with the impedance measurement. The connection diagram is shown in Fig. 5.3.16.
Fig. 5.3.14: Setup to study the effect of the ripple on the stack.

Fig. 5.3.15: Setup for measuring the stack impedance.

Fig. 5.3.16: Connection diagram for the stack impedance measurement.
5.3.4 Long-term Degradation Study

In Section 5.2.1, interaction analysis of the PES on the stack is done. However, the effect of these feedbacks in the long term needs to be investigated for the completion of the study. The developed stack model could not predict any degradation in the long term. Therefore, thousand hours of experimental study is done to investigate the impact of the electrical feedbacks, such as ripple and the load transient on the stack performance in the long run.

5.3.4.1 Long-term Effect of Ripple

Fig. 5.3.17 shows the PES prototype for the long-term ripple study. The PES consists of a boost converter modulated by a biased sinusoid at 60 Hz. The amplitude and bias of the modulating sine wave is adjusted so as to draw 100 percent ripple current from the stack. The degradation study of ripple is conducted on a 5 cell stack connected to a boost converter, and a 5 cell stack connected to the constant load.

The stacks were constructed and operated for a period of ~2000 hours, from mid-November through the end of January. The average current drawn from both the stacks are kept at approximately 13 A. The open circuit voltage of the 5 cell stacks are approximately 5.087 V.

A power outage due to scheduled maintenance at the end of December resulted in a thermal cycle of the stacks. Reheat of the furnace after the power outage encountered some problems with blown fuses and repeated failure to attain temperature. Operating temperature in January was approximately 50 degrees lower than in the earlier portion of the run, which accounts for much of the increase in stack area specific resistance over the thermal cycle. However, the ripple loaded and resistance loaded stacks track each other very closely.

5.3.4.2 Long-term Effect of Load-transient

To study the long term degradation effect due to the load transient, a 25 cell planar stack is connected to a microcontroller programmable PES followed by a load resistance. The PES is programmed to draw 13 A current for first 20 minutes and 2.2 A for the next 10 minutes in every half an hour. Therefore, the average current drawn from the stack is 9.4 A. The open circuit voltage (V_{oc}) of the stack is 24.75 V. Fig. 5.3.18 shows the alternative PES built at UIC for the load transient study. Fig. 5.3.18 shows a typical data captured for the load transient study.
Fig. 5.3.17: PES prototype for long-term ripple study.

Fig. 5.3.18: PES prototype for the long-term load-transient study.
5.4 CONTROL DESIGN AND PARAMETRIC OPTIMIZATION

5.4.1 Design of Power Management Control

To effectively eliminate the effect of the load transient, energy buffering devices like battery are used in conjunction with the fuel cell. A control mechanism is needed to increase the efficacy of this hybrid energy system.

A control system is proposed by Hochgraph et. al, 2004, which would control the state of the charge of battery by manipulating the voltage of the stack through dynamic system modeling of predetermined parameters for the stack and the battery. This control strategy tries to eliminate the need of any input power converter, resulting in the cost reduction of the power conditioning system. However, this strategy neither provide any option to alleviate the degrading effects of the load transient on the stack, nor it considers the efficiency of the power system.

Fig. 5.3.19: Expanded segment of load profile data on 12/08/2005.
In another approach, a fuel cell/battery hybrid system with microprocessor based control is proposed by Early et. al (1990), which tries to alleviate the degrading effects of the load transients by enabling the fuel cell stack to be taken out of the system when a fixed maximum energy output of the stack is exceeded by the load requirement. Since the efficiency and as well the energy density of the battery are small as compared to the fuel cell stack, at higher loads the efficiency of the system goes down. With the battery needs to supply the full load current at high loads, the required energy storage capacity of the battery increases, leading to an increase in the space and cost of the battery and hence the cost of the power system.

In another controlling strategy or fuel cell hybrid vehicle by Droppo et. al (2003), a battery power controller is used to control the power flow from the battery; this provides the additional power to the load when the stack voltage goes below a certain minimum. However, as experimentally investigated in this work, the battery current does not respond to an abrupt load increase immediately and hence could not prevent the zero reactant condition in the stack, unless the operating fuel utilization is inefficiently low. In another approach, as in Jossen et. al (2005), a DC-DC converter is connected at the stack output to deliver a more stable output voltage to the load, and battery is connected at the converter output. During a load transient, the battery provides the additional load current as soon as the bus voltage drops below the voltage of the battery. However, this may lead the battery to handle the full load current until the battery voltage goes below the bus voltage. Again, the higher the bus voltage higher is the number of the batteries required to support the bus voltage, leading to the need of larger number of higher capacity battery.

We propose and design a comprehensive control system with hierarchical control architecture for the fuel cell power system. In this architecture the master control optimizes the controller parameters of the individual subsystems (energy buffering device, BOPS and the PES), which in turn optimizes the performance and efficiency of the overall system while nullifying the effects of load transients on the FCSS.

5.4.1.1 Control Objectives

The high cost of the fuel cell power system leads to higher unit cost of the fuel cell power, and has been one of the bottlenecks in the commercialization of the system. The energy density of the battery being very small as compared to the fuel cells, not only the physical size but also the Ampere-Hour of the battery, which is the indicative of the cost of the battery system, are of prime concern to a designer. Hence optimization of battery size is one of the prime objectives of the control.

The stack efficiency and hence the system efficiency increases with an increase in the fuel utilization in the stack. However as the fuel utilization increases beyond a certain limit, fuels are not supplied evenly to every stack. Slight unequal pass of the fuel in the stack or manifolds cause an uneven distribution of the fuel to the stack, leading to a zero reactant condition in the stack. This condition degrades the anode of the fuel cell degrading the performance of the cell. Hence the fuel utilization should be optimized to obtain high stack efficiency without any reliability issue in the cell.
The presence of low frequency ripple current and anticipated load transient limits the operating range of the fuel utilization. Again the losses in the PES decrease the efficiency of the system. Hence an optimal PES topology is required which will not only minimize the losses in the PES but also reduce the low frequency ripple current magnitude.

The performance of the system is quantified by the ease with which the system reaches the desired value or the steady state when subjected to a transient. To achieve better performance the BOPS should have a very small response time. However the BOPS being a mechanical system, the response time cannot be decreased beyond a certain practical limit. Therefore we need a fast response hybrid system which can provide the required excess load current during a load transient and thereby emulating zero-transient condition for the system.

5.4.1.2 Control Architecture

In a conventional power conditioning systems for fuel cell systems, each individual subsystem is controlled individually and tries to achieve the individual desired objective with the best possible time. The power converters are controlled to provide a constant output voltage (DC or ac) in the steady state and should have minimal overshoot and undershoot during a transient. The BOPS determines the required flow rate of the air and fuel into the FCSS based on the power requirements of the load and maintains the temperature inside the stack. Therefore, it is designed to provide the required amount of fuel and air to the stack in the fastest possible time and maintain the temperature in the stack with minimum variations. The control for the battery or the BMS is designed to provide the additional current during the transient with very fast response.

Because each of the subsystem affects the performance and the operation of other subsystems, optimal operating point of the PCS both in the steady-state and during the transient could not be achieved without information regarding the states of all the subsystems. However, designing a centralized control with all the states of the PCS is a tedious task, given that the BOPS itself has hundreds of states. Similarly, analyzing the stability of the system to obtain an optimal and stable operating point for the PCS of such a high order needs too large a computational time.
To alleviate the computational complexity of a centralized controller, hierarchical control architecture for the fuel cell power system, as shown in Fig. 5.4.1, is conceived. This hierarchical control enables mutually independent control design, leading to higher flexibility, and enables easier and faster calculation of stable operating points for the individual subsystems; this optimizes the system performance and reliability.

5.4.1.3 Proposed Topology

We propose a power electronics topology for the hybrid power management system as shown in Fig. 5.4.2, in which one or multiple DC-DC converters are connected at the output of the stack and the battery, which are then connected in parallel to share the load.

The number of parallel converter modules, \( N \), would depend upon the rated power of the stack and the battery module. The switches \( R_1, \ldots, R_N \) activate and deactivate the converter modules and the number of active DC-DC converter modules at any time depends on the amount of power drawn from the stack and/or the battery and the efficiency of the converter modules at particular power drawn by each of the active converter module. The switch \( R_{bat} \) is used to enable access of the battery for discharging and as well as the charging through multiple converter modules. Now, the current drawn by each of the active converters connected to the stack and/or the battery at any time is calculated based on the total required current and the efficiency of the converter modules, which maximizes the overall efficiency of the PES.

---

**Fig. 5.4.1**: Comprehensive hierarchical controller architecture for the fuel cell based power system.
Efficient Power Sharing Strategy

The efficiency of any DC-DC converter depends upon the power delivered by the converter. At higher output power, the losses increase with increase in the converter current, leading to a drop in the efficiency. On the other hand, at very low output power, the losses become a larger percentage of the output power, which again decreases the converter efficiency.

Mathematically, for each of the $k$ converter modules the efficiency map\(^{14}\) is given as

$$\eta_i = f(p_i) \quad i = 1, 2, ..., k \quad (5.4.1)$$

where $p_i$ is the fraction of the rated output power, $P_{\text{rated}}$ of the converter. Now assuming, $P_i$ to be the input power for the $i^{th}$ converter, such that $\sum_{i=1}^{k} P_i = P_{\text{in}}$, we have, $p_i = \frac{P_i \eta_i}{P_{\text{rated}}}$.\(^{14}\)

\(^{14}\) The efficiency map is experimentally obtained for a converter module.
Now equation (5.4.1) can be rewritten as

\[ \eta_i = f(\eta_i, m_i) \quad i = 1, 2, \ldots, k \]  
where \( m_i = P_i / P_{\text{rated}} \)   \hspace{1cm} (5.4.2)

The iterative equation (2) can be solved to obtain the equation of the \( \eta_i \) in terms of \( m_i \) only

\[ \eta_i = f_m (m_i) \quad i = 1, 2, \ldots, k \]  \hspace{1cm} (5.4.3)

Now the efficiency of the system is given as,

\[ \eta = \frac{1}{P_{\text{in}}} \sum_{i=1}^{k} P_i \eta_i = \frac{P_{\text{rated}}}{P_{\text{in}}} \sum_{i=1}^{k} m_i f_m (m_i) \]  \hspace{1cm} (5.4.4)

To maximize the efficiency of the converter system, the values of \( m_i \) need to be obtained, which maximize the function, \( \sum m_i f_m (m_i) \) for a given input power, and satisfy the constraint \( \sum m_i = P_{\text{in}} / P_{\text{rated}} \), and \( m_i \leq 1 \).

![Graph](image)

**Fig. 5.4.3:** Theoretical efficiency of the 5 kW stack with fuel utilization at various flow rates (moles sec\(^{-1}\)).
Optimal Fuel Utilization Tracking

The stack efficiency and hence the system efficiency increases with an increase in the level of fuel utilization in the stack. However, as the fuel utilization increases beyond a certain limit, the high current density leads to higher drop in the cell voltages and hence the stack voltage, leading to a drop in the stack efficiency.

Fig. 5.4.3 shows the variation of the theoretical stack efficiency with the variation in the fuel utilization at different fuel flow rates levels of the stack and at a constant temperature for a typical fuel cell. As observed, the maximum efficiency is obtained at fuel utilizations beyond 0.95. However, this high level of fuel utilization is not practically achievable due to several reasons.

a. Hydrodynamic leakage: Fuel leakage attributed to the physical leakage, which is directly proportional to the absolute pressure differential across the seal.

b. Diffusive leakage: Diffusion of hydrogen into the electrodes, which is a function of temperature, mole fraction and the concentration.

c. Cell size: With larger cell size, the fuels are not supplied evenly to every cell. Slight unequal pass of the fuel in the stack or manifolds cause an uneven distribution of the fuel to the stack, leading to a local zero reactant condition in the stack.

These three reasons need to be considered to obtain optimal fuel utilization levels for a practical fuel cell stack subsystem. As noticed, all these parameters remain constant, at a constant operating pressure, temperature, fuel constituents and for a given stack and not on the current density inside the cell. Therefore, at higher flow rates of fuel into the stack, the percentage of the leakage (as compared to the flow rates) decreases, and hence higher fuel utilization level can be achieved, i.e., at higher power outputs, the stack can be operated at higher fuel utilization as compared to at lower power outputs.

Therefore, a flow rate-fuel utilization map is designed which will determine the optimal fuel utilization \( \bar{f}_{u} \) at a different levels of the fuel flow rate from the BOPS thereby, maximize the efficiency of the stack. This map is to be designed for each experimental stack based on the leakages and the stack design.

System Control Scheme

The control architecture for this multi-converter approach is shown in Fig. 5.4.4. To enhance the response of the DC-DC boost converter, a tracking control is proposed, which is based on the control of the input current for a desired output voltage (Cortes et al., 2004). The error in the bus voltage is used to calculate the required total current, \( i_{\text{tot}} \) needed to supply the load. During a transient or in the steady-state, the required battery current, is calculated as the difference between the desired total current, \( i_{\text{tot}} \) and the optimal fuel cell stack current, \( i_{\text{FC}} \). The current drawn by each of the active converters connected to the stack and the battery at any time is calculated based on the efficient power sharing strategy discussed earlier.

The total current to be drawn by the active converter or converters connected across the fuel cell stack, \( i_{\text{FC}} \) is calculated from the error between the fuel utilization of the stack, \( f_{u} \) and the desired fuel utilization, \( \bar{f}_{u} \).
Fig. 5.4.4: Optimal fuel utilization tracking based controller architecture for the fuel cell based power system.

5.4.2 BOPS Control Design

5.4.2.1 Control Objectives

A fuel cell stack requires a forced air supply at system pressure. It is important that the flow through each cell should be evenly distributed, especially when diluted reactant gas such as air is used, in order to avoid trapping the partially depleted reactant gas in a relatively restricted flow area. Additionally, when changes in load occur, it is extremely important to keep the appropriate air/hydrogen ratio in the cell in order to avoid cell degradation, high parasitic loads, or starvation induced loads. To assure the flow through each cell at an optimum operating pressure, the air supply system requires coordinated pressure and flow control system. An air compressor with speed control features can be used to supply different amounts of air for a wide range of power demands in order to reduce parasitic power losses.

One of the most important performance criteria for both stationary and mobile fuel cell systems is the transient response to power demands. The fuel cell itself has a very fast dynamic response. However, the response times of the FPS and WRAS subsystems are dependent on system synthesis/design and will affect the overall system transient performance.

For direct hydrogen fuel cell systems, liquid or compress gas hydrogen is stored in a tank. The control task in the hydrogen supply system is to keep the fuel cell flooded with hydrogen and circulated at the same pressure as the air supply pressure, independently of the hydrogen consumed and in proportion to the electrical current drawn. It may also be important to minimize...
the pressure difference between the fuel-supplied anode and the air supplied cathode. The same control issues apply to the onboard or in-place fuel processors. However, in this case additional control issues arise. The control problem encountered in the fuel processor is very complicated. Like any other chemical process it is multi-input/multi-output (MIMO) control system; and to achieve highly efficient chemical conversion, it is important to have precise pressures, temperatures, and mass flow rates of the various reactants at different locations. Furthermore, on overall subsystem controllability analysis is critical in designing proper control algorithms. For instance, controlling the fuel flow to meet the fuel cell power demand and at the same time meet the energy demand at the reformer using exhaust gases may result in an uncontrollable situation. Therefore, accurate control of the reactant ratios at the reactor and at various operational conditions is critical in achieving good overall system performance, fuel economy, and emissions, quite a challenging control task.

5.4.2.2 Control Parameters and Control-variable Set Definitions

A set of system-level control variables have been defined, whose purpose is to keep the component-level dependant variables within acceptable ranges, which in turn can be initially defined as component control limits (e.g., such as maximum stack inlet temperature) or as the output of a trade-off or optimization process (e.g., reformer optimum operating temperature).

The system-level control variables chosen for the BOPS are the steam to methane ratio (SMR), the fuel utilization (FU), the air to fuel ratio (AFR), and the fuel reformate ratio (FRR). The steam to methane ratio allows control of the chemical reaction inside the steam reformer. The fuel utilization affects BOPS energy recovery (in the form of heat and work interactions) and is important for characterizing the reaction in the stack. The air to fuel ratio is the ratio between the air and fuel going to the combustor. It affects the parasitic power requirements and the mass flow and temperature of the combustion gases exiting the combustor as well. Finally, the fuel reformate ratio is the ratio between the methane used in the reformer and the methane burned in the combustor. It permits control of the outlet temperature of the steam-methane reformer. In addition, the proportions at which the stream of hot gases leaving the reformer is divided (one stream to the steam generator and two to two separate compact heat exchangers) and the air stoichiometric ratio in the stack can be used as the system-level control parameters.

5.4.2.3 Fuel and Energy Buffering

SOFCs respond quickly to changes in load while the BOPS responds in times which are several orders of magnitude higher. This response dichotomy can diminish the performance of SOFC electrodes with increasing load as can current and voltage ripples which result from particular PES topologies and operation. Thus, ripples, load changes, and differences in transient response must be approached in a way which ensures not only that efficiency and power density, fuel utilization, and fuel conversion are optimal at all loads but that system response and

Note that the term “control variable” is used here in the sense of a thermodynamic operational decision variable and not in the strict sense of what is directly or physically controlled within the system. For example, physically, there is no such thing as a FU (fuel utilization) controller. Instead, a mass flow rate controller of fuel to the stack for a given current density and load controls the FU. Thus, FU as a control variable has a mathematical sense (i.e. it is an independent variable) but not a physical one.
reliability are maintained at optimal levels for all operating conditions. This can be aided by introducing fuel, air, and electrical energy buffering into the system layout.

As can be seen in Fig. 5.1.25, such buffering has been added to the system configuration. Typically buffering is only used in stationary systems because of the additional weight and volume, which are the operational penalties for transportation systems. However, in this work, the air and fuel tanks considered are very small and light (initial tank designs have yielded 1 liter volumes). It is important to note that the tanks are used to minimize transient effects, to increase response capabilities, and to minimize the subsystems interaction effects during transients. They are not intended for long term storage. With this in mind, it is reasonable to explore a trade-off between the advantages of using buffering devices and the penalties for using them.

The control strategy developed for the BOPS ensures that the fuel and the air in the tanks are never depleted. In addition, during load transients, the load on the SOFC, which is not a stiff voltage source and is, thus, connected to the load through the PES, is met by the batteries until the BOPS is able to supply fuel at the required rates. However, because the batteries (depending on their size) discharge at relatively rapid rates, their duration of operation is relatively small and must, therefore, be combined with a pressurized fuel tank which can rapidly supply fuel to the stack. In addition for transportation applications, the intention is to use the actual battery set of the vehicle instead of a separate battery bank. For stationary applications, batteries can be replaced by the grid.

5.4.2.4 Control Laws and Strategies

Fig. 5.4.5 shows the proposed control scheme for the BOPS integrated to the PES and SOFCs. A multilevel control approach is used in order to help improve the time response of the BOPS. The first level is determined by the air and fuel tank pressures. The objective of the fuel processing and air supply subsystems is to keep the tank pressure at a fixed value. Disturbances in tank pressures appear as the fuel and air stack requirements change. Control strategies should guarantee that the fuel in the tank is never depleted and should ensure that no shut-down process is complete before proper levels of fuel in the tank are reached. Two additional control actions are implemented for the steam methane reformer with the objective of regulating the reformate gases exit composition and temperature. At the steam-methane reformer, the reformate gases temperature and composition are controlled using the hot gases inlet temperature and mass flow, respectively, as control variables. The pairing of the state variables and control variables was determined using the relative gain array matrix (i.e. a common technique of control theory). Table 5.4.1 shows the control and state variables pairing used in order to implement the proposed control strategy.
The second level of control is defined by the hydrogen and air stack requirements. As the load changes, the amount of hydrogen (reformate) out of the tank is changed by regulating the flow valve. The air tank valve is regulated to maintain the proper stoichiometric ratio in the stack. The third level of control is defined by the rate change in load demand and battery bank charge level. For sudden changes in load, the difference between the produced and required power is supplied by the battery bank. The power required to keep the charge level is considered as a parasitic power. Finally, for small increments in power demand, the system is able to assure direct stack response until proper hydrogen mass flow is reached. This is done by increasing the fuel utilization up to safe levels. Reductions in power demand are easier to control, since these can be done by reducing fuel utilization; reducing hydrogen mass flow; and by switching the battery bank to charge mode.
Table 5.4.1: Control and state variables pairing$^{16}$

<table>
<thead>
<tr>
<th>Component</th>
<th>Control Variable</th>
<th>State Variable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Steam-methane reformer</td>
<td>Hot gases inlet temperature</td>
<td>Reformate gas exit temperature</td>
</tr>
<tr>
<td></td>
<td>Anode recirculation fraction</td>
<td>Steam to methane ratio</td>
</tr>
<tr>
<td>Reformate tank</td>
<td>Methane mass flow</td>
<td>Tank Pressure</td>
</tr>
<tr>
<td>Air Tank</td>
<td>Electric Motor volts</td>
<td>Tank Pressure</td>
</tr>
<tr>
<td>Fuel Cell Anode</td>
<td>Valve volts</td>
<td>Reformate mass flow</td>
</tr>
<tr>
<td>Fuel Cell Cathode</td>
<td>Valve volts</td>
<td>Air mass flow</td>
</tr>
</tbody>
</table>

**Start-up strategy with battery bank:**

An analysis of the proposed configuration and control strategies and a consideration of the need for a fast response to load changes lead to the following system start-up control strategy:

1. First the turbo-machinery is started. At this point energy is taken from the battery bank.
2. Once the turbo-machinery is operating, the TMS starts. Fuel and air are delivered to the combustor and hot combustion gases are produced in order to generate steam and heat up the system components.
3. Once the heat source is available, the steam generation process starts. The hot gas mass flow through the steam generator during start-up is higher than at the design point. This is done in order to speed up the convergence to steady state at high values of vapor temperature. The water coming out of the steam generator is recirculated. Thus, no water is wasted and the inlet temperature is increased.
4.1. While adequate vapor temperatures are being reached, hot combustion gases are used for thermal conditioning of heat transfer devices. Thus, hot gases are passed through the hot-side of the system’s heat exchangers and reformer. Hot gas flow through components is constrained by temperature gradient limits.
4.2. At the same time, the SOFCS is conditioned for high temperature operation.
5.1. The streams of hot gases coming out of the TMS are mixed together. If the output temperature is high enough, the PRS starts: the expander is coupled to the air compressor.
5.2. The SOFCS starts using reformate fuel and air from the high pressure tanks: SOFC electrical energy generation commences.
5.3. The SOFC and the PES are coupled in order to start the generation of alternating current.
6. The turbo-machinery stops taking energy from the battery bank, which begins to be recharged.
7.1. With the FPS components and steam at operational temperatures, the steam generator recirculation stops and the fuel processing begins.
7.2. The FPS and the SOFCS are coupled through the high pressure fuel tank. A minimum level of mass in the tank is required at all times.
8. The FPS and air compressor are never shut-down until proper levels in the air and fuel tanks are reached.

$^{16}$ The controller gains are treated as design decision variables in the optimization problem.
5.4.3 Parametric Optimization of BOPS

The procedure followed for the dynamic synthesis/design and operation/control optimization is based on physical decomposition. Time and conceptual decomposition are avoided by using the dynamic models and applying DILGO using the dynamic shadow prices. In the case of physical decomposition, three different subsystems, namely the FPS, SS, and WRAS are taken into account and their coupling functions described.

The interdependence between the three units (subsystems) being synthesized/designed (the SS, FPS, and WRAS) is quite tight. Thus, for example, the FPS’s optimal synthesis/design is affected by the optimal synthesis/design decisions made in the SS and WRAS as well as by the load requirements dictated for the PES. The result is that the fuel cell system at hand constitutes the typical case of a system in which “everything influences everything else”.

Thus, determining the optimal synthesis/design and dynamic operation of the fuel cell system requires that the optimal synthesis/design and dynamic operation of each of the auxiliary power unit subsystems be carried out in an integrated fashion. Individually optimizations of each subsystem without consideration for their integration as a system do not lead to the optimization of the system as a whole. The decomposition approaches, LGO and ILGO are two means by which each subsystem can be individually optimized consistent with their integration into the overall system. However, they are not suited to handle the system dynamics. This is particularly important when optimizing a system operating under transient conditions for a big fraction of its life cycle. Additionally, these systems can be subject to sudden load changes of considerable magnitude. For the reasons stated the DILGO approach is applied to the synthesis/design optimization problem at hand. For a detailed description on the DILGO approach the reader is referred to the work by Muñoz and von Spakovsky (2000a,b,c,d; 2001a,b) and Rancrue and von Spakovsky (2003).

5.4.3.1 System-level Dynamic Synthesis/Design Optimization Problem Definition

Future fuel cell systems present a unique set of requirements not previously addressed. For example, fuel cell based auxiliary power units must be substantially more affordable than comparable systems (battery packs and generators) both in terms of acquisition and operational costs. Future fuel cell systems will likely be high efficiency, high performance systems. To permit an integrated approach to their and other dynamic systems’ optimal synthesis/design and operation/control, it will be necessary to combine them into a single comprehensive model thermodynamic, kinetic, geometry, and control as well as cost functions so that a large number of independent variables related to how different technologies optimally accommodate limited payload spaces can be investigated (Brown, 1999). Thus the system-level optimization problem would be that of minimizing the total cost of the system through its life cycle. Thus the system-level optimization problem is minimizing the total cost of the system through its life cycle. It is formulated as follows in terms of the capital cost of each subsystem and the total operation/control cost:

Minimize

\[
C_T = C_{SS} + C_{FPS} + C_{WRAS} + C_{PES} + C_{BBS} + \int_{t=0}^{T} \dot{C}_{fuel} \, dt
\]

(5.4.5)
\[
\begin{align*}
&\text{w.r.t. } \{\bar{x}_{SS}, \bar{y}_{SS}, \bar{K}_{SS}\}, \quad \{\bar{x}_{FLS}, \bar{y}_{FLS}, \bar{K}_{FLS}\}, \quad \{\bar{x}_{WRAS}, \bar{y}_{WRAS}, \bar{K}_{WRAS}\} \\
\text{subject to } & \\
&\hat{H}_{SS} = 0, \quad \hat{G}_{SS} \leq \bar{G} \quad (5.4.6) \\
&\hat{H}_{FPS} = 0, \quad \hat{G}_{FPS} \leq \bar{G} \quad (5.4.7) \\
&\hat{H}_{WRAS} = 0, \quad \hat{G}_{WRAS} \leq \bar{G} \quad (5.4.8)
\end{align*}
\]

Note that \( C_{BB} \), and \( C_{PES} \) are fixed costs and are, thus, not minimized along with the rest of the objectives, which consist of the total cost of each subsystem and its associated fuel cost penalties. \( C_{SS}, C_{FPS}, \) and \( C_{WRAS} \) represent the capital, amortization, and maintenance costs. \( \dot{C}_{\text{fuel}} \) is the fuel cost rate which is integrated along the total life cycle (from time zero to time \( T \)). For this research work it is important to note that the optimization problem is being solve not only in terms of the synthesis/design and operational decision variables, \( \bar{x} \) and \( \bar{y} \), but also in terms of a set of PID controller gains, \( \bar{K} \), which are intended to optimize the system with respect to not only total cost but also the time response. Here, the system’s time response to the changes in load is set as a constraint.

In order to synthesize/design the proposed fuel cell system (FCS), the energy requirements for a representative residential building\(^{17}\) must be established. The types of residential loads considered are the following:

- Electrical load.
- Space heating load.
- Space cooling load.

The electrical load, in particular, includes the electricity needed to power the lights and appliances of the residence as well as the fans of the HVAC equipment. The profiles of these three different loads depend greatly on the geographical location of the residence and the corresponding weather conditions. The residential energy demands as well as the environmental conditions given in Figs. 5.4.6 and 5.4.7 are representative of Atlanta, Georgia, and are based on an analysis of detailed load profile data obtained from Gunes and Ellis (2001).

\(^{17}\) Based on the work by Gunes and Ellis (2001), a representative residential building is a 195 m\(^2\) typical single-family residence for the United States. Residential energy surveys indicate that a typical family includes four members, i.e. two adults and two children.
Fig. 5.4.6: Electrical energy use for peak cooling day in Atlanta, Georgia on 07/11 (Gunes and Ellis, 2001).

Fig. 5.4.7: Electrical energy use for peak heating day in Atlanta, Georgia on 01/12 (Gunes and Ellis, 2001).

Now, for purposes of this project, the entire load/environmental profile has been simplified into a two-day load profile, i.e. typical summer day plus typical winter day. This two-day profile seen in Fig. 5.4.8 is a simplification of the original profiles of Figs. 5.4.6 and 5.4.7 in that only major load transitions are taken into account. It is believed that this sufficiently models the load changes for the synthesis/design process. However, to ensure conditions which properly challenge the control systems, two abrupt large changes in load have been introduced at time 1 and 24 hours. The resulting total load profile shown in Fig. 5.4.8 is multiplied by 180 days in order to account for a whole year.
5.4.3.2 Decomposition and Coupling Function Definitions

In order to apply the DILGO method to the optimization problem the FCS is broken down into the subsystems mentioned earlier, i.e. the SS, FPS, and WRAS. Simplified breakdown of the FCS, as well as its interactions with the environment and the material and energy streams connecting its three subsystems, are shown in Fig. 5.4.9 Therefore, the physical decomposition of the proposed FCS configuration into three units leads to the decomposition of the system-level synthesis/design optimization problem into three optimization sub-problems, one for the SS, one for the FPS, and one for the WRAS. In order to apply DILGO to the system-level optimization problem for total life cycle cost, system-level, unit-based optimization problems are defined for the units to be optimized. The boundaries of each unit (subsystem), their associated local decision variables as well as the coupling functions connecting each unit with the rest are clearly seen in Fig. 5.4.9. This figure illustrates the decomposition of the system-level problem for FCS synthesis/design into four separate but integral sub-problems (the PES is not considered here).

The material and energy streams linking the above three units are identified as the coupling functions of the FCS. The coupling functions are considered as intermediate products and/or feedbacks going to or coming from the units. The application of the DILGO decomposition technique makes it necessary to define the coupling functions shown in Fig. 5.4.9. A more detailed description of these coupling functions is given below in Fig. 5.4.10. A list per subsystem appears in Table 5.4.2.
Fig. 5.4.9: Subsystems (including controllers) and subsystem coupling functions.
Table 5.4.2: Coupling function definition.

<table>
<thead>
<tr>
<th>Subsystem</th>
<th>Coupling Function</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>SS</td>
<td>Hydrogen molar flow</td>
<td>$\dot{n}_H_2$</td>
</tr>
<tr>
<td>SS</td>
<td>System tank pressure</td>
<td>$P_{FPS}$ and $P_{WRAS}$</td>
</tr>
<tr>
<td>SS</td>
<td>Air molar flow</td>
<td>$\dot{n}_{Air}$</td>
</tr>
<tr>
<td>WRAS</td>
<td>Motor parasitic power</td>
<td>$\dot{E}_{WRAS}$</td>
</tr>
<tr>
<td>FPS</td>
<td>Hot gases exit temperature</td>
<td>$T_{HOT\text{gas}}$</td>
</tr>
<tr>
<td>FPS</td>
<td>Hot gases molar flow</td>
<td>$\dot{n}_{HOT\text{gas}}$</td>
</tr>
</tbody>
</table>

The SOFCS must satisfy (apart from its internal parasitic power demand and the residential total electrical load) the power demand, $\dot{E}_{WRAS}$, required to run the WRAS. In order for the SOFCS to produce the required gross power, the necessary molar flow rate of hydrogen in the hydrogen-rich gas stream, $\dot{n}_H_2$, must be supplied by the FPS. In the same way, the necessary molar flow rate of air, $\dot{n}_{Air}$, must be supplied by the WRAS. In addition, the FPS provides hot gases to the WRAS at a given rate and temperature, $\dot{n}_{HOT\text{gas}}$ and $T_{HOT\text{gas}}$, used to recover work at the expander. Moreover, the pressure of the hydrogen-rich gas and air streams, $P_{FPS}$ and $P_{WRAS}$, exiting the FPS and WRAS, respectively, must match the inlet stack pressure of the SOFCS. In addition to the coupling functions mentioned above, the hydrogen and oxygen utilization factors...
can be defined as functions linking the SOFCS, FPS, and WRAS units. In the consideration of optimizing the BOPS, however, these two factors are treated as fixed parameters in the SOFCS model for reasons of simplicity.

Given the high fidelity of the simulations and the number and type of decision variables and constraints (Table 5.4.3 to Table 5.4.6), it can be seen that one is confronted with a very complex, large-scale, mixed integer, non-linear, dynamic optimization problem. The difficulties associated with solving this problem are exacerbated by the following:

- The dynamic simulation tools are not specifically designed to handle large scale optimizations. Each time a simulation is run, it is necessary to launch the program and read the necessary software licenses. This is computationally expensive.
- The presence of both continuous and discrete decision variables makes it necessary to use a heuristic approach: either a genetic algorithm or simulated annealing. There are no general gradient-based methods able to solve this dynamic mixed integer, non-linear programming (DMINLP) problem. However, heuristic algorithms impose a significant computational penalty in terms of solution time.

5.4.3.3 SOFCS System-level, Unit-based Optimization Problem Definition

The SOFC stack unit-based, system-level optimization problem is formulated as follows

Minimize

\[ C_{SS}^* = C_{SS} + C_{FPS} + C_{WRAS} + C_{fuel}^* \]

\[ + \int_{t=0}^{T} \lambda_{H_2} (t) \Delta \dot{n}_{H_2} (t) dt + \int_{t=0}^{T} \lambda_{Air} (t) \Delta \dot{n}_{Air} (t) dt \]

\[ + \int_{T=0}^{T} \lambda_{pres_{FPS}} (t) \Delta P_{FPS} (t) dt + \int_{T=0}^{T} \lambda_{pres_{WRAS}} (t) \Delta P_{WRAS} (t) dt \]

w.r.t. \( n_{cell}, A_{air}, K_{SS} \)

subject to

\[ \bar{h}_{SS} = \bar{0} \]

\[ \bar{g}_{SS} \leq \bar{0} \]

\[ \left[ \dot{E}_{WRAS} - \dot{E}_{WRAS}^* \right] = \bar{0} \] (5.4.10)

where the vector of equality constraints, \( \bar{h}_{SS} \), represents the thermodynamic model of the SOFC stack while the vector of inequality constraints, \( \bar{g}_{SS} \), represents physical limitations imposed upon the subsystem. Equations (5.4.10) indicate that the coupling function \( \dot{E}_{WRAS} \) must take the proper values dictated by the solution of the WRAS unit-based, system-level optimization problem described in the following section. The synthesis/design and operational decision variables for the SOFC stack along with their ranges, as well as the physical constraints imposed upon the subsystem, are shown in Table 5.4.3. It has been assumed in equation (5.4.10) that the dynamic shadow prices are constant for a particular operational point over the range of hydrogen and air mass flow and FPS pressure. Note that the coupling functions have been represented in the above equations by mole flow rates and pressure differences. The work of Muñoz and von
Spakovsky (2000b) suggest that there is a mathematical advantage with the use of quantities as coupling functions that make the shadow prices monotonic and, ideally, linear.

### Table 5.4.3: SOFCS decision and principal dependent optimization variables and constraints.

<table>
<thead>
<tr>
<th>Synthesis/Design Decision Variable Description</th>
<th>Constraints</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_{cells}$</td>
<td>Number of cells</td>
</tr>
<tr>
<td>$A_{cell}$</td>
<td>Cell active area (cm$^2$)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operational Decision Variable Description</th>
<th>Constraints</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_{FCoper}$</td>
<td>Stack operating pressure (bar)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Dependent Variable Description</th>
<th>Constraints</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_{cell}^{actual}$</td>
<td>Actual cell voltage (V)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Operational Parameter</th>
<th>Constraints</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{oper}$</td>
<td>Stack temperature</td>
</tr>
</tbody>
</table>

#### 5.4.3.4 FPS System-level, Unit-based Optimization Problem Definition

The unit-based, system-level optimization problem for the FPS is defined as Minimize

$$C'_{FPS} = C_{FPS} + C_{fuel} + C_{SS} + C_{WRAS}$$

$$+ \int_{t=0}^{T} \dot{\lambda}_{T_{HOTgas}}(t) \Delta T_{HOTgas}(t) dt + \int_{t=0}^{T} \dot{\lambda}_{n_{HOTgas}}(t) \Delta n_{HOTgas}(t) dt$$

w.r.t. $\{\tilde{x}_{FPS}, \tilde{y}_{FPS}, \tilde{K}_{FPS}\}$ subject to

$$\tilde{h}_{FPS} = \tilde{0}$$

$$\tilde{g}_{FPS} \leq \tilde{0}$$

$$\begin{bmatrix} \dot{n}_{H_2} - \dot{n}_{H_2}^* \\ \dot{n}_{Air} - \dot{n}_{Air}^* \end{bmatrix} = \tilde{0}$$

where the vector of equality constraints, $\tilde{h}_{FPS}$, represents the thermodynamic, kinetic, and geometric models of the FPS unit while the vector of inequality constraints, $\tilde{g}_{FPS}$, represents physical limitations imposed upon the subsystem. Equations (5.4.12) indicate that the coupling functions $\dot{n}_{H_2}$ and $\dot{n}_{Air}$ must take the appropriate values provided by solving the SOFC stack and WRAS unit-based, system-level optimization problems. The synthesis/design and operational decision variables for the FPS along with their ranges are presented in Table 5.4.4 and Table 5.4.5.

### Table 5.4.4: FPS synthesis/design decision variables and constraints.

<table>
<thead>
<tr>
<th>Component</th>
<th>Synthesis/Design Decision Variable</th>
<th>Constraints</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Component</th>
<th>Synthesis/Design Decision Variable</th>
<th>Constraints</th>
</tr>
</thead>
<tbody>
<tr>
<td>SMR reactor</td>
<td>$d_i^{SMR}$</td>
<td>$0.01 \leq d_i^{SMR} \leq 0.02$</td>
</tr>
<tr>
<td></td>
<td>$n_{tubes}^{SMR}$</td>
<td>$100 \leq n_{tubes}^{SMR} \leq 500$</td>
</tr>
<tr>
<td></td>
<td>$L_{SMR}$</td>
<td>$0.05 \leq L_{SMR} \leq 1$</td>
</tr>
<tr>
<td>Steam generator</td>
<td>$d_i^{SG}$</td>
<td>$0.01 \leq d_i^{SG} \leq 0.02$</td>
</tr>
<tr>
<td></td>
<td>$n_{tubes}^{EG}$</td>
<td>$100 \leq n_{tubes}^{EG} \leq 500$</td>
</tr>
<tr>
<td></td>
<td>$L_{EG}$</td>
<td>$0.05 \leq L_{EG} \leq 1$</td>
</tr>
<tr>
<td>Compact heat exchangers</td>
<td>$N_{plates}$</td>
<td>$4 \leq N_{plates} \leq 60$</td>
</tr>
<tr>
<td></td>
<td>$L_h$</td>
<td>$0.03 \leq L_h \leq 1.5$</td>
</tr>
<tr>
<td></td>
<td>$L_c$</td>
<td>$0.03 \leq L_c \leq 1.5$</td>
</tr>
</tbody>
</table>

### Component Synthesis/Design Decision Variable Constraints

<table>
<thead>
<tr>
<th>Component</th>
<th>$K_P$</th>
<th>Proportional gain</th>
<th>$10^{-8} \leq K_P \leq 10^{-2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>SMR control</td>
<td>$K_I$</td>
<td>Integral gain</td>
<td>$10^{-13} \leq K_I \leq 10^{-8}$</td>
</tr>
<tr>
<td>Reformate pressure control</td>
<td>$K_P$</td>
<td>Proportional gain</td>
<td>$0.1 \leq K_P \leq 500$</td>
</tr>
<tr>
<td></td>
<td>$K_I$</td>
<td>Integral gain</td>
<td>$10^{-2} \leq K_I \leq 10$</td>
</tr>
<tr>
<td>Reformate temperature control</td>
<td>$K_P$</td>
<td>Proportional gain</td>
<td>$0.1 \leq K_P \leq 500$</td>
</tr>
<tr>
<td></td>
<td>$K_I$</td>
<td>Integral gain</td>
<td>$10^{-2} \leq K_I \leq 10$</td>
</tr>
<tr>
<td>Reformate tank output control</td>
<td>$K_P$</td>
<td>Proportional gain</td>
<td>$0.1 \leq K_P \leq 500$</td>
</tr>
<tr>
<td></td>
<td>$K_I$</td>
<td>Integral gain</td>
<td>$10^{-2} \leq K_I \leq 10$</td>
</tr>
</tbody>
</table>
Table 5.4.5: FPS operational decision variables and constraints.

<table>
<thead>
<tr>
<th>Component</th>
<th>Operational Decision Variable</th>
<th>Constraints</th>
</tr>
</thead>
<tbody>
<tr>
<td>SMR reactor</td>
<td>( T_{\text{SMR}}^{o} )</td>
<td>SMR reactor outlet temperature, °C</td>
</tr>
<tr>
<td></td>
<td>τₜₜₜ</td>
<td>550 ( \leq T_{\text{SMR}}^{o} ) ( \leq 1300 )</td>
</tr>
<tr>
<td>Reformate mixer</td>
<td>( \zeta_{u,p/\text{ca}} )</td>
<td>Steam-to-methane ratio</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1.5 ( \leq \zeta_{u,p/\text{ca}} ) ( \leq 6 )</td>
</tr>
</tbody>
</table>

5.4.3.5 WRAS System-level, Unit-based Optimization Problem Definition

The unit-based, system-level optimization problem for the WRAS is defined as

Minimize

\[
C_{\text{WRAS}}^{\ast} = C_{\text{WRAS}} + C_{\text{FPS}}^{\ast} + C_{\text{fuel}}^{\ast} + C_{\text{SS}}^{\ast} + \int_{t=0}^{\tau} \dot{E}_{\text{WRAS}} \Delta t
\]

w.r.t. \( \{\bar{x}_{\text{WRAS}}, \bar{y}_{\text{WRAS}}, \bar{K}_{\text{WRAS}}\} \)

subject to

\[
\begin{bmatrix}
\hat{h}_{\text{WRAS}} = \hat{0} \\
\bar{g}_{\text{WRAS}} \leq \bar{0} \\
\begin{bmatrix}
\hat{n}_{\text{Air}} - \hat{n}_{\text{Air}} \\
\hat{n}_{\text{HOTgas}} - \hat{n}_{\text{HOTgas}} \\
\hat{T}_{\text{HOTgas}} - \hat{T}_{\text{HOTgas}}
\end{bmatrix} = \bar{0}
\end{bmatrix}
\]

(5.4.14)

where the vector of equality constraints, \( \hat{h}_{\text{WRAS}} \), represents the thermodynamic, kinetic, and geometric models of the WRAS while the vector of inequality constraints, \( \bar{g}_{\text{WRAS}} \), represents the physical limitations imposed upon the subsystems. Equations (5.4.14) indicate that the coupling functions \( \hat{n}_{\text{Air}} \), \( \hat{n}_{\text{HOTgas}} \), and \( T_{\text{FPS}}^{\ast} \) must take the appropriate values provided by solving the SOFC stack and FPS unit-based, system-level optimization problems. The synthesis/design and operational decision variables for the WRAS along with their ranges are presented in Table 5.4.6.
Table 5.4.6: WRAS decision and principal dependent optimization variables and constraints.

<table>
<thead>
<tr>
<th>Component</th>
<th>Synthesis/Design Decision Variable</th>
<th>Constraints</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compressor</td>
<td>$P_{\text{designCOMP}}$ Compressor design pressure (bar)</td>
<td>$3 \leq P_{\text{designCOMP}} \leq 10$</td>
</tr>
<tr>
<td></td>
<td>$F_{\text{designCOMP}}$ Compressor design flow (kmol/sec)</td>
<td>$3 \cdot 10^{-6} \leq F_{\text{designCOMP}} \leq 10 \cdot 10^{-5}$</td>
</tr>
<tr>
<td>Expander</td>
<td>$P_{\text{designEXP}}$ Expander design pressure (bar)</td>
<td>$3 \leq P_{\text{designEXP}} \leq 10$</td>
</tr>
<tr>
<td></td>
<td>$F_{\text{designEXP}}$ Expander design flow (kmol/sec)</td>
<td>$3 \cdot 10^{-6} \leq F_{\text{designEXP}} \leq 10 \cdot 10^{-5}$</td>
</tr>
<tr>
<td>Air tank control</td>
<td>$K_P$ Proportional gain</td>
<td>$0.1 \leq K_P \leq 500$</td>
</tr>
<tr>
<td></td>
<td>$K_I$ Integral gain</td>
<td>$10^{-2} \leq K_I \leq 10$</td>
</tr>
<tr>
<td>Electric motor control</td>
<td>$K_P$ Proportional gain</td>
<td>$10^{-4} \leq K_P \leq 10^{-1}$</td>
</tr>
<tr>
<td></td>
<td>$K_I$ Integral gain</td>
<td>$10^{-5} \leq K_I \leq 10^{-2}$</td>
</tr>
</tbody>
</table>
6. RESULTS AND DISCUSSION

6.1 VALIDATION RESULT OF ELECTRICAL FEEDBACK EFFECTS

6.1.1 Validation of Stack Characteristics

Fig. 6.1.1 shows the comparison of I-V characteristics of the 25 cell stack model and the 25 cell stack experimental unit. The response of the model is verified during several electrical feedbacks to prove its accuracy during the transients.

![Graph showing I-V characteristics comparison](image)

Fig. 6.1.1: Steady-state I-V characteristics comparison of the planar SOFC stack.

6.1.2 Validation of Load Transients

We analyze the effects of load transient on the output of the PSOFC stack. A programmable electronic load operating in constant current mode is connected across the stack output, and a current transient of 2.2 A to 12 A and subsequently 12 A to 2.2 A is applied after 1400 seconds. Figs. 6.1.2(a) and 6.1.2(b) shows the drop in the output voltage of the stack model and the experimental stack prototype respectively.

Due to the subjected load transient, the mean temperature in the stack increases as shown in Fig. 6.1.3. (The mean temperature profile near the no-load to full-load transient is skewed due to manual turning off of the electronic load at t = 2000 sec accidentally). The increase in the stack temperature is attributed to the increased rate of the exothermic reaction. However, the thermal time constant of the stack being much larger than that of the SOFC electrochemistry/PES time constant, the cell temperature gradually reaches the steady state value after approximately 600 s.
Fig. 6.1.2: a) Effect of load current transient (2.2 A to 12 A) on the voltage of the stack model. b) The experimental validation of its effect on the planar stack, scope channel 1 (10 V/div) and channel 4 (2 A/div) measures the stack voltage and current respectively.

Fig. 6.1.3: Validation of the effect of load transient (no load (NL) – full load (FL) – no load (NL)) on the planar SOFC stack temperature. Actual no load to full load transient occurs at 2077 seconds.

To investigate the effect of multiple load transient, we subject the system to multiple small duration loads. The duration of the load is kept fixed at 300 seconds followed by 300 seconds of no load condition. Due to multiple set of transient load, the temperature of the PSOFC does not have sufficient time to drop back to its initial value as shown in Fig. 6.1.4. Hence the multiple load transients may lead to a higher temperature inside the PSOFC.
Fig. 6.1.4: Validation of the effect of multiple load transient (NL-FL-NL) on the planar SOFC stack temperature.

6.1.3 Validation of the Ripple Effect

Fig. 6.1.5: a) Effect of 40 percent current ripple on the stack voltage of the model. b) Experimental validation of the ripple effect on planar SOFC stack, scope channels A and D show the stack voltage and current respectively.

To study the effect of the ripple, the power electronics prototype, which consists of a bidirectional DC-DC boost converter, is connected across the stack. The duty ratio of switches of the converter is modulated using a sinusoidal signal of 60 Hz, producing 60 Hz AC voltage at the
output. The current drawn from the stack contains 120 Hz ripple. The load connected across the boost converter is adjusted so that the magnitude of the ripple is 40 percent of the mean stack current. Figs. 6.1.5(a) and 6.1.5 (b) show the effect of a low frequency (120 Hz) ripple on the stack model and the experimental prototype respectively.

### 6.2 ANALYSIS OF STACK DEGRADATION RESULT

Fig. 6.2.1 shows the percentage degradation of the ASR (area specific resistance) in the stacks after approximately 900 hrs of study. This shows that, the degradation of the ASR due to the load transient is very high as compared to the stack carrying constant current. Similarly, increase in the ASR of the stack with low-frequency ripple current is higher as compared to the stack feeding constant current.

![Comparison of long-term ASR degradation due to low-frequency ripple, constant current and load transient.](image)

The degradation in the ASR due to the ripple is found to be 0.06 $\Omega \text{cm}^2$ higher as compared to the constant current case after 880 hrs of operation. The increase in the ASR degradation leads to a drop in the power output of the stack. The percentage drop in the output power is given as

$$
\Delta P_{drop} = V_{fc} I_{fc} - V_{fc} I_{fc} = \left( \frac{\text{ASR}'}{A_{cell}} - \frac{\text{ASR}_b}{A_{cell}} \right) I_{fc}^2 = \left( \frac{\Delta \text{ASR}}{A_{cell}} \right) I_{fc}^2 \times \frac{\%}{100} \times \frac{I_{fc}^2}{A_{cell}} \times \text{ASR}_b
$$

where $I_{fc}$ is the average current drawn from the fuel cell, $A_{cell}$ is the electro-active area of the planar cell, $\text{ASR}_b$ is the base ASR of the stack, and $\text{ASR}'$ is the ASR of the stack after degradation.
Comparing the efficiencies of the stacks, the stack carrying 100 percent ripple in the current is found to have an additional drop of 1.72 percent to that of the stack carrying constant current. And the efficiency of the stack with the load transient drops by 10.32 percent as compared to the constant current stack.

The analysis of the long term degradation experiment above indicates that the ASR of the cell degrades with time, when a current is drawn from the stack. However, this degradation is enhanced due to the presence of the ripple in the current and due to the load transients. The degradation of the ASR of the cell deteriorates its efficiency. The load transient, even though at a smaller rate as compared to the frequency of the ripple poses higher threat to the performance and the efficiency of the planar stack. Figs 6.2.2(a) and 6.2.2(b) show the drop in the available power from a planar cell due to the load transients and the low frequency ripple current.

![Fig. 6.2.2: The drop in the output power of the PSOFC due to ASR degradation caused by a) load transient and b) low-frequency ripple. The solid lines and the dotted lines refer to the profiles before the start of the degradation study, and after 912 hrs of the study respectively.](image)
6.3 Parametric Study of the Effect of Electrical-feedbacks

6.3.1 Effects of Load-transients

As discussed in Section 5.2.1.1, the load transient affects the fuel utilization in the stack, with sudden increase due to increase in the load and drop with decrease in the level of the load demand. The total increase in the fuel utilization depends on the severity of the load transient as shown in Fig. 6.3.1.

![Graph showing the effect of load transient on fuel utilization and mean stack temperature.](image)

**Fig. 6.3.1**: Effect of severity of the load transient on the fuel (hydrogen) utilization and mean stack temperature.

It is found that, the level of increase in the mean temperature of the stack is dependent only on the initial and the final load current drawn from the stack, as shown in Fig. 6.3.1, and independent of the slew rate of the load current during the transient. Fig. 6.3.2 shows the increase in the mean temperature for various slew rates of load current.

Since the interfaces among the electrolyte and the electrodes are potentially subjected to the residual stresses, a detailed analysis of the stress developed at those interfaces is done. Figs 6.3.3 and 6.3.4 show the residual stresses at the four interfaces of a planar SOFC before and after the load transient, respectively. The stress levels are measured in MPa. A residual tensile stress is potentially degrading for the components of the SOFC. As shown in Fig. 6.3.4, the electrolyte interface with cathode sees a level of high tensile stress due to the higher temperature gradient caused by the load transient. Therefore, the electrolyte is more prone to failure.
Fig. 6.3.2: Effect of the duration of load transient on the increase in the mean stack temperature.

The results of the biaxial test are analyzed using Weibull statistics to determine the failure stress of each specimen. And the probability of the failure according to ASTM C1239, is obtained by the exponential of the integration over all regions of the specimen volume (Ke An, 2003) and is defined as

$$P_f = 1 - \exp\left[-\int_V \left(\frac{\sigma}{\sigma_\theta}\right)^m dV\right], \sigma > 0$$

$$P_f = 0, \sigma \leq 0$$

(6.3.1)

where $\sigma$ is the failure stress of the elemental volume and $\sigma_\theta$ is the characteristic Weibull strength of the material and is estimated using the equation

$$\sigma_\theta = \left[\frac{1}{N} \sum_i (\sigma_i)^m\right]^{1/m}$$

(6.3.2)

where $\sigma_i$ is the failure stress of the $i^{th}$ specimen, for $0 < i < N$, and $m$ is the Weibull modulus and is estimated using the equation

$$\frac{\sum_i (\sigma_i)^m \ln(\sigma_i)}{\sum_i (\sigma_i)^m} - \frac{1}{N} \sum_i \ln(\sigma_i) - \frac{1}{m} = 0$$

(6.3.3)
Fig. 6.3.3: Residual stress at different interfaces before the load transient.
The risk of rupture intensity $(\sigma/\sigma_0)^m$ of the electrolyte is shown in Fig. 6.3.5. The estimated probability of failure after the load transient is calculated using the surface integral of the risk of rupture intensities using (6.3.2). And the probability of failure, $P_f$, for the electrolyte is calculated as 0.84 percent after the load transient. Assuming the failure of the electrolyte lead to the failure of the cell, the reliability of an M cell stack is given as in (Stolten, 2004)

$$R = (1 - P_f)^M$$

(6.3.4)
Fig. 6.3.5: Risk of rupture intensities at the interface of electrode with cathode after the load transients.

Fig. 6.3.6: Estimated stack reliability with probability of failure of a cell.
Fig. 6.3.6 shows the reliability of the stack with variation of probability of failure of a single cell. As can be seen, the reliability of the stack, for a given cell failure probability, decreases drastically with an increase in the number of cells in the stack. Therefore, even a small failure rate of estimated 0.84% induced due to residual stress is detrimental to the reliability of a long stack.

6.3.2 Effects of Load Power Factor

In Section 5.2.1.1 we analyze the effect of the load power factor on the ripple current drawn by the planar SOFC stack. Fig. 6.3.7 shows the effect of load power factor variation on the stack current ripple at various capacitances and at a constant active power drawn by the load. In the next subsection, it is discussed that, the available power from the stack decreases with an increase in the current ripple magnitude. Therefore, a decrease in the load power factor decreases the efficiency of the stack.

However, as discussed under the effect of the ripple, and since the variation in the power drawn from the stack due to ripple is negligible at various power factor loads drawing the same active power, the increase in the mean temperature should be minimal. Fig. 6.3.8 illustrates the effect of load power factor variation on the mean temperature of the stack.

Fig. 6.3.7: Effect of power factor of the load on the magnitude of stack current ripple.
6.3.3 Effects of Load Harmonics

An increase in the THD (ratio of the rms of the harmonic components to the rms of the fundamental, $U_h/U_1$) of the AC load increases the distortion in the output AC current due to increase in the magnitude of the harmonic components as well their phase. This distortion in the AC current also introduces distortion in the current drawn from the planar stack. Fig. 6.3.9 shows the effect of the variation of the THD at different power factors on the ripple magnitude in the stack current. At a fixed power factor of the fundamental current, the percentage ripple in the stack current decreases with an increase in the THD of the load (refer to the analysis and calculation in the Section 5.2.1.1 for the effect of THD). However, due to minimal variation in the power drawn from the stack, the effect of the THD on the increase in the mean temperature is minimal as shown in Fig. 6.3.10.
Fig. 6.3.9: Effect of THD on the stack current ripple.

Fig. 6.3.10: Effect of THD on the increase in the mean temperature of the stack.
6.3.4 Effects of Ripple

We have discussed in Section 5.2.1.2 that, an increase in the ripple magnitude forces to decrease the maximum average stack current to a lower level. This leads to a decrease in the operable fuel utilization. Fig. 6.3.11 shows the decrease in the maximum operable fuel utilization with increase in the magnitude of the current ripple. This decrease in the operating fuel utilization in the stack, decrease the steady state stack efficiency as shown in Fig. 6.3.12.

Fig. 6.3.13 shows the effect of the ripple on the stack temperature. Since the thermal time constant of the planar cell is much higher as compared to the time scale of the low frequency ripple, the stack temperature would not reflect any variation in a small time scale. The stack temperature depends on the power drawn from the stack. Since even with a 100 percent ripple the increase in the RMS current drawn from the stack is approximately 5.91 percent, the increase in the stack current in the steady state is negligible.

![Graph showing the effect of low frequency ripple on operable fuel utilization.](image1.png)

**Fig. 6.3.11:** Effect of low frequency ripple on operable fuel utilization.

![Graph showing the effect of low frequency ripple on achievable efficiency of the stack.](image2.png)

**Fig. 6.3.12:** Effect of low frequency ripple on achievable efficiency of the stack.
6.4 POWER MANAGEMENT CONTROL RESULTS

The performance of the energy management control as discussed in Section 5.4.1 is tested on a 5 kW PSOFC stack model, which is an upscale version of validated stack model. It is assumed that the response, dynamics and the characteristics of the upscale stack model will follow the validated model.

First of all, the efficacy of the hierarchical control is verified assuming a fixed desired fuel utilization, \( f_u^* = 0.78 \). The hybrid system in the steady state is subjected to a load transient from 2 kW to 3 kW at time \( t = 0.02 \) sec. It is hypothetically assumed that flow rate of the stack will reach the steady state in 0.2 sec. Fig. 6.4.1 shows the response of the battery current to the load transient to provide the additional power, till the fuel flow rate of the stack reaches the steady-state value. Since the current drawn form the stack is independent of the load current, the stack current remains unaltered, and hence the stack fuel utilization remains unaltered as shown in Fig. 6.4.2. However, the bus voltage sags for a short duration, till the battery completely provides the additional load demand as shown in Fig. 6.4.2.
Fig. 6.4.1: Response of the battery current due to the load transient and flow adjustment.

Fig. 6.4.2: Response of the bus voltage and fuel utilization to a sudden load transient which is followed by the flow adjustment of BOPS for a fixed fuel utilization of 0.78.
Next, to enhance the efficiency of the stack subsystem in the steady state, optimal fuel utilization is obtained from a fuel utilization – flow rate map and is fed to the BOPS control as an input which determines the required flow rate based on the power demand and desired fuel utilization. Hence the flow rates of fuel and air from the BOPS in the steady-state are optimized to maximize the efficiency of the power system.

Using the performance map as derived above, the response of the control is obtained for a typical fuel cell power system (SOFC based) subjected to load transient at time $t = 0.04$ seconds. Fig. 6.4.3 shows actual variation of the conversion efficiency of the stack due to a change in the fuel flow rate of the stack after the transient. The change in the fuel utilization due to variation of fuel flow rate is shown in Fig. 6.4.4.

**Fig. 6.4.3:** Efficiency of the stack before and after the load transient.
The efficiency of the power converter system is maximized using efficient power sharing among the converters. Fig. 6.4.5 shows the overall converter system efficiency for a five module DC-DC boost converter using the efficient power sharing strategy. The fraction of the input power drawn by the converter module-1 $P_1/P_{in}$ to attain maximum efficiency is also obtained in the range of the input power. The efficiency map for the boost converter module is shown in Fig. 6.4.5.

The control strategy completely eliminates the effect of the load transient on the fuel cell stack by providing the additional load current from the battery. Secondly, in the steady state it maximizes the efficiency of the system by optimizing the fuel utilization in the stack.

Fig. 6.4.4: Fuel utilization variation due to change in the fuel flow rate after the load transient.
Fig. 6.4.5: Multi-converter system efficiency as compared to the single 5 kW converter and power sharing using five converter modules.

6.5 Optimization and Control of BOPS

An important objective of Phase I of this project was to establish feasible system super-configuration which provides high efficiency and reliability. Based on this super-configuration, detailed dynamic models for each component were developed and then coupled in order to generate a system level dynamic model. Using the system level dynamic model, parametric studies were done in order to determine system behavior for various combinations of system-level parameters and components locations and dimensions. The results of the parametric studies were used to determine the most promising subset of this super-configuration i.e. reduced super-configuration based on system response, fuel consumption, capital cost, operational constraints, etc. During Phase II, the resulting reduced super-configuration was subjected to a large scale synthesis/design optimization while taking into account its effects on system operation, i.e. on the dynamic response of the system. The parametric studies showed this configuration to provide adequate fuel efficiency. However, the system cannot offer proper control of the temperature difference between the anode and the cathode inlets. Current solid oxide fuel cell stack materials
require that the temperature gradients along and across the stack to be controlled within a very small range. This information is mostly proprietary and not available in the literature. However, at a 2004 fuel cell conference in Rochester, New York; a 5 K difference between anode and cathode inlets was suggested by several manufacturers. Therefore, this value was used for the project.

The main reason for a high temperature difference at the stack inlet is the fact that the mass flow at the cathode exit is reduced due to oxygen conversion during the electrochemical reactions. This reduction is in fact significant due to the relatively low oxygen to hydrogen ratio used to run the stack. Here, the oxygen to hydrogen ratio was set to 2.2 based on available information. Additionally, the mass flow at the cathode exit has a time delay with respect to the mass flow at the inlet. This behavior is most critical while driving the system from low to high load. During this operational condition, the mass flow of cold gases through heat exchanger II increases rapidly while the hot gases coming out of the stack increase at a slower rate due to the stack time delay. The same phenomenon is present in the anode and heat exchanger I. This behavior makes the stack inlet temperature difficult to control unless additional control forces are integrated (e.g., hot gases and cathode products mixing). This solution is not desirable because it implies additional capital and operational costs.

In order to provide a system-level solution for the problem mentioned above, heat exchanger I is relocated. Instead of transferring energy from the anode exit to the anode inlet stream, heat exchanger I is used to transfer energy from the reformate tank exit stream to the cathode exit stream. The products of the cathode at a higher temperature are then passed through heat exchanger II. This modification has proved to be effective in controlling both the anode and the cathode inlet temperatures. The stack exit temperature is held constant at 1000 K by separately controlling it with a fan based cooling system. Furthermore, in general the anode inlet mass flow is much smaller that the cathode’s. This means that the heat exchanger I hot gas exit temperature (i.e. anode inlet temperature) is always very close to 1000 K. Furthermore, the additional energy put into the cathode exhaust helps to level the heat exchanger II cold stream exit temperature (i.e. cathode inlet temperature) rapidly and closer to 1000 K.

Regarding the anode exhaust, if was found that recirculating a fraction of it back into the steam-methane mixer provides sufficient water content for the steam-methane reformer, thus, eliminating the need for a steam generator during regular operation and even during transients. This in fact elevates the system efficiency due to the elimination of all parasitics related to the steam generator operation (i.e. pump motor and hot gases). The steam generator is still required for start-up. It was also concluded that due to the high temperature of the recirculated anode products, heat exchanger III was not required at this location. This component was, thus, relocated in order to transfer energy to the hot gases going into the expander so as to reduce the dependence of the WRAS on the electrical motor. Fig. 6.5.1 shows the resulting reduced super-configuration established at the end of Phase I. This Phase I/Phase II reduced super-configuration is used in order to perform the dynamic synthesis/design and operational/control optimization of the SOFC system, resulting in the final optimal system configuration. The resulting optimum configuration is not shown because of pending patent considerations.
6.5.1 Cost Optimization Results

As mentioned above, the DILGO physical decomposition technique for dynamic system is used in order to optimize the SOFC based APU synthesis/design and operational/control for an entire residential load profile. The solutions to the FPS, WRAS, and SOFC stack unit-level and system-level, unit-based optimization problems in terms of life cycle cost for the first and the final iteration of the DILGO approach as well as the corresponding total life cycle cost for the SOFC system (BOPS/SOFC stack) are presented in Table 6.1.
Table 6.1: Optimum cost of the total SOFC system and subsystem for the first and the final iteration of the DILGO approach.

<table>
<thead>
<tr>
<th>DILGO Iteration No.</th>
<th>BOPS/SS ($)</th>
<th>FPS ($)</th>
<th>WRAS ($)</th>
<th>SS ($)</th>
<th>Fuel ($)</th>
<th>Percentage Improvement</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>38,230</td>
<td>10,947</td>
<td>2,203</td>
<td>5,541</td>
<td>19,539</td>
<td>---</td>
</tr>
<tr>
<td>6</td>
<td>24,843</td>
<td>6,239</td>
<td>1,625</td>
<td>3,752</td>
<td>13,227</td>
<td>35.017</td>
</tr>
</tbody>
</table>

What is believed to be the global optimum value for the total life cycle cost of the BOPS/SOFC stack is obtained in six iterations of DILGO. A significant improvement in the value of the system-level objective function is observed upon completion of each DILGO iteration. In particular, the final total life cycle cost is 35.017% lower than that of the first iteration. To verify that the DILGO process had reached global optimum value, the problem was run a seventh time with no observable change in the independent variables or the system-level objective function.

**Optimal Costs**

The optimal costs for the proposed SOFC based APU configuration are based on a production volume of 200,000 units per year and a maximum net power output of 6.6 kW. Obviously, a significant change in the number of units produced per year could significantly modify these costs.

The breakdown of the FPS and WRAS purchase costs can be seen in Fig. 6.5.2 and Fig. 6.5.3, respectively. It is obvious that the FPS cost is well distributed among the three major components (i.e. reactor, steam generator, and heat exchangers). The WRAS purchase cost breakdown displayed in Fig. 6.5.3 clearly shows that the expander dominates the WRAS purchase cost. This comes as no surprise, taking into account that this component introduces new technology in order to maintain high pressures for all operational conditions, especially in a system with relatively small flow rates. Fig. 6.5.4 shows the breakdown of the BOPS/SOFC stack total cost. This cost includes the operating cost of the BOPS/SOFC stack over the entire load profile. Fig. 6.5.4 indicates that the cost associated with the consumption of natural gas (methane) throughout the lifetime of the BOPS/SOFC stack is the major contributor to the total cost of the BOPS/SOFC stack and that the FPS is the second most costly subsystem. Detailed optimum cost function values appear in Table 6.2.
Fig. 6.5.2: FPS purchase cost breakdown (based on a production volume of 200,000 units/year).

Fig. 6.5.3: WRAS purchase cost breakdown (based on a production volume of 200,000 units/year).

Fig. 6.5.4: SOFC system total cost breakdown (based on a production volume of 200,000 units per year).
Table 6.2: WRAS, and SOFC stack optimum capital and operational cost\textsuperscript{19}.

<table>
<thead>
<tr>
<th>Component</th>
<th>Cost (US$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SOFCS (US$)</td>
<td>24,843</td>
</tr>
<tr>
<td>FPS (US$)</td>
<td>6,239</td>
</tr>
<tr>
<td>WRAS (US$)</td>
<td>1,625</td>
</tr>
<tr>
<td>SOFC stack (US$)</td>
<td>3,752</td>
</tr>
<tr>
<td>Fuel (US$)</td>
<td>13,227</td>
</tr>
<tr>
<td>WRAS (US$)</td>
<td>1,625</td>
</tr>
<tr>
<td>Compressor</td>
<td>487</td>
</tr>
<tr>
<td>Expander</td>
<td>745</td>
</tr>
<tr>
<td>Motor</td>
<td>243</td>
</tr>
<tr>
<td>Auxiliary</td>
<td>147</td>
</tr>
<tr>
<td>FPS (US$)</td>
<td>6,239</td>
</tr>
<tr>
<td>HX I</td>
<td>611</td>
</tr>
<tr>
<td>HX II</td>
<td>358</td>
</tr>
<tr>
<td>HX III</td>
<td>15.28</td>
</tr>
<tr>
<td>HX IV</td>
<td>487</td>
</tr>
<tr>
<td>HX V</td>
<td>0</td>
</tr>
<tr>
<td>Bare Reactor</td>
<td>1,212</td>
</tr>
<tr>
<td>Catalyst</td>
<td>1,928</td>
</tr>
<tr>
<td>Steam Generator</td>
<td>1,618</td>
</tr>
<tr>
<td>SOFCS (US$)</td>
<td>3,752</td>
</tr>
</tbody>
</table>

6.5.2 Start-up Results

For start-up, the BOPS was first analyzed at the component level. Before the production of hydrogen starts at the reformer, it is necessary to generate steam at temperatures above 800 °K. To reach these conditions as soon as possible while assuring material integrity, the temperature and mass flow of the hot gases are controlled. The higher the gas inlet conditions the faster the steam reaches operational conditions.

To reach these conditions, one of two procedures can be followed. In the first approach, both cold water and hot gases are passed through the steam generator; and until operational conditions are reached, the water coming out of the steam generator is recirculated to the water tank. Two advantages result from this approach. No water is wasted, and the water inlet temperature increases with time, which increases the rate at which the metal heats up. Fig. 6.5.5 shows the spatial and temporal thermal responses of steam generator start-up on the water side. It can be seen how water exit temperatures higher than 800 °K are reached in about 300 sec while steady state is reached in 600 sec.

\textsuperscript{19} Cost includes purchase cost, amortization cost, and maintenance cost.
Fig. 6.5.5: Steam generator start-up temporal and spatial thermal responses on the water side.

In the second approach, the water coming out of the steam generator is recirculated directly back into the steam generator. Again, this approach results in no water being wasted and the water inlet temperature increases with time, however, at a much higher rate than with the first approach. Fig. 6.5.6 shows a comparison between the transient responses for the two procedures. For the case with direct recirculation, the water takes 195 seconds to reach 850 °K. Note how immediately after stopping the direct recirculation (at 200 sec), the steam temperature is above 850 °K; and it is ready to be used in the reformer. In the case with tank recirculation, it takes the steam 300 sec to reach temperatures above 800 °K. In both cases, the rate of temperature increase of the steam reformer walls and the water stream depends on the mass flow and temperature of the hot gases and on the mass of the steam generator.

Fig. 6.5.6: Steam generator start-up comparison of thermal responses on the water side.
During transient operation, especially at start-up and shut-down, material resistance to thermal stresses were taken into account in order to assure the integrity of all components. This was controlled by introducing temperature gradient and heat flux constraints into the synthesis/design and operational problem. For the present study, it was found that the heat flux occurring throughout the steam generator during start-up is less than 150 kW/m², which is significantly less than the maximum allowable value (burnout flux) of 340 kW/m².

Fig. 6.5.7 shows the spatial and temporal performance of the steam-methane reactor during start-up. Notice that the plot starts at 200 seconds, which is the time that it takes for the steam generator to start up and at which point the recirculation is stopped. During recirculation, all thermal components are pre-heated. This means that hot gases are passed through these components without any cold-side flow. The final conditions (metal temperature) after the pre-heating period depend on the mass flow and temperature of the hot gases and on the mass of the component. Again, temperature gradients must be taken into account. To generate Fig. 6.5.7, the synthesis/design point mass flow of hot gases was used during pre-heating (0.000503 kmol/sec). It took the reformer 410 seconds to reach steady state at a maximum methane conversion rate of 90%. Without pre-heating, steady state is reached in 1050 seconds. The duration of the transient depends on the degree of pre-heating and the mass flow conditions on both sides of the reactor. Notice that the initial conversion rate at the reformer exit may not be zero if the pre-heating is high enough.

![Conversion of CH4 vs Position Ratio Along the Reformer and Time](image)

**Fig. 6.5.7:** Steam-methane reformer start-up dynamic response for low pre-heating.

Fig 6.2.8 shows the reformer wall temperature response during start-up. The first 200 sec corresponds to the preheating period. Initially, the temperature of the metal starts increasing at a higher rate on the hot-gas inlet side. At the end of the pre-heating period, the temperature of the metal close to the hot-gas inlet side (position ratio 10.0 at 200 sec) is slightly higher than the steady state temperature; and the temperature of the metal close to the reformate-gas inlet side (position ratio 0.0 at 200 sec) is lower than the steady state temperature. This behavior produces higher thermal stress in the axial direction than those present during steady state operation. Thus,
for start-up, both control variables and physical limits or constraints should be taken into account during the synthesis/design process.

![Graph showing steam methane reformer wall temperature start-up response for high pre-heating.](image)

**Fig. 6.5.8:** Steam methane reformer wall temperature start-up response for high pre-heating.

A comparison between the thermal responses of heat exchanger III for the cases with and without pre-heating is shown in Fig. 6.5.9. Again, the pre-heating time is 200 sec. When pre-heating finishes and cold-side flow starts, conditions are such that the cold stream exit temperature is at operational conditions. If no pre-heating is used, 195 additional seconds are required to reach operational conditions.

![Graph showing compact heat exchanger III start-up thermal time response comparison between pre-heating and no pre-heating.](image)

**Fig. 6.5.9:** Compact heat exchanger III start-up thermal time response comparison between pre-heating and no pre-heating.
Finally, the heat exchanger model uses a two-dimensional grid of 400 discrete elements, which allows a detailed and fairly accurate prediction of the temperature distribution in each compact heat exchanger. Fig. 6.5.10 shows this two-dimensional temperature distribution on the cold side for heat exchanger III. The y and x axes are scaled on the basis of the number of discrete segments in each direction.

### 6.5.3 System Dynamic Response

The dynamic independent (decision) and dependent decision variables are defined as system outputs or state variables. As state variables, they are regulated by a set of controllers. These variables are also called controlled variables and serve as reference values for the controllers. The variables that are manipulated in order to keep controlled variables at their optimum values are defined as control variables. Fig. 6.5.11 to Fig. 6.5.20 show the dynamic optimum trajectories of the dynamic independent (decision) and dependent variables along with the dynamic trajectories of their respective control variables. Fig. 6.5.11 illustrates the close following of the actual reformate tank pressure to that of the optimum pressure trajectory. It should be noticed how the optimum tank pressure (i.e. in effect the system pressure) is a function of system demand. At high loads the optimum pressure is higher. This is explained by the fact that a low loads both the SOFC stack and FPS efficiency is higher and the pressure increase has only a minor effect on the stack efficiency increment. On the other hand, the WRAS is less efficient at low loads; and therefore, the parasitic power due to the electrical motor at low load increases as the system pressure increases.
The insert in Fig. 6.5.11 shows the behavior of the system pressure during a very strong operation change at 86,400 sec (24 hr). At this point the load changes from 1.5 kW to 5.55 kW and the optimum operational pressure changes from 297 kPa to 472 kPa. The system pressure matches the optimum system pressure after approximately 1300 sec (21.7 min). The apparent slow response is not due to the lack of system capacity but rather to the need to take into account efficient operation during the transient, since as the mass flow of the steam-methane mixture into the reformer increases, the reformer conversion efficiency decreases due to the reduction in gas residence time and the slow dynamics of the heat transfer process through the reformer walls. Thus, an indiscriminate increase in methane mass flow would rapidly increase the reformate tank pressure, but the hydrogen mole fraction would drop.

Fig. 6.5.12 shows the dynamic trajectory of the methane flow rate into the reformer, which in turn is the control variable to the reformate tank pressure. This mass flow is in fact regulated by a flow control valve. The rapid increase in the mass flow at 86,400 sec is due to the sudden change in the reference pressure which produces an instantaneous error signal, which the controller tries to correct.
Fig. 6.5.12: Steam-methane reformer optimum inlet methane mass flow (control variable).

Fig. 6.5.13 shows how the actual air tank pressure very closely follows the optimum system pressure trajectory. Again the optimum system pressure is a function of system demand. In general, the faster the response with respect to the reformate tank is due to the fact that a higher loads the expander is able to provide all the energy required by the compressor.

Fig. 6.5.13: Air tank pressure (state variable) optimum dynamic response.
Fig. 6.5.14 shows the optimum and the actual dynamic trajectory for the steam-methane reformer reformate exit temperature. This figure shows how the actual reformate exit temperature very closely follows the optimum temperature trajectory. This, optimum reformate exit temperature is a function of system demand. At high loads, the optimum temperature is higher. This is explained by the fact that at high loads the reformate residence time is lower; thus, the conversion efficiency is lower. In order to increase the conversion capacity an increase in the reformate’s exit temperature is required. However, a temperature increase is restricted by the additional fuel consumption. Again, let us analyze the system behavior as a very strong operational change occurs at 86,400 sec (24 hr). At this point the load changes from 1.5 kW to 5.55 kW and the optimum reformate exit temperature changes from 1051.8 K to 1061.4 K. The system pressure matches the optimum system pressure after approximately 1450 sec (24.2 min). The apparent slow response is due to the slow transient of the heat transfer process through the reformer walls.

![Temperature vs Time Graph](image)

**Fig. 6.5.14:** Steam-methane reformer gas exit temperature (state variable) optimum dynamic response.

Fig. 6.5.15 shows the dynamic trajectory of the hot gases reformer inlet temperature, which in turn is the control variable for the reformate exit temperature. The rapid increase in the hot gases temperature is due to two reasons. The first is the sudden change in the reference temperature (optimum temperature) which produces an instantaneous error signal, and the second is the change in reformate exit temperature due to the change in mass flows. Both conditions introduce an error which the controller tries to correct.
Fig. 6.5.15: 3D depiction of the steam-methane reformer optimum hot gases inlet temperature (control variable) dynamic response.

Fig. 6.5.16 shows the most important system operational constraint’s dynamic response. As mentioned above, regulating the temperature difference between the anode and the cathode inlet is extremely important in order to avoid thermal stresses. The maximum acceptable absolute temperature difference allowed was 5 K. As can be seen, this constraint is met through the entire load profile, including during the strong transients present at 3,600 sec (1 hr) and 84600 sec (24 hr). The higher temperature difference is present at very low loads. In general, the temperature difference is a function of the operational conditions (e.g., mass flow and temperatures). Due to configurational reasons explained below, the anode inlet temperature is easy to regulate (the chosen stack operational temperature is 1000 K). However, the cathode inlet temperature depends more strongly on system synthesis/design, which is used instead of an additional controller. This solution is more fuel efficient and more reliable.
Fig. 6.5.16: Anode and cathode inlet temperature optimum dynamic behavior.

Fig. 6.5.17: Methane conversion optimum dynamic response.
Fig. 6.5.17 shows the methane conversion optimum dynamic trajectory. As expected, the conversion at low load (low mass flows) is higher even though the reformate exit temperature is lower. This is explained by the higher residence time through the reformer. In addition, after the step load change at 86,400 sec (24 hr) the methane conversion decreases suddenly due to the rapid increase in reformate mass flow. The methane conversion stabilizes at about 89,000 sec (24.7 hr). Fig. 6.5.18 shows the optimum dynamic response of the methane conversion along the reformer for the step-up load change. In general, it should be pointed out as a major conclusion that the capacity of the system to reach steady state is faster for a step-down in load (at 3600 sec (1 hr)) than for a step-up in load (at 84600 sec (24 hr)).

Fig. 6.5.19 shows the stack hydrogen requirements compared to the BOPS hydrogen supply from the reformate tank. The rapid response is evident. This unique and very desirable feature is due to the existence of reformate and air buffers. It should be pointed out that the time response is a limiting characteristic of SOFC systems when applied to APUs. First, the methane and the anode products are subject to transport delays. Second, an increase in mass flow through the reformer implies a reduction in conversion, which from Fig. 6.5.18 takes about 400 sec (6.7 min) to stabilize. Finally, a faster response requires a stronger intervention on the part of the hot gases (i.e. an increase in the hot gases temperature above efficient values) which additionally may introduce excessive temperature gradients in the reformer. Furthermore, without buffering, a reduction in load would generate waste, since the extra hydrogen generated during the transient cannot be used in the stack and instead must be used in the burner.
Fig. 6.5.19: Stack hydrogen requirements and BOPS optimum hydrogen supply (part of the reformate mass flow which is a state variable) from the reformate tank.

Fig. 6.5.20 shows the reformer fuel tank pressure response for a non-optimized PID controller responding to a decrease in load demand starting from full load. The change in load demand induces a change in hydrogen demand from the fuel tank. In the cases plotted in Fig. 6.5.20, the load demand decreases, thus, reducing the required hydrogen from the fuel tank. This causes the tank pressure to increase. Even though the pressure in the tank takes about 1300 sec to stabilize at a final value, the controller is able to keep the error below 2% even for the largest possible load change (80%). Also note that the larger the perturbation in load, the larger the maximum error in tank pressure is. Faster pressure controllers are possible to implement and were in fact modeled. However, it was observed that decreasing the pressure response time increases perturbations in methane conversion, since this increases the rate at which the reformate flow through the reformer changes. This is an illustration of closely coupled system.
Fig. 6.5.20: Fuel tank pressure transient with PID controller for decreasing changes in load demand starting from full load.

Fig. 6.5.21 shows the methane conversion control at the reformer for a set of non-optimized PID controllers for decreasing load demand starting from full load. After a decrease in load occurs, a spike in the conversion rate results for all cases of load change due to a reduction in reactant flows. The size of the spike depends on the size of the load perturbation. The spike reveals how the energy stored in the reactor walls and catalyst affects the dynamic response. The higher the load perturbation, the bigger the conversion spikes are. For the case of 80% load demand perturbation, the induced change in reactant flows leads to a peak of almost 100% conversion. Note how the controller reaches steady state faster for the 80% perturbation. However, the maximum error is also the highest for this case. On the other hand, for the other cases, the response is slower, but the maximum error is reduced. This feature points to the need for a non-linear controller to increase the controller gain for moderate and small changes in load.

Fig. 6.5.21: Methane conversion transient with PID controller for decreasing changes in load demand starting from full load.
6.5.4 System Efficiency

Fig. 6.5.22 shows the FPS and SOFC system optimum efficiencies through the entire load profile. The BOPS efficiencies are not shown because they coincide with the FPS efficiency except for and small interval of time at the start of the profile and even in this interval the deviations are very small.

![Graph showing FPS, SOFC stack, and SOFC system optimum dynamic efficiency profile.]

**Fig. 6.5.22:** FPS, SOFC stack, and SOFC system optimum dynamic efficiency profile.

There are several interesting features and behaviors that should be noted from Fig. 6.5.23. First, FPS efficiencies higher than one are due to the fact that no additional energy is required to generate steam. Therefore, the required extra heat is used only for the methane reforming.
Moreover, the extensive heat and work recovery achieved by the optimum system configuration enhances the FPS efficiency. Note that the WRAS is able to provide the required power for air compression for most of the load profile, and even during the low load segment, additional parasitic power is small. The synergy effect of recirculating the anode exhaust is increased by the fact that the steam is at high temperature, eliminating the need for methane pre-heating.

As expected the FPS efficiency is higher at low load regimes. This is due to reasons previously mentioned (i.e. the residence time in the reformer increases, improving the conversion). In the same manner, the efficiency of the SS at lower loads increases. The same behavior is true for the system total efficiency. The high value and relatively flat behavior of system efficiency with respect to the load requirement is one of the characteristics that make fuel cell systems appealing over conventional technologies. A total system efficiency ranging from 0.3 at low load (86,400 sec or 24 hr) to 0.94 at high load (3,600 sec or 1 hr) shows a remarkable system performance. As shown in Fig. 6.5.23 during the two drastic step changes in load at 3,600 sec and 86,000 sec dramatic changes in system efficiency are generated due to the system dynamic effects such as transport delays, the slow transients of the reformer, and control effects. This shows the importance of considering the dynamic effects when optimizing the system configuration, component designs, and controls in order to minimize the negative effects and take advantages of the positive ones.

Fig. 6.5.24 shows the effect of one of the dynamic operational decision variables on SOFC system efficiency. An incremental increase in the reformer reference temperature (optimum reformate exit temperature) with respect to the optimum reduces the system efficiency due to the extra fuel required to maintain a hotter temperature. A reduction in this temperature with respect to the optimum reduces the system efficiency due to the reduction in the reforming efficiency (i.e. the higher the temperature the better the demethanation reaction) and the reduction in the hot gases inlet temperature into the expander. This shows, once again, the delicate balance to be achieved in order to find the optimum synthesis/design and dynamic operational decision variable values.

![Fig. 6.5.24: Reformer reference temperature effect on system efficiency.](image-url)
6.5.5 Design Variable Effects on System Dynamics and Operational Costs

Fig. 6.5.25 shows the effect of the steam-methane reformer size on the temperature difference between the anode and cathode inlet streams, which in turn is the most important operational constraint applied.

Fig. 6.5.26 shows the effect of the steam-methane reformer size on the fuel and component capital costs. The figure shows how a reformer 10% larger than the optimum generates a temperature difference larger than that allowed (i.e. 5 K). Additionally, the reduction in fuel consumption due to a larger reformer does not compensate the increase in capital cost. Hence, this option is not feasible from an operational and an economical standpoint. A reformer 10% smaller still meets the temperature difference constraint. However, the reduction in capital cost does not compensate the increment in fuel consumption, yielding a more expensive system than the optimum. Therefore, this option is not economically optimal.

![Fig. 6.5.25: Effects of variations in steam-methane reformer size on system dynamics.](image)

![Table 6.3: Effects of variation in steam-methane reformer size on life cycle costs.](table)

<table>
<thead>
<tr>
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<th>10% Smaller</th>
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<td>US$ 2,080</td>
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<td><strong>Total</strong></td>
<td>US$ 15,529</td>
<td>US$ 15,616</td>
<td>US$ 15,591</td>
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Fig. 6.5.26 and Fig. 6.5.27 show the effect of variation in the steam-methane reformer size on the cost rate. As previously concluded, the larger the reformer the lower the cost rate. However, Fig. 6.5.26 shows clearly that the variation in cost rate depends on the operational condition, i.e.
load requirement. At low loads, the reformer size effect is small compared to its effect at high loads. Additionally, Fig. 6.5.28 shows a zoom-in of Fig. 6.5.26 exactly at the moment of the step load increment at 86,400 sec (24 hr). As can be seen, the same trend as before applies. The cost rate during the transient is lower as the reformer size goes up. Hence, one can conclude that the operational/control cost goes down as the reformer size goes up. Obviously, the optimum balance between reformer size and cost rate is a trade-off problem, which has been successfully solved by implementing dynamic shadow price rates.

Fig. 6.5.29 shows the effects of variations in the heat exchanger II size on the temperature difference between the anode and cathode inlet streams. Table 6.4 shows this effect on the fuel and component capital costs. This figure shows how a reformer 10% larger than the optimum generates a temperature difference larger than that allowed (i.e. 5 K) during the step-up change in load at 86,400 sec (24 hr). A heat exchanger 10% smaller violates the temperature difference constraint at low loads (about 21,600 sec (6 hr)). Therefore, both modifications are operationally unacceptable. Table 6.4 shows that a smaller heat exchanger is economically feasible if higher temperature difference are allowed. This effect shows how progress in one technology (i.e. stack materials) can produce FPS cost reductions.

![Fig. 6.5.26: Effect of variation in steam-methane reformer size on cost rate.](image)

![Fig.6.5.27: Effect of variation in steam-methane reformer size on cost rate at 1 hr and 24 hr.](image)
**Fig. 6.5.28**: Zoom-in at 24 hr of the effects of variation in steam-methane reformer size on cost rate.

**Fig. 6.5.29**: Effect of variation in heat exchanger II size on system dynamics.

**Table 6.4**: Effects of variation in heat exchanger II size on life cycle costs.

<table>
<thead>
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6.6 EXPERIMENTAL RESULT OF THE NOVEL PES PROTOTYPE

6.6.1 Performance of ZRBC

In our experimental prototype a small external tunable inductor was used in series with secondary winding of the coupled-inductor in order to obtain a finer control over the HF current ripple. Fig. 6.6.1(b) shows the percentage of ripple reduction achieved by the coupled inductor as the external inductance is tuned. For an external inductance of 7.6 µH the fuel cell HF current ripple is reduced to 20% of the maximum possible HF ripple. The rest 80% of the HF current ripple is supplied by the secondary winding of the coupled inductor as shown in Fig. 6.6.1 (a).

Fig. 6.6.1: Coupled inductor performance results: (a) input current split between the DC and the AC windings for an optimum value of external inductance; and (b) experimentally-observed input ripple-current variation in the DC winding with variation in external inductance.
Fig. 6.6.2 demonstrates the low frequency current injection by the APF. From the figure it can be seen that the PES low frequency peak input current is reduced to 15% of the maximum possible input current ripple. The remaining 85% of the current ripple flows through the secondary winding of coupled inductor. Such a reduction in fuel cell current ripple will significantly improve the stack efficiency and probably enhance the life of the fuel cell stack.

Fig. 6.6.3(a) is the experimentally obtained efficiency plot for the individual subsystem and the overall PES. The obtained overall efficiency at full load is approximately 92% and the peak efficiency of 92.4% is obtained at 3 kW of output power. Fig. 6.6.3(b) is the predicted overall system efficiency, when the fuel cell stack is connected to PCS. The obtained efficiency numbers in Fig. 6.6.3(b) is a product of measured PCS overall efficiency and modeled fuel cell stack efficiency values for different values of current ripple varying from 5% to 97%.

6.6.2 Performance of the DC-AC Converter

For the HF inverter, the PSZVS SPWM is implemented using the UC3875. The gating pulses for all 4 switches and the transformer primary current and voltage waveforms are shown in Figs. 6.6.4 (a) and 6.6.4 (b), respectively.

The ZVS range is predicted using the following equation:
\[ \frac{t_{ZVS}}{t_{\text{LineCycle}}} = \frac{2}{\pi} \sin^{-1} \left( \frac{1}{4} \left( \frac{V_{DC}^2}{3C_{\text{oss}}} + \frac{1}{2} \frac{C_T}{C_{\text{out}}L_{\text{lk}}} \right) \right)^{1/2} \] (6.5)

where

- \( V_{DC} \) is the input voltage to the DC-AC converter
- \( L_{\text{lk}} \) is the leakage inductance of the primary transformer
- \( C_{\text{oss}} \) is the effective output capacitance of the MOSFETs of the HF inverter
- \( C_T \) is the equivalent parasitic capacitance of the HF transformer
- \( t_{\text{LineCycle}} \) is the line-cycle time period (for a 60 Hz line frequency it is 16.67 ms).

For a given average power, the load power factor has a minimal impact on the duration of ZVS operation. Fig. 6.6.5(a) is the plot for available ZVS range for various values of leakage inductances. It can be seen that for low values of leakage inductance, the ZVS is lost for a large output power range (upto 40% loss in ZVS for 100 nH of leakage). However, such low values of leakage may not be achievable for a 20 kHz transformer design. Therefore, for leakage values of 500 nH and above, significant reduction in the turn-on losses can be achieved over the entire load range.

Fig. 6.6.5(b) is plotted for 6 different values of leakage inductances for output voltage of the DC-AC converter. It is seen that with increase in the leakage and output power, the efficiency of the transformer degrades significantly. Therefore, it is necessary to design and wind a transformer for very low leakage inductance. Two possible winding arrangements are shown in Fig. 6.6.6 and obtained values of leakage inductances for Figs. 6.6.6(a) and 6.6.6(b) are 1.2 \( \mu \)H and 450 nH, respectively. We selected the second design for the PCS.
Fig. 6.6.3: (a) Measured efficiency for the proposed PCS and its subsystems (b) Combined efficiency of stack and PES for various fuel cell ripple current.
Fig. 6.6.4: Illustration of the HF inverter operation: (a) gating pulse for HF inverter switches (b) transformer primary voltage and current waveforms.
Fig. 6.6.5: (a) Parametric plot showing the percentage ZVS achievable versus load current for different values of leakage inductances (b) Transformer efficiency versus output power for various values of leakage inductances.
Fig. 6.6.6: Two different winding arrangements for a 5 kW, 25 kHz isolation transformer fabricated using P-49925-UC, ferrite core. (a) Primary and secondary windings on the same leg using a AWG 10 solid copper wire. The leakage inductance was measure to be 1.2 µH. (b) Primary and secondary windings distributed over the entire length of the core using a 2 strand AWG 14 copper wire. The leakage inductance was measure to be 450 nH.

The above discussed 5 kW prototype of the PES can potentially enhance the fuel cell durability and currently, achieves a peak efficiency of 92.4%. A new zero-ripple filter is proposed, which significantly reduces the low- and high-frequency (HF) current ripples seen by the fuel cell stack, thereby increasing the fuel cell hydrogen utilization and stack efficiency. The HF inverter improves the PCS reliability by reducing the voltage stress and the zero-voltage-switching (ZVS) ensures lossless commutation and improves the overall efficiency. The cost of fabrication of the actual prototype with a single phase output (designed for 5 kW) meets DOE cost constraint of $40/kW (for a volume of around 100,000 units). The proposed power-conditioning system (PCS) can be easily extended to applications with power rating higher than 20 kW by paralleling the power modules and can be operated in a rectifier mode to feed power back into a regenerative fuel cell. Also, the isolated DC-AC inverter stage can be used for photovoltaic applications (which typically has much higher input DC voltage) yielding even higher efficiency.
7. CONCLUSIONS

**Modeling:** One of the key challenges with the comprehensive system modeling, optimization, and parametric analyses is high computation overhead due to a significant difference in the time-scales of the SOFC, BOPS, and PES and AL subsystems, aggravated primarily by the switching discontinuity of the PES and large order of the BOPS. To reduce the computational burden and time, a novel reduced-order modeling approach has been developed. This enables the prototype to (a) resolve significant time-scale variations between the SOFC and BOPS and PES without losing resolution, (b) accomplish system-level analysis in minutes rather than in days, (c) enable long-term performance and reliability modeling without losing resolution, (d) reduce the cost of the simulation platform, and (e) enable the prototype for real-time simulation (RTS). RTS can serve as springboard for simulating larger scale fuel-cell power system simulation (e.g., 300 – 500 MW power plants or power-train models of vehicles). To attain the optimal compromise between comprehensive and reduced-order model, a hybrid-modeling approach has also been devised. In such an approach, the type of a subsystem model is selected based on the nature of the analysis. Thus, the hybrid modeling approach using reduced-order models solves a difficult problem in SOFC system simulation and has tangible implications for SECA industry team members and national laboratories (e.g., PNNL and ORNL).

**Electrical-feedback Effects:** The experimental validation of the model predictions (under steady-state and transient conditions) using detailed but simple set of experimental strategies (that can be easily replicated by SECA industry members) proved successful. It also showed the accuracy of the physics-based models of the planar SOFC and the power-electronics. Using the validated model, extensive parametric analyses was carried out to ascertain the effect of electrical feedbacks (resulting from PES topology variations, load type and load fluctuations on the stack) on the SOFC and our conclusions are as follows:

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21 For instance, while analyzing the effect of transients of the application load on the stack, variations of the average current has a much more significant effect on stack temperature than the switching-ripple dynamics. Hence, for SOFC-system interaction analysis, average model of the PES and the reduced-order model of the BOPS (whose dynamics change much more slowly than the current transient) are appropriate choices. On the other hand, to investigate the effect of the switching-current ripple on the stack, the discontinuous model of the PES is used together with the temporal of the SOFCS and the reduced-order model of the BOPS in the hybrid prototype.

22 Such a model is an invaluable to resolve potential component and system synthesis/design problems; analyze interactions among the various subsystems and application loads on a system as well as a detailed component level (e.g., component geometries in general and the internal dynamics and properties of SOFC stacks in particular) during steady-state, transient, and rapid start-up conditions; predict stack lifetimes and component electrical and thermal behavior; investigate, formulate and design the system control; and conduct analyses, investigations, and predictions using mathematical optimization and/or trade-off studies.
A. **Transient Electrical Effects:**
   a. The effect of a single load-current transient on the stack temperature depends on the increase in magnitude of the load current and not on the slew rate of the load or on very short term current overshoot;

   b. While, the variation in the stack temperature due to a single load transient is small as compared to a single thermal cycling of the stack, repetitive current transient enhances the stack temperature rise. So, load cycling needs close attention on the part of the SOFC system manufacturers;

   c. A (specific case study) on thermal stress analysis (subsequent to single load transient) revealed minor increase in level of residual stress (leading to a minor increase in the probability of failure) at the interface of the electrolyte with cathode in a planar SOFC. This is attributed to non-uniform temperature gradient and differences in the CTEs and elastic properties among the SOFC components. It is not clear, however, what the impact of repetitive load transients will be on the durability of the stack over longer periods of time;

   d. Unlike an increase in load current, decrease in the same, poses different challenges including i) increase in stack voltage, ii) need for a mechanism to dissipate the power till the BOPS adjusts control for the new steady state, and iii) stack may cool by a small amount (because while the amount of exothermic reactions reduces due to reduced load current, the air-flow rate may take a little while, governed by the bandwidth of the BOPS, to adjust to the new load). The effect of (i) is on the breakdown voltage of the PES and a higher breakdown voltage for a power semiconductor device may have implications for the efficiency of the PES.

B. **Steady-state Electrical Effects:**
   a. For single-phase inverters, the presence of low-frequency (SOFC) current ripple reduces the active-power capability of the stack if it is directly interfaced to the inverter. One way to partially mitigate this problem is to use a passive or active filter. The former may be bulky depending on how much stack ripple reduction is required, while the latter may slightly reduce the PES efficiency. Using a DC-DC converter (e.g., boost converter) in between the stack and the inverter, will not make much difference unless the capacitor (decoupling the DC-DC converter and the inverter is large). For this case, the overall efficiency of the PES will be a product of the individual efficiencies of the inverter and the DC-DC converter. With a (single-stage) inverter and active-filter approach, this is not the case; however, high-frequency (galvanic isolation) transformer design requires close attention. A related study by the PI (not outlined in this report) revealed that for three-phase systems, under balanced condition, input ripple can be significantly minimized depending on the choice of the topology. However, under unbalanced and harmonic-load conditions, fuel-cell current ripple may still exist;

   b. When a SOFC stack is subjected to large current ripple, its fuel utilization swings as well depending on the magnitude of the ripple (usually percentage current ripple
without mitigating circuit is high). Attempt should be made not to allow the peak fuel utilization to reach unacceptably high values. Further, because the stack efficiency reduces on either side of the optimal efficiency point, a large ripple needs to be avoided from stack efficiency and the overall energy-system efficiency standpoint;

c. Current ripple was found to have practically no effect at all on the stack temperature due to a large difference in the ripple duration and thermal time constant of the SOFC stack;

d. The power factor of passive (linear) loads and the harmonics due to nonlinear loads affect the magnitude of the ripple current. For the former case, deviation of the power factor from the best possible case of 1.0 led to even higher current ripple (for the same active current). The implications of this are outlined in (a) and (b) above. Load total harmonic distortion (THD) also has a clear impact on the fuel-cell current ripple. However, it was observed that this relationship is not a one-to-one and is more complex;

e. High-frequency ripple (of usually small magnitude as compared to the average stack current) has a negligible impact on the SOFC in short term with regard to stack temperature. If, however, the nature of the high-frequency current is pulsating, although we still expect the stack temperature to have very little effect, what the effect will be on stack voltage due to this micro-load cycles is not clear. For such a scenario, our experimental study did show large voltage swings of the stack output. However, it was not clear whether this swing is due to the PES or the impedance of the electrical interconnect between the SOFC stack and the PES;

f. The stack impedance is primarily resistive at lower frequencies (e.g., 60 Hz grid frequency), but attains a higher reactive component near converter switching frequency. This is another reason why the switching current ripple should not be high.

C. (Case-specific) Experimental Long-term (1000 hours) Effect: A long term experimental study devised to investigate if the current ripple and the load transients, for the same average stack current, has any different impact on the degradation (using a measure of ASR) of the stack. These results were compared with a benchmark case, where the stack was subjected to the same average current as for either of the case, but, without any current ripple. The (case-specific) result shows that load transient accelerates increase in ASR (which translates to loss of stack power) as compared to the benchmark case. The trend is the same when the stack is subjected only to ripple current; however, the increase in ASR is lesser in this case. For this case, however, the experimental study could not distinguish if the effect on ASR was primarily due to the high- or low-frequency ripple alone or due to a combined effect.

Novel Optimal Power Electronics: A (patent filed) novel, efficient, reliable, and cost-effective fuel-cell PES topology has been realized, which can meet $40/kW price target in volume
production and enhance the durability of SOFC stack. The novelty of the PES lies in the architecture of the system, which comprises two stages. The first stage practically eliminates low- and high-frequency (fuel-cell) current ripple and also boosts the low stack voltage in a very efficient manner due to the current-sharing modularity of the converter. The implications and necessity of ripple mitigation has been outlined above. The second stage comprises an isolated inverter, whose front end is a soft-switched multilevel high-frequency inverter. This leads to very high efficiency as well enables the converter to operate at higher power and using larger output voltage energy sources such as photovoltaic arrays (in this case, the efficiency of the PES will be even higher because the first (boost) stage is not required). The back end of the second stage comprises a cycloconverter, which directly converts AC output of the high-inverter without requiring intermediate power conversion. Most importantly, cycloconverter operates at line-frequency, which practically eliminates the switching losses. The developed PES is suitable for grid connection, can be extended for higher power, and can be interfaced to other fuel-cell stacks, regenerative fuel cells, as well as photovoltaic arrays.

Novel Topological Control: Finally, a (patent filed) novel control scheme (based on distributed power management and multi-hierarchical feedback) is realized. It has several advantages over other conventional system and is applicable to several PES topologies. Firstly, it eliminates the requirement of 2 dedicated DC-DC power conditioners for the battery and the fuel cell, by eliminating one of them. This saves cost, weight, and space. Second, the power-management scheme of the control, ensure an almost flat efficiency across the power range unlike a drooping efficiency curve or a conventional approach converter. This is achieved by using a distributed power architecture and ensuring that only optimal number of converters are actuated to meet a given load. Third, the multi-hierarchical feedback control effectively mitigates the effect of the load transient on the stack. Further, it lets the battery use the distributed PES to provide the additional load power immediately after a transient, but relinquish the battery power as governed by the BOPS bandwidth.
8. LIST OF ACRONYMS

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<tr>
<th>Acronym</th>
<th>Description</th>
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<tbody>
<tr>
<td>AFR</td>
<td>Air-to-fuel Ratio</td>
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<tr>
<td>APU</td>
<td>Auxiliary Power Unit</td>
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<tr>
<td>BOPS</td>
<td>Balance-of-plant Subsystem</td>
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<tr>
<td>CFD</td>
<td>Computational Fluid Dynamics</td>
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<td>CSI</td>
<td>Current-source Inverter</td>
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REFERENCES


APPENDICES

A. PES MODELS

A.1 PES Simulink and SimPowerSystems Schematic Models

(Simulink switching model of the residential system)
(Simulink average model of the residential system)

(Controller for the boost converter)
(Controller for voltage source inverter)

(PSOFC PCS System Model)
A.2 Flow Chart of the Multi-converter Control for Power Management System
B. BOPS MODEL CODES

B.1 Main Processing Routine

UNIT
  Interface AS OL_Master_Interface

SET
  WITHIN Interface DO
    WITHIN Master DO
      WITHIN MM DO
        axial := [CFDM, 2, 20] ;
        PROPERTIES_REFOR.AXIAL := [CFDM, 2, 20] ;
        PROPERTIES_OUT.AXIAL := [CFDM, 2, 20] ;
        ENTHALPY_REFOR.AXIAL := [CFDM, 2, 20] ;
        RateR.C_W := [CFDM, 2, 20] ;
      END
      ReactorLength := 0.40000000000000 ;
      WITHIN HX1 DO
        PlateThickness := 0.010000000000000 * 2.5400000000000 / 100 ;
      END
      WITHIN HX2 DO
        PlateThickness := 0.010000000000000 * 2.5400000000000 / 100 ;
      END
      WITHIN HX4 DO
        PlateThickness := 0.010000000000000 * 2.5400000000000 / 100 ;
      END
      WITHIN HX3 DO
        PlateThickness := 0.010000000000000 * 2.5400000000000 / 100 ;
      END
      WITHIN HX5 DO
        PlateThickness := 0.010000000000000 * 2.5400000000000 / 100 ;
      END
  END

ASSIGN
  WITHIN Interface DO
    WITHIN Master DO
      MM.Temp_o := 900 ;
      jam.m_ref := 0.0077918500000000 ;
      jam.Bias := 50 ;
      oxigen_util := 0.35000000000000 ;
      Kv := 0.0080000000000000 ;
      Ka := 7.7500000000000E-005 ;
      Kb := 1.5500000000000E-005 ;
      WITHIN MM DO
        d_i := 0.012000000000000 ;
        P := 300 ;
        n_tubes := 300 ;
        thickness := 0.0005000000000000 ;
        X1_ref := 0.91463200000000 ;
        KA_2 := 0.00015209000000000 * 1.6000000000000 ;
        KB_2 := 1929.1300000000 / 0.30000000000000 ;
        minimum_output_1 := 6.0000000000000E-008 ;
        maximum_output_1 := 1.3000000000000E-006 ;
        KA := 22.150500000000 ;
        KB := 27.283000000000 ;
        T_ref := 1098.6700000000 ;
        KA_3 := 2.6285900000000E-010 * 14.7000000000000 ;
KB_3 := 445.99600000000 / 1 ;
minimum_output := 5.0000000000000E-007 ;
maximum_output := 0.00025000000000000 ;
SMR_ref := 1.8773000000000 ;
KA_4 := 1.4626700000000 / 100 * 1350 ;
KB_4 := 0.0048389000000000 * 10 * 1350 ;
Tank.Volume := 0.00200000000000000 ;
END
WITHIN HX1 DO
  FinTypePRI := 15 ;
  LengthHX(1) := 0.040000000000000 ;
  LengthHX(2) := 0.040000000000000 ;
  NoPlates := 6 ;
END
WITHIN HX2 DO
  FinTypePRI := 15 ;
  LengthHX(1) := 0.150000000000000 ;
  LengthHX(2) := 0.150000000000000 ;
  NoPlates := 10 ;
END
WITHIN HX4 DO
  FinTypePRI := 15 ;
  LengthHX(1) := 0.150000000000000 ;
  LengthHX(2) := 0.150000000000000 ;
  NoPlates := 40 ;
END
WITHIN HX3 DO
  FinTypePRI := 15 ;
  LengthHX(1) := 0.300000000000000 ;
  LengthHX(2) := 0.300000000000000 ;
  NoPlates := 60 ;
END
WITHIN HX5 DO
  FinTypePRI := 15 ;
  LengthHX(1) := 0.200000000000000 ;
  LengthHX(2) := 0.200000000000000 ;
  NoPlates := 20 ;
END
WITHIN jam DO
  P2s := 3 ;
  P_tank_ref := 290000 ;
  scale_factor := 0.050000000000000 ;
  Kv := 0.00015583700000000 ;
  Kb := 5.5015210000000 * 2 * 5 ;
  Ka := 0.00081270000000000 * 120 ;
  minimum_output := 10 ;
  maximum_output := 300 ;
  WITHIN turb DO
    scale_factor := 0.035000000000000 ;
    Kb := 5.5015210000000 * 50000 * 0.500000000000000 / 2 ;
    Ka := 0.00081270000000000 * 200000 * 15 / 2 ;
    minimum_output := 1.1000000000000 ;
    maximum_output := 2.8000000000000 ;
  END
END
END
END
INTERFACE.MASTER.Y_ANO_OUT_3.SIGNAL := 0.20771500000000 ;
INTERFACE.MASTER.V1_CONTROL_SIGNAL_1.SIGNAL := 0.018687200000000 ;
INTERFACE.MASTER.Y_ANO_OUT_7.SIGNAL := 0.00000000000000 ;
INTERFACE.MASTER.Y_CAT_OUT_5.SIGNAL := 0.00000000000000 ;
INTERFACE.MASTER.Y_ANO_OUT_4.SIGNAL := 0.12091700000000 ;
INTERFACE.MASTER.Y_CAT_OUT_4.SIGNAL := 0.00000000000000 ;
INTERFACE.MASTER.TEMP_ANO_OUT_1.SIGNAL := 1000.0000000000 ;
INTERFACE.MASTER.Y_CAT_OUT_1.SIGNAL := 0.00000000000000 ;
INTERFACE.MASTER.GROSSP.SIGNAL := 5080.0000000000 ;
INTERFACE.MASTER.Y_ANO_OUT_6.SIGNAL := 0.00000000000000 ;
INTERFACE.MASTER.F_CH4_NEW_CONTROL_SIGNAL_1.SIGNAL := 6.04682000000000E-005 ;
INTERFACE.MASTER.Y_CAT_OUT_6.SIGNAL := 0.13783300000000 ;
INTERFACE.MASTER.RECIRCULATION_CONTROL_SIGNAL_1.SIGNAL := 0.54017400000000 ;
INTERFACE.MASTER.Y_ANO_OUT_1.SIGNAL := 0.014104200000000 ;
INTERFACE.MASTER.F_ANO_IN_1.SIGNAL := 0.00011510500000000 ;
INTERFACE.MASTER.Y_CAT_OUT_3.SIGNAL := 0.00000000000000 ;
INTERFACE.MASTER.Y_ANO_OUT_2.SIGNAL := 0.57419200000000 ;
INTERFACE.MASTER.Y_CAT_OUT_7.SIGNAL := 0.79771400000000 ;
INTERFACE.MASTER.Y_ANO_OUT_5.SIGNAL := 0.083072200000000 ;
INTERFACE.MASTER.TGASIN_CONTROL_SIGNAL_1.SIGNAL := 1331.5600000000 ;
INTERFACE.MASTER.F_ANO_OUT_1.SIGNAL := 0.00011510500000000 ;
INTERFACE.MASTER.TEMP_CAT_OUT_1.SIGNAL := 1000.0000000000 ;
INTERFACE.MASTER.Y_CAT_OUT_2.SIGNAL := 0.064453100000000 ;
INTERFACE.MASTER.F_CAT_OUT_1.SIGNAL := 0.00034150600000000 ;
INTERFACE.MASTER.NETP.SIGNAL := 5000.0000000000 ;
INTERFACE.MASTER.P2S_P1S_CONTROL_SIGNAL_1.SIGNAL := 2.4540100000000 ;
INTERFACE.MASTER.VOLT_CONTROL_SIGNAL_1.SIGNAL := 74.116100000000 ;
INTERFACE.MASTER.F_OUT_CONTROL_SIGNAL_1.SIGNAL := 9.1446300000000E-007 ;

PRESET
RESTORE "Try_37"
INITIAL
WITHIN Interface DO
  WITHIN Master DO
    F_reformat = 0.00011510500000000 ;
    EE = 1193.5500000000 ;
    FOR z := 0 TO MM.ReactorLength DO
      MM.$T_w(z) = 0 ;
      MM.$T_cat(z) = 0 ;
    END
    MM.F_out_2 = 9.1446300000000E-007 ;
    MM.Total_Feed_4 = 6.04682000000000E-005 ;
    MM.EE = 1640.2100000000 ;
    MM.EE_2 = 24.174000000000 ;
    MM.EE_3 = 6979400.0000000 ;
    MM.EE_4 = 1.7870400000000 ;
    MM.Tank.M(1) = 0.0003934660000000 ;
    MM.Tank.M(2) = 0.0068904700000000 ;
    MM.Tank.M(3) = 0.0138355000000000 ;
    MM.Tank.M(4) = 0.0085173000000000 ;
    MM.Tank.M(5) = 0.0368840000000000 ;
    MM.Tank.M(6) = 0 ;
    MM.Tank.M(7) = 0 ;
    MM.Tank.M_total = 0.0646464000000000 ;
    MM.Tank.T = 1098.5540000000 ;
    FOR k := 1 TO 7 DO
      MM.F_recir_2(k) = MM.F_recir(k) ;
    END
    FOR k := 1 TO HX1.KK DO
      FOR i := 1 TO HX1.NN DO
        HX1.$T_Metal(i, k) = 0 ;
      END
      FOR k := 1 TO HX2.KK DO
        FOR i := 1 TO HX2.NN DO
          HX2.$T_Metal(i, k) = 0 ;
        END
      FOR k := 1 TO HX4.KK DO

5/6/2006
FOR i := 1 TO HX2.NN DO
    HX4.$T_Metal(i, k) = 0 ;
END

END

FOR k := 1 TO HX3.KK DO
    FOR i := 1 TO HX3.NN DO
        HX3.$T_Metal(i, k) = 0 ;
    END
END

FOR k := 1 TO HX5.KK DO
    FOR i := 1 TO HX5.NN DO
        HX5.$T_Metal(i, k) = 0 ;
    END
END

jam.mot.$Ia = 0 ;
jam.mot.$Sw = 0 ;
jam.EE = 40930.900000000 ;
jam.$tm = 0 ;
jam.turb.$tm = 0 ;
jam.volt_2 = jam.volt ;
jam.M_tur = jam.M_mixer ;
FOR k := 1 TO 7 DO
    jam.Tank.$M(k) = 0 ;
END
jam.Tank.M_total = 0.16572700000000 ;
jam.Tank.$T = 0 ;
jam.turb.P2s_P1s_2 = 2.5135400000000 ;
jam.turb.EE = 125.16400000000 ;
END

END

SOLUTIONPARAMETERS
ReportingInterval := 1000.00
NLSolver := "NLSOL" [  
    "OutputLevel" := 0,
    "ConvergenceTolerance" := 1.0000000000000E-007
  ]
DASolver := "DASOLV" [
    "AbsoluteTolerance" := 1.0000000000000E-007,
    "RelativeTolerance" := 1.0000000000000E-007,
    "Absolute1stTimeDerivativeThreshold" := 0,
    "Relative1stTimeDerivativeThreshold" := 0,
    "Relative2ndTimeDerivativeThreshold" := 0,
    "OutputLevel" := 0
  ]

SCHEDULE
LINEARISE
INPUT
INTERFACE.MASTER.Y_CAT_OUT_7.SIGNAL;
INTERFACE.MASTER.Y_CAT_OUT_6.SIGNAL;
INTERFACE.MASTER.Y_CAT_OUT_5.SIGNAL;
INTERFACE.MASTER.Y_CAT_OUT_4.SIGNAL;
INTERFACE.MASTER.Y_CAT_OUT_3.SIGNAL;
INTERFACE.MASTER.Y_CAT_OUT_2.SIGNAL;
INTERFACE.MASTER.F_ANO_IN_1.SIGNAL;
INTERFACE.MASTER.Y_CAT_OUT_1.SIGNAL;
INTERFACE.MASTER.Y_ANO_OUT_7.SIGNAL;
INTERFACE.MASTER.Y_ANO_OUT_6.SIGNAL;
INTERFACE.MASTER.Y_ANO_OUT_5.SIGNAL;
INTERFACE.MASTER.Y_ANO_OUT_4.SIGNAL;
INTERFACE.MASTER.Y_ANO_OUT_3.SIGNAL;
INTERFACE.MASTER.Y_ANO_OUT_2.SIGNAL;
INTERFACE.MASTER.Y_ANO_OUT_1.SIGNAL;
INTERFACE.MASTER.F_ANO_OUT_1.SIGNAL;
INTERFACE.MASTER.GROSSP.SIGNAL;
INTERFACE.MASTER.TEMP_ANO_OUT_1.SIGNAL;
INTERFACE.MASTER.F_CAT_OUT_1.SIGNAL;
INTERFACE.MASTER.NETP.SIGNAL;
INTERFACE.MASTER.TEMP_CAT_OUT_1.SIGNAL;
INTERFACE.MASTER.P2S_P1S_CONTROL_SIGNAL_1.SIGNAL;
INTERFACE.MASTER.RECIRCULATION_CONTROL_SIGNAL_1.SIGNAL;
INTERFACE.MASTER.TGASIN_CONTROL_SIGNAL_1.SIGNAL;
INTERFACE.MASTER.V1_CONTROL_SIGNAL_1.SIGNAL;
INTERFACE.MASTER.VOLT_CONTROL_SIGNAL_1.SIGNAL;
INTERFACE.MASTER.F_CH4_NEW_CONTROL_SIGNAL_1.SIGNAL;
INTERFACE.MASTER.F_OUT_CONTROL_SIGNAL_1.SIGNAL;

OUTPUT

INTERFACE.MASTER.F_CAT_IN_1.SIGNAL;
INTERFACE.MASTER.TEMP_ANO_IN_1.SIGNAL;
INTERFACE.MASTER.XI_1.SIGNAL;
INTERFACE.MASTER.TEMP_CAT_IN_1.SIGNAL;
INTERFACE.MASTER.Y_ANO_IN_1.SIGNAL;
INTERFACE.MASTER.Y_ANO_IN_2.SIGNAL;
INTERFACE.MASTER.Y_ANO_IN_3.SIGNAL;
INTERFACE.MASTER.Y_ANO_IN_4.SIGNAL;
INTERFACE.MASTER.Y_ANO_IN_5.SIGNAL;
INTERFACE.MASTER.Y_ANO_IN_6.SIGNAL;
INTERFACE.MASTER.Y_ANO_IN_7.SIGNAL;
INTERFACE.MASTER.Y_CAT_IN_1.SIGNAL;
INTERFACE.MASTER.Y_CAT_IN_2.SIGNAL;
INTERFACE.MASTER.Y_CAT_IN_3.SIGNAL;
INTERFACE.MASTER.Y_CAT_IN_4.SIGNAL;
INTERFACE.MASTER.Y_CAT_IN_5.SIGNAL;
INTERFACE.MASTER.Y_CAT_IN_6.SIGNAL;
INTERFACE.MASTER.Y_CAT_IN_7.SIGNAL;
INTERFACE.MASTER.M1_1.SIGNAL;
INTERFACE.MASTER.M_TUR_1.SIGNAL;
INTERFACE.MASTER.P_TANK_1.SIGNAL;
INTERFACE.MASTER.P_TANK_2.SIGNAL;
INTERFACE.MASTER.P_TANK_REF_1.SIGNAL;
INTERFACE.MASTER.T_REF_1.SIGNAL;
INTERFACE.MASTER.TEMP_1.SIGNAL;
INTERFACE.MASTER.X_REF_1.SIGNAL;
INTERFACE.MASTER.P_TANK_REF_2.SIGNAL;
INTERFACE.MASTER.SMR_1.SIGNAL;
INTERFACE.MASTER.SMR_REF_1.SIGNAL;
INTERFACE.MASTER.T1.SIGNAL;
INTERFACE.MASTER.X_1.SIGNAL;

END

B.2 Modelling the Master_Interface

# PARAMETER
# ParameterName AS INTEGER || REAL || LOGICAL < DEFAULT Value >
# ParameterName AS ARRAY ( Size < , ... > ) OF INTEGER || REAL || LOGICAL < DEFAULT Value >
# ParameterName AS FOREIGN_OBJECT < "ForeignObjectClass" > < DEFAULT "ForeignObjectValue" >

UNIT

Master AS Master_Model
F_ano_out       AS Constant
F_cat_out       AS Constant
Gross_P         AS Constant
Net_P           AS Constant
Y_ano_out_1     AS Constant
Y_ano_out_2     AS Constant
Y_ano_out_3     AS Constant
Y_ano_out_4     AS Constant
Y_ano_out_5     AS Constant
Y_ano_out_6     AS Constant
Y_ano_out_7     AS Constant
Y_cat_out_1     AS Constant
Y_cat_out_2     AS Constant
Y_cat_out_3     AS Constant
Y_cat_out_4     AS Constant
Y_cat_out_5     AS Constant
Y_cat_out_6     AS Constant
Y_cat_out_7     AS Constant
Temp_ano_out    AS Constant
Temp_cat_out    AS Constant

# Hydrogen Tank Valve Controller
V1_Control_signal    AS Constant

# Electric Motor Controller
Volt_Control_signal   AS Constant

# Expander pressure ratio Controller
P2s_P1s_Control_signal   AS Constant

# Stema Methane Ration Controller
Recirculation_Control_signal   AS Constant

# Hydrogen tank Pressure Controller
F_Ch4_new_Control_signal    AS Constant

# Reformer Degree of Reaction Controller
F_out_Control_signal       AS Constant

# Reformer output temperature Controller
TGasIn_Control_signal      AS Constant

TOPOLOGY
F_ano_out.Output         = Master.F_ano_out_1;
F_cat_out.Output         = Master.F_cat_out_1;
Gross_P.Output           = Master.GrossP;
Net_P.Output             = Master.NetP;
Temp_ano_out.Output      = Master.Temp_ano_out_1;
Temp_cat_out.Output      = Master.Temp_cat_out_1;
Y_ano_out_1.Output = Master.y_ano_out_1;
Y_ano_out_2.Output = Master.y_ano_out_2;
Y_ano_out_3.Output = Master.y_ano_out_3;
Y_ano_out_4.Output = Master.y_ano_out_4;
Y_ano_out_5.Output = Master.y_ano_out_5;
Y_ano_out_6.Output = Master.y_ano_out_6;
Y_ano_out_7.Output = Master.y_ano_out_7;
Y_cat_out_1.Output = Master.y_cat_out_1;
Y_cat_out_2.Output = Master.y_cat_out_2;
Y_cat_out_3.Output = Master.y_cat_out_3;
Y_cat_out_4.Output = Master.y_cat_out_4;
Y_cat_out_5.Output = Master.y_cat_out_5;
Y_cat_out_6.Output = Master.y_cat_out_6;
Y_cat_out_7.Output = Master.y_cat_out_7;

# Hydrogen Tank Valve Controller
V1_Control_signal.Output = Master.V1_Control_signal_1;

# Electric Motor Controller
Volt_Control_signal.Output = Master.Volt_Control_signal_1;

# Expander pressure ratio Controller
P2s_P1s_Control_signal.Output = Master.P2s_P1s_Control_signal_1;

# Stema Methane Ration Controller
Recirculation_Control_signal.Output = Master.Recirculation_Control_signal_1;

# Hydrogen tank Pressure Controller
F_Ch4_new_Control_signal.Output = Master.F_Ch4_new_Control_signal_1;

# Refeormer Degree of Reaction Controller
F_out_Control_signal.Output = Master.F_out_Control_signal_1;

# Refeormer output temperature Controller
TGasIn_Control_signal.Output = Master.TGasIn_Control_signal_1;

### B.3 Modeling the Master Model

PARAMETER
ReactorLength   AS  REAL
NoComp          AS INTEGER
NoPoints        AS INTEGER
Tstandard       AS  REAL
a, b, c, d      AS ARRAY (NoComp) OF  REAL
Hformation      AS ARRAY (NoComp) OF  REAL
MolarMass       AS ARRAY (NoComp) OF  REAL

UNIT
MM       AS CH4_Reformer_Dynamis_2
HX1      AS CompactHX_2
HX2  AS CompactHX_2  
HX4  AS CompactHX_2  
HX3  AS CompactHX_2  
HX5  AS CompactHX_2  
Mix1  AS Reformer_mixer  
Mix2  AS Reformer_mixer  
Mix3  AS Reformer_mixer  
CMIX  AS Combustor_mixer  
COMB  AS Burner  
jam  AS comp_alt

PORT

XI_1 AS PMLControl

Y_ano_out_1 AS PMLControl
Y_ano_out_2 AS PMLControl
Y_ano_out_3 AS PMLControl
Y_ano_out_4 AS PMLControl
Y_ano_out_5 AS PMLControl
Y_ano_out_6 AS PMLControl
Y_ano_out_7 AS PMLControl

Y_cat_out_1 AS PMLControl
Y_cat_out_2 AS PMLControl
Y_cat_out_3 AS PMLControl
Y_cat_out_4 AS PMLControl
Y_cat_out_5 AS PMLControl
Y_cat_out_6 AS PMLControl
Y_cat_out_7 AS PMLControl

Y_ano_in_1 AS PMLControl
Y_ano_in_2 AS PMLControl
Y_ano_in_3 AS PMLControl
Y_ano_in_4 AS PMLControl
Y_ano_in_5 AS PMLControl
Y_ano_in_6 AS PMLControl
Y_ano_in_7 AS PMLControl

Y_cat_in_1 AS PMLControl
Y_cat_in_2 AS PMLControl
Y_cat_in_3 AS PMLControl
Y_cat_in_4 AS PMLControl
Y_cat_in_5 AS PMLControl
Y_cat_in_6 AS PMLControl
Y_cat_in_7 AS PMLControl

F_ano_out_1 AS PMLControl
F_cat_out_1 AS PMLControl

Temp_ano_out_1 AS PMLControl
Temp_cat_out_1 AS PMLControl

Temp_ano_in_1 AS PMLControl
Temp_cat_in_1 AS PMLControl
F_cat_in_1 AS PMLControl

# Hydrogen Tank Valve Controller

GrossP  AS PMLControl
NetP  AS PMLControl
# Reformer output temperature Controller

# The error of this controller is defined as
# where e = T_ref - Temp(ReactorLength);
# Temp(ReactorLength) is the output temperature of the reformer
# T_ref is the the reference value

F_Ch4_new_Control_signal_1 AS PMLControl
F_out_Control_signal_1 AS PMLControl
m_1 AS PMLControl
M_tur_1 AS PMLControl
P2s_Pls_Control_signal_1 AS PMLControl
P_tank_1 AS PMLControl
P_tank_2 AS PMLControl
P_tank_ref_1 AS PMLControl
P_tank_ref_2 AS PMLControl
Recirculation_Control_signal_1 AS PMLControl
SMR_1 AS PMLControl
SMR_ref_1 AS PMLControl
T_ref_1 AS PMLControl
Temp_1 AS PMLControl
TGasIn_Control_signal_1 AS PMLControl
V1_Control_signal_1 AS PMLControl
Volt_Control_signal_1 AS PMLControl
X_1 AS PMLControl
X_ref_1 AS PMLControl
F_ano_in_1 AS PMLControl

VARIABLE

Y AS ARRAY(NoPoints,NoComp) OF general
Fmix AS ARRAY(NoPoints) OF MolarFlowRate
Temp AS ARRAY(NoPoints) OF Temperature
Ho AS ARRAY(NoComp) OF General
Hcomp AS ARRAY(NoPoints,NoComp) OF General
HcompTotal AS ARRAY(NoPoints,NoComp) OF General
Hmix AS ARRAY(NoPoints) OF General
Q_SMR_hot AS General
Q_SMR_cold AS General

YVAP_in AS General
Y_cat_in AS ARRAY(NoComp) OF General
Y_cat_out AS ARRAY(NoComp) OF General
F_Cathode_in_H2O AS General
F_Cathode_in_wet_total AS General
oxygen_util AS General
F_02_in AS General
F_02_out AS General
F_Cathode_in AS General
F_N2_in AS General
F_N2_out AS General
F_Cathode_out AS General
Kv AS General
Ka AS General
Kb AS General
Tao AS General
F_reformate AS General
e AS General
EE AS General
ii AS General
iiii AS General
GrossPower AS General
GrossPower_2 AS General
NetPower AS General
NetPower_ref AS General
F_ano_in1 AS General
F_cat_in1 AS General
F_ano_out1 AS General
F_cat_out1 AS General
y_ano_out1 AS ARRAY (NoComp) OF General
y_cat_out1 AS ARRAY (NoComp) OF General
Temp_ano_out1 AS General
Temp_cat_out1 AS General

SET

Tstandard := 273.15 + 25;
NoComp := 7;
NoPoints := 34;
a := [104.0, 180.0, 62.8, -55.6, 79.5, 10.3, 72.0];
b := [-77.8, -85.4, -22.6, 30.5, -26.3, 5.4, -26.9];
c := [20.1, 15.6, 4.6, -1.96, 4.23, -0.18, 5.19];
d := [-1.3, -0.858, -0.272, 0.0, -0.197, 0.0, -0.298];
Hformation := [-74900, -242000, -110600, -393800, 0.0, 0.0, 0.0]; # KJ/ Kmol
MolarMass := [16.043, 18.015, 28.010, 44.010, 2.016, 31.999, 28.013]; #kg/kmol

EQUATION

# Identification of the constituent enthalpy and mixture's specific enthalpy
# vectors Hcomp and Hmix respectively
Ho = a*Tstandard + (4/5)*b*Tstandard^(5/4) + (2/3)*c*Tstandard^(3/2) +
(4/7)*d*Tstandard^(7/4);

FOR j := 1 TO NoPoints DO
    FOR i := 1 TO NoComp DO
        Hcomp(j,i) = a(i)*Temp(j) + (4/5)*b(i)*Temp(j)^(5/4) +
        (2/3)*c(i)*Temp(j)^(3/2) + (4/7)*d(i)*Temp(j)^(7/4);
        HcompTotal(j,i) = Hformation(i) + Hcomp(j,i) - Ho(i);
    END
    Hmix(j) = sigma(Y(j,1:NoComp)*HcompTotal(j,1:NoComp));
END

# Prereformer mixer
# CH4 Reformer
Temp(1) = 310;
Temp(2) = 310;
Temp(3) = 310;
Temp(4) = 310; # There is not need for heat exchanger
Temp(5) = Temp_ano_out1;#HX5.T_hot_out_1;
Temp(6) = Mix1.Temp_3;
Temp(7) = MM.TGasIn;
Temp(8) = MM.T_out(0);
Temp(9) = MM.Temp(ReactorLength);
Temp(10) = jam.T2;
Temp(11) = MM.Tank.T;
Temp(12) = Temp_ano_out1;#1000; #Temperature coming out of the cell
Temp(13) = Temp(5);
Temp(14) = Temp(5);
Temp(15) = HX4.T_hot_out_1;
Temp(16) = Temp(1);
Temp(17) = CMIX.Temp_Burner_1;
Temp(18) = MIX2.Temp_3;
Temp(19) = HX3.T_cold_out_1;
Temp(20) = Temp_cat_out1;#1000; #Temperature coming out of the cell
Temp(21) = HX5.T_cold_out_1;
Temp(22) = HX3.T_hot_out_1;
Temp(23) = HX4.T_cold_out_1;
Temp(24) = HX4.T_cold_in_1;
Temp(25) = Temp(8);
Temp(26) = HX4.T_hot_out_1;
Temp(27) = HX1.T_hot_out_1; #this temperature can not be too high
Temp(28) = Temp(27);
Temp(29) = jam.tank.T;
Temp(30) = HX1.T_cold_out_1;
Temp(31) = Mix3.Temp_3;
Temp(32) = jam.turb.T2;
Temp(33) = Temp(32);
Temp(34) = Temp(4);

# Element specification of the above vectors and matrices
# Specification of the elements of the mole fraction matrix Y

# Methane heat Exchanger
y(1,1) = 1;
FOR i := 2 TO NoComp DO
  Y(1,i) = 0;
END
y(2,1) = 1;
FOR i := 2 TO NoComp DO
  Y(2,i) = 0;
END
y(3,1) = 1;
FOR i := 2 TO NoComp DO
  Y(3,i) = 0;
END

# CH4 Reformer
Y(4,) = Y_cat_in;
Y(5,) = MM.Y_recir;
Y(6,) = MM.Y_combin;
Y(7,) = MM.Y_combustion_gas;
Y(8,) = Y(7,);
Y(9,) = MM.RateR.Y_reactor(,ReactorLength);
Y(10,) = Y_cat_in;
# mass flow in kmol

\[
\begin{align*}
F_{\text{mix}}(1) &= F_{\text{mix}}(2) + F_{\text{mix}}(3); \\
F_{\text{mix}}(2) &= \text{MM.F_Ch4_new}/100; \\
F_{\text{mix}}(3) &= \text{CMIX.FlowRate_CH4_new}; \\
F_{\text{mix}}(4) &= F_{\text{mix}}(10); \\
F_{\text{mix}}(5) &= \text{MM.F_recir_total}/1000; \\
F_{\text{mix}}(6) &= F_{\text{mix}}(2); \\
F_{\text{mix}}(7) &= \text{COMB.FlowRate_out}; \\
F_{\text{mix}}(8) &= F_{\text{mix}}(7); \\
F_{\text{mix}}(9) &= \text{MM.Total_to_tank}/1000; \\
F_{\text{mix}}(10) &= F_{\text{mix}}(24) + F_{\text{mix}}(29); \\
F_{\text{mix}}(11) &= \text{MM.Tank.F_cell}; \\
F_{\text{mix}}(12) &= \text{MM.F_ano_out}; \\
F_{\text{mix}}(13) &= F_{\text{mix}}(22); \\
F_{\text{mix}}(14) &= \text{MM.F_ano_out} - \text{MM.F_recir_total}/1000; \\
F_{\text{mix}}(15) &= F_{\text{mix}}(11); \\
F_{\text{mix}}(16) &= F_{\text{mix}}(3); \\
F_{\text{mix}}(17) &= \text{CMIX.FlowRate_Burner}; \\
F_{\text{mix}}(18) &= \text{Mix2.FlowRate_3}; \\
F_{\text{mix}}(19) &= F_{\text{Cathode_in_wet_total}};
\end{align*}
\]

\[
\begin{align*}
F_{\text{mix}}(20) &= F_{\text{Cathode_out}}; \\
F_{\text{mix}}(21) &= F_{\text{mix}}(20); \\
F_{\text{mix}}(22) &= F_{\text{mix}}(21); \\
F_{\text{mix}}(23) &= F_{\text{mix}}(19); \\
F_{\text{mix}}(24) &= F_{\text{mix}}(23); \\
F_{\text{mix}}(25) &= F_{\text{mix}}(8); \\
F_{\text{mix}}(26) &= F_{\text{mix}}(25); \\
F_{\text{mix}}(27) &= \text{Mix2.FlowRate_1}; \\
F_{\text{mix}}(28) &= F_{\text{mix}}(13) - F_{\text{mix}}(27); \\
F_{\text{mix}}(29) &= \text{Mix2.FlowRate_2}; \\
F_{\text{mix}}(30) &= F_{\text{mix}}(26); \\
F_{\text{mix}}(31) &= \text{Mix3.FlowRate_3}; \\
F_{\text{mix}}(32) &= F_{\text{mix}}(31); \\
F_{\text{mix}}(33) &= F_{\text{mix}}(31); \\
F_{\text{mix}}(34) &= F_{\text{mix}}(10);
\end{align*}
\]
####### HX1
HX1.T_hot = Temp(22);
HX1.T_cold = Temp(26);
HX1.Moles_hot = F_Cathode_out;
HX1.Moles_cold = MM.Total_hot_gas;
HX1.Ymix(2,) = Y(26,);
HX1.Ymix(1,) = Y(22,);

####### HX2
HX2.T_hot = Temp(32);
HX2.T_cold = Temp(4);
HX2.Moles_hot = Fmix(32);
HX2.Moles_cold = Fmix(10);
HX2.Ymix(2,) = Y(4,);
HX2.Ymix(1,) = Y(32,);

####### Reformer Mixer
Mix1.FlowRate_1 = MM.F_CH4_new/1000;
Mix1.Y_1 = Y(1,);
Mix1.FlowRate_2 = MM.F_recir_total/1000;
Mix1.Y_2 = MM.Y_recir;
Mix1.EnthalpyMix_2 = Hmix(5);
Mix1.EnthalpyMix_1 = Hmix(4);

####### Combustor Mixer
# CMIX.FlowRate_CH4_new = 3.39345e-006*2.2;
# CMIX.FlowRate_Air = 0.0002524;
# CMIX.FlowRate_Anode = MM.F_recir_total*(1-MM.Recirculation)/1000;
if MM.Recirculation >= 0.99 then
    CMIX.FlowRate_Anode = MM.F_recir_total*(1-0.99)/1000;
else if MM.Recirculation <= 0.01 then
    CMIX.FlowRate_Anode = MM.F_recir_total*(1-0.01)/1000;
else
    CMIX.FlowRate_Anode = MM.F_recir_total*(1-MM.Recirculation)/1000;
end
end
CMIX.EnthalpyMix_CH4_new = Hmix(16);
CMIX.EnthalpyMix_Air = Hmix(18);
CMIX.EnthalpyMix_Anode = Hmix(14);
CMIX.Y_CH4_new = Y(16,);
CMIX.Y_Anode = Y(14,);  # See the mole fraction
if CMIX.FlowRate_Air < F_Cathode_out then
    CMIX.Y_Air = Y_cat_out;
else
    CMIX.Y_Air = MIX2.Y_3;
end
CMIX. T_CH4_new = Temp(16);
CMIX. T_Anode = Temp(14);
CMIX. T_Air = Temp(18);

####### Combustor
COMB.FlowRate_in = CMIX.FlowRate_Burner;
COMB.EnthalpyMix_in = Hmix(17);
COMB.Y_BURNER_in = CMIX.Y_Burner;
COMB.T_design_BURNER = MM.TGasIn;
COMB.FlowRate_out = MM.Total_hot_gas;

# CH4 Reformer

#
MM.Temp(0) = Mix1.Temp_3;
Q_SMR_cold = MM.RateR.FT(ReactorLength)/1000*Hmix(6);
MM.F_combin_total/1000*Hmix(6);
Q_SMR_hot = MM.Total_hot_gas*(Hmix(7)-Hmix(8));
MM.Y_combustion_gas = COMB.Y_BURNER_out;

##### # Heat Exchanger IV

HX4.T_hot = MM.T_out(0);
HX4.T_cold = jam.Tank.T;
HX4.Ymix(2,) = Y_cat_in;
HX4.Ymix(1,) = Y(7,);
HX4.Moles_hot = MM.Total_hot_gas;
HX4.Moles_cold = F_Cathode_in_wet_total;

#### Cathode Fuel Cell

# Specification of the component mole fractions at the exit of the anode

YVAP_in = 0.06;
Y_cat_in(1) = 0;
Y_cat_in(2) = YVAP_in;
FOR k := 3 TO 7-2 DO
  Y_cat_in(k) = 0;
END
Y_cat_in(6) = 0.21*(1 - YVAP_in);
Y_cat_in(7) = 0.79*(1 - YVAP_in);

F_Cathode_in_H2O = (1/0.21)*YVAP_in*F_02_in / (1 - YVAP_in);
F_Cathode_in_wet_total = F_Cathode_in + F_Cathode_in_H2O;

F_02_in = MM.Tank.F_cell * MM.Tank.X(5) * MM.F_U / 2 / oxigen_util;
F_02_out = F_02_in - MM.Tank.F_cell * MM.Tank.X(5) * MM.F_U / 2;
F_Cathode_in = F_02_in / 0.21;
F_N2_in = F_Cathode_in - F_02_in;
F_N2_out = F_N2_in;
#F_Cathode_out = F_Cathode_in - (F_02_in-F_02_out);

{ 
  Y_cat_out(1) = 0;
  Y_cat_out(2) = F_Cathode_in_H2O/(F_Cathode_out+F_Cathode_in_H2O);
  FOR k := 3 TO 5 DO
    Y_cat_out(k) = 0;
  END
  Y_cat_out(6) = F_02_out/(F_Cathode_out+F_Cathode_in_H2O);
  Y_cat_out(7) = F_N2_out/(F_Cathode_out+F_Cathode_in_H2O);
}

# Y_cat_out = y_cat_out1;

##### # Heat Exchanger III

HX3.T_hot = HX5.T_cold_out_1;#1000;
HX3.T_cold = HX4.T_cold_out_1;
HX3.Ymix(2,) = Y_cat_in;
HX3.Ymix(1,) = Y_cat_out;
HX3.Moles_hot = F_Cathode_out;
HX3.Moles_cold = F_Cathode_in_wet_total;

######## # Heat Exchanger V

HX5.T_hot = MM.Tank.T;
HX5.T_cold = Temp(20);# 1000;
HX5.Moles_hot = MM.Tank.F_cell;
HX5.Ymix(2,) = Y_cat_out;
HX5.Ymix(1,) = MM.Tank.X;

#######    Air Mixer

if CMIX.FlowRate_Air < F_Cathode_out then
    Mix2.FlowRate_2 = 0;
    Mix2.Y_1 = Y(27,);
    Mix2.Y_2 = Y(29,);
    Mix2.EnthalpyMix_2 = Hmix(29);
    Mix2.EnthalpyMix_1 = Hmix(27);
    Mix2.FlowRate_3 = CMIX.FlowRate_Air;
else
    Mix2.FlowRate_1 = F_Cathode_out;
    Mix2.Y_1 = Y(27,);
    Mix2.Y_2 = Y(29,);
    Mix2.EnthalpyMix_2 = Hmix(29);
    Mix2.EnthalpyMix_1 = Hmix(27);
    Mix2.FlowRate_3 = CMIX.FlowRate_Air;
end

#######    Turbomachinery

jam.Tank.F_Cathode = F_Cathode_in;
jam.turb.T1 = Mix3.Temp_3;

#######    Expander Mixer

if CMIX.FlowRate_Air < F_Cathode_out then
    Mix3.FlowRate_1 = F_Cathode_out-Mix2.FlowRate_3;
    Mix3.FlowRate_2 = MM.Total_hot_gas;
    Mix3.Y_1 = Y(27,);
    Mix3.Y_2 = Y(26,);
    Mix3.EnthalpyMix_2 = Hmix(30);
    Mix3.EnthalpyMix_1 = Hmix(28);
else
    Mix3.FlowRate_1 = 0;
    Mix3.FlowRate_2 = MM.Total_hot_gas;
    Mix3.Y_1 = Y(27,);
    Mix3.Y_2 = Y(26,);
    Mix3.EnthalpyMix_2 = Hmix(30);
    Mix3.EnthalpyMix_1 = Hmix(28);
end

#######    anode fuel cell inlet valve controller

Tao = 0.2;
$F_reformate = Kv/Tao*iiii - Kv/Tao*.004 - F_reformate/Tao;
e = NetPower_ref - NetPower;
$EE = 0;
ii = (Ka*e + kb*EE);
#iiii = 0.0186872;  
#iiii = V1_Control_signal_1;  
#if ii < 0.004 then  
#iiii = 0.004;  
#else if ii > 0.024 then  
#iiii = 0.024;  
#else  
#iiii = ii;  
#end  
#end

GrossPower_2 = 4E+07*F_reformate + 594;  
NetPower = GrossPower_2-jam.mot.pow_m;  
#NetPower = GrossPower-jam.mot.pow_m;  
#NetPower_ref = 5000;

############  Interfacing  ############

MM.Tank.F_cell          = F_ano_in1;  
MM.Tank.F_cell          = F_reformate;  
F_Cathode_in_wet_total  = F_cat_in1;  
F_ano_in_1.signal       = F_ano_in1;  
F_cat_in_1.signal       = F_cat_in1;  
F_ano_out_1.signal      = F_ano_out1;  
F_cat_out_1.signal      = F_cat_out1;  
Temp_ano_out_1.signal   = Temp_ano_out1;  
Temp_cat_out_1.signal   = Temp_cat_out1;  
Temp_ano_in_1.signal    = HX5.T_Hot_OUT_1;  
Temp_cat_in_1.signal    = HX3.T_Cold_OUT_1;  
XI_1.signal             = MM.X1(ReactorLength);  
Y_ano_out_1.signal      = y_ano_out1(1);  
Y_ano_out_2.signal      = y_ano_out1(2);  
Y_ano_out_3.signal      = y_ano_out1(3);  
Y_ano_out_4.signal      = y_ano_out1(4);  
Y_ano_out_5.signal      = y_ano_out1(5);  
Y_ano_out_6.signal      = y_ano_out1(6);  
Y_ano_out_7.signal      = y_ano_out1(7);  
Y_cat_out_1.signal      = y_cat_out1(1);  
Y_cat_out_2.signal      = y_cat_out1(2);  
Y_cat_out_3.signal      = y_cat_out1(3);  
Y_cat_out_4.signal      = y_cat_out1(4);  
Y_cat_out_5.signal      = y_cat_out1(5);  
Y_cat_out_6.signal      = y_cat_out1(6);  
Y_cat_out_7.signal      = y_cat_out1(7);  
Y_ano_in_1.signal       = MM.Tank.X(1);  
Y_ano_in_2.signal       = MM.Tank.X(2);  
Y_ano_in_3.signal       = MM.Tank.X(3);  
Y_ano_in_4.signal       = MM.Tank.X(4);  
Y_ano_in_5.signal       = MM.Tank.X(5);  
Y_ano_in_6.signal       = MM.Tank.X(6);  
Y_ano_in_7.signal       = MM.Tank.X(7);  
Y_cat_in_1.signal       = Y_cat_in(1);  
Y_cat_in_2.signal       = Y_cat_in(2);  
Y_cat_in_3.signal       = Y_cat_in(3);  
Y_cat_in_4.signal       = Y_cat_in(4);
Y_cat_in_5.signal = Y_cat_in(5);
Y_cat_in_6.signal = Y_cat_in(6);
Y_cat_in_7.signal = Y_cat_in(7);

y_ano_out1 = MM.Y_recir;
MM.F_recir = F_ano_out1*1000*y_ano_out1*MM.Recirculation;

y_cat_out1 = Y_cat_out;
F_Cathode_out = F_cat_out1;

# Hydrogen Tank Valve Controller
V1_Control_signal_1.signal = iii;
GrossP.signal = GrossPower;
NetP.signal = NetPower_ref;

# Electric Motor Controller
Volt_Control_signal_1.signal = Jam.volt;
P_tank_ref_1.signal = jam.P_tank_ref;
P_tank_1.signal = jam.Tank.P_tank;

# Expander pressure ratio Controller
P2s_P1s_Control_signal_1.signal = Jam.turb.P2s_P1s;
M_tur_1.signal = jam.M_tur;
M1_1.signal = jam.Turb.M1;

# Stema Methane Ration Controller
Recirculation_Control_signal_1.signal = MM.Recirculation_1;
SMR_ref_1.signal = MM.SMR_ref;
SMR_1.signal = MM.SMR;

# Hydrogen tank Pressure Controller
F_Ch4_new_Control_signal_1.signal = MM.F_Ch4_new_1;

P_tank_ref_2.signal = MM.P_tank_ref;
P_tank_2.signal = MM.Tank.P_tank;

# Reformer Degree of Reaction Controller
F_out_Control_signal_1.signal = MM.F_out;
X_1.signal = MM.X1(ReactorLength);
X_ref_1.signal = MM.X1_ref;

# Reformer output temperature Controller
TGasIn_Control_signal_1.signal = MM.TGasIn;

# The error of this controller is defined as
# where e = T_ref - Temp(ReactorLength);
# Temp(ReactorLength) is the output temperature of the reformer
# T_ref is the the reference value
T_ref_1.signal = MM.T_ref;
Temp_1.signal = MM.Temp(ReactorLength);
B.4 Modeling the Methane Reformer

PARAMETER

ReactorLength AS REAL
StoiCoeff_smr AS ARRAY(7) OF REAL
StoiCoeff_Shift AS ARRAY(7) OF REAL
StoiCoeff_total AS ARRAY(7) OF REAL
Hformation AS ARRAY(7) OF REAL
Tstand AS REAL
Sformation AS ARRAY(7) OF REAL
a AS ARRAY(7) OF REAL
b AS ARRAY(7) OF REAL
c AS ARRAY(7) OF REAL
d AS ARRAY(7) OF REAL
M_vector AS ARRAY(7) OF REAL
NoComp AS INTEGER
af AS ARRAY(7) OF REAL
bf AS ARRAY(7) OF REAL
Mcoef_A AS ARRAY(7) OF REAL
Mcoef_B AS ARRAY(7) OF REAL

UNIT

Tank AS Fuel_Tank
RateR AS Rate
Enthalpy_Refor AS Enthalpy
#Enthalpy_out AS Enthalpy
Properties_Refor AS Properties
Properties_out AS Properties
HT_Coeff AS Heat_Transf_Coeff

DISTRIBUTION_DOMAIN

axial AS [ 0 : ReactorLength ]

VARIABLE

F AS DISTRIBUTION (axial) OF General
X1 AS DISTRIBUTION (axial) OF General
TT AS DISTRIBUTION (axial) OF General
d_i AS General
p AS General
Fo AS General
Fl AS General
F AS General
R AS General
Temp AS DISTRIBUTION (axial) OF General
CP_reformate AS DISTRIBUTION (axial) OF General
Cp AS General
Delta_H_CH4_shift AS General
Delta_H_CH4_smr AS General
Rho_wall AS General
Cp_wall AS General
d_o AS General
h_out AS DISTRIBUTION (axial) OF General
A_out AS General
CP_out AS DISTRIBUTION (axial) OF General
F_out AS General
T_w AS DISTRIBUTION (axial) OF General
T_out AS DISTRIBUTION (axial) OF General
n_tubes AS General
A_in AS General
Delta_H_f AS General
v AS General
Temp_o AS General
thickness AS General
Y_combustion_gas AS ARRAY(7) OF General
Dp AS General
h_cold AS DISTRIBUTION (axial) OF General
Rho_cat_1 AS General
Cp_cat AS General
h_cat AS DISTRIBUTION (axial) OF General
Ac AS General
T_cat AS DISTRIBUTION (axial) OF General
e_e AS General
jh AS DISTRIBUTION (axial) OF General
SMR AS General

Total_H2_out AS General
Total_out AS ARRAY(7) OF General
hMix AS DISTRIBUTION (axial) OF General
KA_2 AS General
KB_2 AS General
E_2 AS General
Pro_2 AS General
Assintotic_2 AS General
EE_2 AS General
F_out_1 AS General
F_out_2 AS General
dswitch_1 AS General
X1_ref AS General
Pro_int_2 AS General
minimum_output_1 AS General
maximum_output_1 AS General
Total_to_tank AS General
F_out_cell AS ARRAY(7) OF General
Recirculation AS General
Recirculation_1 AS General
F_U AS General
F_recir AS ARRAY(7) OF General
F_recir_2 AS ARRAY(7) OF General
F_recir_total AS General
Y_recir AS ARRAY(7) OF General
F_Ch4_new AS General
F_Ch4_new_1 AS General
F_combin AS ARRAY(7) OF General
F_combin_total AS General
F_combin_total_per_tube AS General
Y_combin AS ARRAY(7) OF General

FCH4 AS General
FH2O AS General
FH2 AS General
FCO AS General
FCO2 AS General
KA AS General
KB AS General
T_ref AS General
e AS General
EE AS General
Pro AS General
Pro_int AS General
TGasIn AS General
P_tank_ref AS General
e_3            AS General
Pro_3          AS General
Pro_int_3      AS General
Ka_3           AS General
kb_3           AS General
Total_Feed_3   AS General
minimum_output AS General
maximum_output AS General
Assintotic_1   AS General
EE_3           AS General
Total_Feed_4   AS General
dswitch        AS General
SMR_ref        AS General
e_4            AS General
EE_4           AS General
Pro_4          AS General
Ka_4           AS General
Pro_int_4      AS General
kb_4           AS General
P_SMR    AS DISTRIBUTION (axial) OF General
P_SMR_1  AS DISTRIBUTION (axial) OF General
F_o      AS General
Phi      AS General
gc       AS General
Rho_1    AS DISTRIBUTION (axial) OF General
vel      AS DISTRIBUTION (axial) OF General
vis_1    AS DISTRIBUTION (axial) OF General
G        AS DISTRIBUTION (axial) OF General
Total_hot_gas       AS General
F_ano_out           AS General

SELECTOR

# StopIntegrator    AS (active, inactive)         DEFAULT inactive
# StopIntegrator_1  AS (active_1, inactive_1)     DEFAULT inactive_1
# Assint            AS (Low_bound, High_bound)    DEFAULT High_bound

SET

StoiCoeff_smr         := [-1, -1, 1, 0.0, 3, 0.0, 0.0 ] ;
StoiCoeff_Shift       := [0.0, -1, -1, 1, 0.0, 0.0, 0.0 ] ;
M_vector              := [16.043, 18.015, 28.01, 44.01, 2.016, 31.99, 28.014 ];
StoiCoeff_total       := [-1, -3/2, 1/2, 1/2, 7/2, 0.0, 0.0 ];
Hformation            := [-74900, -242000, -110600, -393800, 0.0, 0.0, 0.0 ]; # KJ/
Kmol
Tstand                := 273.15 + 25 ;
NoComp                := 7;

# Data taken from Gyftopoulos Table 29.4, page 549
Sformation := [-80.6, -44.4, 89, 7, 2.9, 0.0, 0.0, 0.0 ]; # KJ/ Kmol K

Data:

a        := [104.0, 180.0, 62.8, -55.6, 79.5, 10.3, 72.0];
b        := [-77.8, -85.4, -22.6, 30.5, -26.3, 5.4, -26.9];
c        := [20.1, 15.6, 4.6, -1.96, 4.23, -0.18, 5.19];
d        := [-1.3, -0.858, -0.272, 0.0, -0.197, 0.0, -0.298];
af       := [-13.213, -6.866, 10.098, -0.010, 0.0, 0.0];
bf       := [-10735, -29911, -13808, -47575, 0.0, 0.0];
Mcoef_A  := [3.2324e-7, -0.000001820, 3.4278e-7, 1.2918e-7, 0.0000021356, 3.3018e-7, 1.5005e-7];
Mcoef_B := [1.4398e-9, 0.0000000023, 1.1426e-9, 7.9496e-10, 8.2800e-9, 1.2227e-9, 1.8060e-9];

#BOUNDARY
# Input and Output
# Y(0) = RateR.Y_CH4(0);
# Y(ReactorLength) = signal_out;

EQUATION

RateR.d_i = d_i;
pi        = 3.1416;
R         = 8.3134;
HT_Coeff.d_i = d_i;
HT_Coeff.thickness = thickness;

RateR.FCH4(0) = Fo * Y_combin(1)*1000;
RateR.FH2O(0) = Fo * Y_combin(2)*1000;
RateR.FH2(0)  = Fo * Y_combin(5)*1000;
RateR.FCO(0)  = Fo * Y_combin(3)*1000;
RateR.FCO2(0) = Fo * Y_combin(4)*1000;

FCH4 = F_combin(1)/n_tubes;
FH2O = F_combin(2)/n_tubes;
FH2  = F_combin(5)/n_tubes;
FCO  = F_combin(3)/n_tubes;
FCO2 = F_combin(4)/n_tubes;

FOR z := 0 TO ReactorLength DO
    Enthalpy_Refor.Temperature(z)   = Temp(z);
    Enthalpy_Refor.Ycomp(,z)        = RateR.Y_reactor(,z);
    #  Enthalpy_out.Temperature(z)     = T_out(z);
    #  Enthalpy_out.Ycomp(,z)          = Y_combustion_gas;
    Properties_Refor.Temperature(z) = Temp(z);
    Properties_Refor.Ycomp(,z)      = RateR.Y_reactor(,z);
    Properties_out.Temperature(z)   = T_out(z);
    Properties_out.Ycomp(,z)        = Y_combustion_gas;
    P*1000                          = Properties_out.Pressure(z);
    P_SMR_1(z)                      = Properties_refor.Pressure(z);

    HT_Coeff.TMix(z)                = Temp(z);
    HT_Coeff.YMix(,z)               = RateR.Y_reactor(,z);
    HT_Coeff.TGas(z)                = T_out(z);
    HT_Coeff.F(z)                   = F(z);
    HT_Coeff.FlowMixIn(z)           = F(z);
END

HT_Coeff.PMix                   = P*1000;
HT_Coeff.PGas                   = P*1000;
HT_Coeff.YGasIn                 = Y_combustion_gas;
HT_Coeff.FlowGasIn              = F_out;
HT_Coeff.NTubes                 = n_tubes;

FOR z := 0 TO ReactorLength DO
    RateR.T(z)   = Temp(z);
    RateR.Po(z)  = P_SMR_1(z)/1000000;
END
\[ \text{Dp} = 0.002; \]
\[ \text{P}_\text{SMR}(0) = \text{P}_o; \]
\[ \text{P}_o = \text{P} \times 1000 \times 0.02089; \]
\[ \Phi_i = 0.46; \]
\[ \text{gc} = 32.; \]

\[
\text{FOR } z := 0 \text{ TO ReactorLength} \text{ DO}
\]
\[ \text{Rho}_1(z) = \text{Properties_Refor.Rho}(z) \times 0.062297; \]
\[ \text{vel}(z) = \text{HT_Coeff.uMix}(z) \times 11808; \]
\[ \text{vis}_1(z) = \text{Properties_Refor.Viscosity}(z) \times 75.20; \]
\[ \text{G}(z) = \text{Rho}_1(z) \times \text{vel}(z); \]
\[ \text{P}_\text{SMR}_1(z) = \text{P}_\text{SMR}(z) / 0.02089; \]
\[
\text{END}
\]

\[
\text{FOR } z := 0 |+ \text{ TO ReactorLength} \text{ DO}
\]
\[ \text{PARTIAL(P}_\text{SMR}(z), \text{axial}) = #0; \]
\[ (-\text{G}(z)) / (\text{Rho}_1(z) \times \text{gc} \times \text{Dp}) \times ((1 - \Phi_i) / (\Phi_i^3)) \times (150 \times (1 - \Phi_i) \times \text{vis}_1(z) / (\text{Dp} + 1.75 \times \text{G}(z))); \]
\[
\text{END}
\]

\[ \text{Cp} = 39; \]
\[ \text{Delta}_H_{\text{CH4 shift}} = \text{SIGMA(StoiCoeff_shift*Hformation)}; \]
\[ \text{Delta}_H_{\text{CH4 smr}} = \text{SIGMA(StoiCoeff_smr*Hformation)}; \]
\[ \text{A}_\text{in} = 2 \times \pi \times d_i \times \text{ReactorLength} / 100; \]
\[ \text{Delta}_H_f = \text{SIGMA(StoiCoeff_total*Hformation)}; \]
\[ \nu = \text{SIGMA(StoiCoeff_total)}; \]

\[
\{\begin{align*}
\text{Y_combustion_gas(1)} &= 0; \\
\text{Y_combustion_gas(2)} &= 0.25; #0.154808; \\
\text{Y_combustion_gas(3)} &= 0; \\
\text{Y_combustion_gas(4)} &= 0.10; #0.0643497; \\
\text{Y_combustion_gas(5)} &= 0; \\
\text{Y_combustion_gas(6)} &= 0.05; #0.118469; \\
\text{Y_combustion_gas(7)} &= 0.6; #0.662372; \\
\end{align*}\}
\]

\[
\{\begin{align*}
\text{Y_combustion_gas(1)} &= 0; \\
\text{Y_combustion_gas(2)} &= 0.121446; #0.25; #0.154808; \\
\text{Y_combustion_gas(3)} &= 0; \\
\text{Y_combustion_gas(4)} &= 0.060723; #0.10; #0.0643497; \\
\text{Y_combustion_gas(5)} &= 0; \\
\text{Y_combustion_gas(6)} &= 0.116509; #0.05; #0.118469; \\
\text{Y_combustion_gas(7)} &= 0.701322; \\
\end{align*}\}
\]

\[ \text{F1} = \text{Fo*RateR.Y_CH4(0)}; \]
\[ \text{X1(0)} = 0; \]
\[ \text{F} = \text{Fo} + 2 \times \text{RateR.X1*F1}; \]

\[
\text{FOR } z := 0 |+ \text{ TO ReactorLength} \text{ DO}
\]
\[ \text{RateR.X1(z)} = \text{X1(z)}; \]
\[
\text{END}
\]

\[
\text{FOR } z := 0 \text{ TO ReactorLength} \text{ DO}
\]
\[ \text{h_out(z)} = \text{HT_Coeff.hExGas(z)}; \]
\[ \text{h_cold(z)} = \text{HT_Coeff.hExMix(z)}; \]
\[
\text{END}
\]

\[
\text{FOR } z := 0 \text{ TO ReactorLength} \text{ DO}
\]
\[ \text{TT(z)} = 900 + z / .0045 \times 4; \]
\[
\text{END}
\]

\[
\text{FOR } z := 0 |+ \text{ TO ReactorLength} \text{ DO}
\]

5/6/2006
\[
\text{PARTIAL(CP\_reformate(z)\*F(z)\*Temp(z),axial)} = \\
h\_cold(z)\*\pi*d\_i^2*(T\_w(z)-T\_out(z)) + h\_cat(z)\*669.29\*(\pi*d\_i^2/4)*(T\_cat(z)-T\_out(z)) \\
\text{PARTIAL(F(z)\*hMix(z),axial);}
\]

\[
\text{FOR z := 0 TO ReactorLength DO} \\
\quad \text{Properties\_Refor.CP(z) = CP\_reformate(z);} \\
\quad \text{Properties\_out.CP(z) = CP\_out(z);} \\
\text{END}
\]

\[
\text{FOR z := 0 TO ReactorLength DO} \\
\quad h\_Mix(z) = \text{Enthalpy\_Refor.Hmixture(z);} \\
\text{END}
\]

\[
\text{Rho\_wall} = 7800; \\
\text{Cp\_wall} = 0.6113; \\
\text{d\_o} = d\_i + 2*\text{thickness;} \\
\text{A\_out} = \pi*d\_o^2/4;
\]

\[
\text{FOR z := 0 TO ReactorLength DO} \\
\quad \text{PARTIAL(T\_out(z)\*CP\_out(z),axial)} = - h\_out(z)\*\pi*d\_o*(T\_w(z)-T\_out(z))/F\_out; \\
\text{END}
\]

\[
\text{Rho\_cat\_1} = 1200; \\
\text{Cp\_cat} = 1.0262; \\
\text{Ac} = 669.29*\text{ReactorLength}\*\pi*d\_i^2/4; \\
\text{e\_e} = 0.469;
\]

\[
\text{FOR z := 0 TO ReactorLength DO} \\
\quad jh(z) = 0.725 / (100)^{0.36} / e\_e; \quad \#\text{for 30 < Re < 10^2} \\
\quad h\_Cat(z) = 0.5*jh(z)*\text{HT\_Coeff.uMix(z)*HT\_Coeff.RhoMix(z)/2*CP\_reformate(z)/(0.72^{(2/3));} \\
\text{END}
\]

\[
\text{FOR z := 0 TO ReactorLength DO} \\
\quad 0 = \text{Rho\_cat\_1}\*\text{Cp\_cat}\*T\_cat(z) - h\_Cat(z)\*669.29*(Temp(z) - T\_cat(z)); \\
\text{END}
\]

\[
\text{FOR z := 0 TO ReactorLength DO} \\
\quad \text{Rho\_wall}\*(d\_o^2 - d\_i^2) * \text{Cp\_wall} * T\_w(z) \\
\quad \quad = 4*h\_out(z)\*d\_o*(T\_out(z) - T\_w(z)) - 4*h\_cold(z)\*d\_i*(T\_w(z) - T\_out(z)); \\
\text{END}
\]

\[
\text{Total\_H2\_out} = \text{n\_tubes}\* F(\text{ReactorLength})*\text{RateR.Y\_H2(ReactorLength)*1000}; \quad \#\text{in moles/s} \\
\text{Total\_out} = \text{n\_tubes}\* F(\text{ReactorLength})*\text{RateR.Y\_reactor(,ReactorLength)*1000}; \quad \#\text{in moles/s} \\
\text{Total\_to\_tank} = \text{SIGMA(Total\_out);} \\
\text{E\_2} = X1\_ref - X1(\text{ReactorLength}); \\
\text{Pro\_2} = Ka\_2*E\_2; \\
\text{Pro\_int\_2} = Ka\_2*EE\_2/kb\_2; \\
\text{F\_out\_1} = Pro\_2 + Pro\_int\_2;
\]

\[
\text{Assintotic\_2} = 0.0000001; \\
\text{EE\_2} = 0; \\
\text{#F\_out} = F\_out\_2; \\
\text{$F\_out\_2} = -0.5*F\_out\_2 + 0.5*F\_out\_1;\#0.000001;
\]

\[
\{ \\
\text{CASE Assint OF}
\]
WHEN Low_bound:
  \( Assintotic_2 = 0.0000001; \)
  \[
  \text{SWITCH TO High_bound IF (F\_out\_1 > (minimum\_output\_1))};
  \]
WHEN High_bound:
  \( Assintotic_2 = \text{maximum\_output\_1 + dswitch\_1}; \)
  \[
  \text{SWITCH TO Low_bound IF (F\_out\_1 < (minimum\_output\_1))};
  \]
END

CASE StopIntegrator\_1 OF
  WHEN inactive\_1:
    \( EE_2 = E_2; \)
    \( \#F\_out = F\_out\_2; \)
    \( F\_out\_2 = -0.5*F\_out\_2 + 0.5*F\_out\_1; \)
    \( \text{SWITCH TO active\_1 IF ((F\_out\_1 < (minimum\_output\_1 - dswitch\_1)) OR (F\_out\_1 > (maximum\_output\_1 + dswitch\_1))));} \)
  WHEN active\_1:
    \( EE_2 = 0; \)
    \( \#F\_out = F\_out\_2; \)
    \[ F\_out\_2 = -0.5*F\_out\_2 + 0.5*Assintotic_2; \]
    \( \text{SWITCH TO inactive\_1 IF ((F\_out\_1 > minimum\_output\_1) AND (F\_out\_1 < maximum\_output\_1))}; \)
END #CASE

dswitch\_1 = 0.000000015 ;
\[
\text{T\_out(ReactorLength) = TGasIn};
\]
\#KA = 22.1505;
\#KB = 27.283;
\#T\_ref = 1098.67;
e = T\_ref - Temp(ReactorLength);
$EE = 0;
Pro = Ka*e;
Pro\_int = Ka*EE/kb;
#TGasIn = Pro + Pro\_int;
#TGasIn = 1331.56;

Tank.F\_reformer = Total\_to\_tank/1000;
Tank.T\_in = Temp(ReactorLength);
Tank.Y\_reformer = RateR.Y\_reactor(,ReactorLength);

F\_Ch4\_new = F\_Ch4\_new\_1 * n\_tubes;
P\_tank\_ref = P\_SMR\_1(ReactorLength);
e\_3 = P\_tank\_ref - Tank.P\_tank;
Pro\_3 = Ka\_3*e\_3;
Pro\_int\_3 = Ka\_3*EE\_3/kb\_3;
Total\_Feed\_3 = Pro\_3 + Pro\_int\_3;
Assintotic\_1 = 0.00000045;
$EE\_3 = 0;
#F\_Ch4\_new\_1 = Total\_Feed\_4;
#Total\_Feed\_4 = -0.15*Total\_Feed\_4 + 0.15*Total\_Feed\_3;#0.000001;

if Total\_Feed\_3 < minimum\_output then
  Assintotic\_1 = 0.00000045;
else
  Assintotic\_1 = maximum\_output;
CASE StopIntegrator OF
    WHEN inactive:
        $EE_3 = e_3;
        #F_Ch4_new_1 = Total_Feed_4;
        $Total_Feed_4 = -0.15*Total_Feed_4 + 0.15*Total_Feed_3;#0.0000001;
        SWITCH TO active IF ((Total_Feed_3 < (minimum_output - dswitch)) OR (Total_Feed_3 > (maximum_output + dswitch)));
        WHEN active:
            $EE_3 = 0;
            #F_Ch4_new_1 = Total_Feed_4;
            $Total_Feed_4 = -0.15*Total_Feed_4 + 0.15*Assintotic_1;#Total_Feed_3;#minimum_output;
        SWITCH TO inactive IF ((Total_Feed_3 > minimum_output) AND (Total_Feed_3 < maximum_output ));
    END #CASE
}
dswitch = 0.00000004;

SMR = RateR.FH2O(0)/RateR.FCH4(0);
e_4 = SMR_ref - SMR;
$EE_4 = 0;
Pro_4 = Ka_4*e_4;
Pro_int_4 = Ka_4*EE_4/kb_4;
Recirculation = Recirculation_1;

F_out_cell = Tank.F_cell * Tank.X*1000;
F_U = 0.85;
#F_recir(1) = F_out_cell(1)*Recirculation;
#F_recir(2) = (F_out_cell(2)+F_out_cell(5)*F_U)*Recirculation;
#F_recir(3) = F_out_cell(3)*Recirculation;
#F_recir(4) = F_out_cell(4)*Recirculation;
#F_recir(5) = (1-F_U)*F_out_cell(5)*Recirculation;
#F_recir(6) = F_out_cell(6)*Recirculation;
#F_recir(7) = F_out_cell(7)*Recirculation;
$F_recir_2 = -0.1*F_recir_2 + 0.1*F_recir;
F_recir_total = SIGMA(F_recir);
F_ano_out = F_recir_total/Recirculation/1000;
F_combin(1) = F_recir_2(1) + F_Ch4_new ;
F_combin(2) = F_recir_2(2);
F_combin(3) = F_recir_2(3);
F_combin(4) = F_recir_2(4);
F_combin(5) = F_recir_2(5);
F_combin(6) = 0;
F_combin(7) = 0;
F_combin_total = SIGMA(F_combin);
F_combin_total_per_tube = SIGMA(F_combin)/n_tubes/1000;
Fo = F_combin_total_per_tube ;
Y_combin(1) = F_combin(1)/F_combin_total;
Y_combin(2) = F_combin(2)/F_combin_total;
Y_combin(3) = F_combin(3)/F_combin_total;
Y_combin(4) = F_combin(4)/F_combin_total;
Y_combin(5) = F_combin(5)/F_combin_total;
Y_combin(6) = 0;
Y_combin(7) = 0;
Total_hot_gas = F_out*n_tubes;

B.5 Modeling the Compact Heat Exchanger

# ===================================================================================================
# #                  Compact Plate-Fin Heat Exchanger Model
# #
# # - Remarks
# # i) The effectiveness relation used in the current model is valid for cross
# #    flow (single pass) arrangement with both fluids unmixed
# # ii) Thermophysical Properties Calculations: The linear fits for the thermal
# #    conductivity and the dynamic Viscosity of the mixture's components were
# #    provided by the EES software. The curve fits for the water/steam were
# #    provided by MS Excel.
# # iii) The plate-fin heat exchanger design is based on the methodology and
# #    the example problems presented in the following references
# # - References
# # i) "Heat Exchangers: Selection, Rating, and Thermal Design", Sadik Kakac,
# #    Hongtan Liu
# # ii) "Fundamentals of Heat and Mass Transfer", Frank Incropera, David Dewitt
# #
# # ===================================================================================================

PARAMETER
NoComp                  AS INTEGER
Kfin                    AS REAL
PlateThickness          AS REAL
MaterialDensity         AS REAL
a, b, c, d              AS ARRAY (NoComp) OF REAL
Kcoef_A, Kcoef_B        AS ARRAY (NoComp) OF REAL
Mcoef_A, Mcoef_B        AS ARRAY (NoComp) OF REAL
Cp_metal                AS REAL
KK, NN                  AS INTEGER

UNIT
FinChoice               AS FinTypeModel_1
Colburn                 AS ColburnFactor_1

VARIABLE
NoPlates                AS General
MolesReformate, MolesCombMix AS MolarFlowRate
Treformate_IN, Treformate_OUT AS Temperature
TcombMix_IN, TcombMix_OUT AS Temperature
Ymix                    AS ARRAY (2, NoComp) OF General
HeightHX                AS Length
Tavg_Reformate, Tavg_CombMix AS Temperature
Cmin, Cmax, Cratio      AS Positive
NTU, UA                 AS Positive
Effectiveness           AS General
TotalMass               AS Positive
PlateVolume, PlateMass  AS Positive
LengthHX, FinLength     AS ARRAY (2) OF Length
MolarFlow AS ARRAY (2) OF MolarFlowRate
FreeFlowArea, FrontalArea AS ARRAY (2) OF Positive
HeatTransferArea, Volume AS ARRAY (2) OF Positive
FinVolume, FinMass AS ARRAY (2) OF Positive
N_fin, N_overall AS ARRAY (2) OF Positive
Reynolds, G, m, HTC AS ARRAY (2) OF Positive
CP, Conductivity, Viscosity AS ARRAY (2) OF ThermoPhysical
Temperature AS ARRAY (2) OF Temperature
CPcomp, Kcomp, Mcomp AS ARRAY (2, NoComp) OF ThermoPhysical
mCp_HOT AS Positive
mCp_COLD AS Positive
FinTypePRI AS Positive
Temp AS ARRAY (4) OF General
T_hot_IN_1 AS General
T_hot_OUT_1 AS General
T_Cold_OUT_1 AS General
T_Cold_IN_1 AS General
T_hot AS General
T_cold AS General
Moles_hot AS General
Moles_cold AS General
T_Cold_IN AS ARRAY (NN+1,KK) OF General
T_Hot_IN AS ARRAY (NN,KK+1) OF General
T_Hot_OUT AS ARRAY (NN,KK+1) OF General
T_Metal AS ARRAY (NN,KK) OF General
Q_Hot_Metal AS ARRAY (NN,KK) OF General
Q_Metal_Cold AS ARRAY (NN,KK) OF General
Tavg_Hot AS ARRAY (NN,KK) OF General
Tavg_Cold AS ARRAY (NN,KK) OF General

SET
Kfin := 0.035;
MaterialDensity := 7800;
Kcoef_A := [-0.028545, -0.0224088296, 0.010559, -0.0053149, 0.081635, 0.0090033, 0.01197];
Kcoef_B := [0.00019266, 0.0001171410, 0.000055063, 0.0000755, 0.00034784, 0.000063871, 0.00005238];
Mcoef_A := [3.2324e-7, -0.0000001820, 3.4278e-7, 1.2918e-7, 0.0000021356, 3.3018e-7, 1.5005e-7];
Mcoef_B := [1.4398e-9, 0.0000000023, 1.1426e-9, 7.9496e-10, 8.2800e-9, 1.2227e-9, 1.8060e-9];
NoComp := 7;
# Data taken from Gyftopoulos' Table 20.2, page 320.
a := [104.0, 180.0, 62.8, -55.6, 79.5, 10.3, 72.0];
b := [-77.8, -85.4, -22.6, 30.5, -26.3, 5.4, -26.9];
c := [20.1, 15.6, 4.6, -1.96, 4.23, -0.18, 5.19];
d := [-1.3, -0.858, -0.272, 0.0, -0.197, 0.0, -0.298];
Cp_metal := 0.41; # 0.6113 KJ/Kg
KK :=20;
NN :=20;

EQUATION
# Average temperatures necessary for properties calculations

\[
T_{\text{avg\_Reformate}} = \frac{(T_{\text{reformate\_IN}} + T_{\text{reformate\_OUT}})}{2} ;
\]
\[
T_{\text{avg\_CombMix}} = \frac{(T_{\text{combMix\_IN}} + T_{\text{combMix\_OUT}})}{2} ;
\]

\[
\text{Temperature}(1) = T_{\text{avg\_Reformate}} ; \quad \text{#hot stream}
\]
\[
\text{Temperature}(2) = T_{\text{avg\_CombMix}} ; \quad \text{#cold stream}
\]

\[
\text{Temp}(1) = T_{\text{reformate\_IN}} ;
\]
\[
\text{Temp}(2) = T_{\text{reformate\_OUT}} ;
\]
\[
\text{Temp}(3) = T_{\text{combMix\_IN}} ;
\]
\[
\text{Temp}(4) = T_{\text{combMix\_OUT}} ;
\]

# Properties Calculations

\[
T_{\text{hot}} = T_{\text{reformate\_IN}} ;
\]
\[
T_{\text{cold}} = T_{\text{combMix\_IN}} ;
\]
\[
\text{Moles\_hot} = \text{Moles\_Reformate} ;
\]
\[
\text{Moles\_cold} = \text{Moles\_CombMix} ;
\]

\[
\text{FOR } k := 1 \text{ TO NoComp-5 DO}
\]
\[
\text{FOR } i := 1 \text{ TO NoComp DO}
\]
\[
CP_{\text{comp}}(k,i) = a(i) + b(i) * T_{\text{temperature}}(k)^{(1/4)}
\]
\[
+ c(i) * T_{\text{temperature}}(k)^{(1/2)} + d(i) * T_{\text{temperature}}(k)^{(3/4)} ;
\]
\[
K_{\text{comp}}(k,i) = K_{\text{coef\_A}}(i) + K_{\text{coef\_B}}(i) * T_{\text{temperature}}(k) ;
\]
\[
M_{\text{comp}}(k,i) = M_{\text{coef\_A}}(i) + M_{\text{coef\_B}}(i) * T_{\text{temperature}}(k) ;
\]
\[
\text{END}
\]
\[
CP(k) = \sigma(Y_{\text{mix}}(k,1:\text{NoComp})*CP_{\text{comp}}(k,1:\text{NoComp})) ;
\]
\[
\text{Conductivity}(k) = \sigma(Y_{\text{mix}}(k,1:\text{NoComp})*K_{\text{comp}}(k,1:\text{NoComp})/1000) ;
\]
\[
\text{Viscosity}(k) = \sigma(Y_{\text{mix}}(k,1:\text{NoComp})*M_{\text{comp}}(k,1:\text{NoComp})) ;
\]
\[
\text{END}
\]

# Geometry Calculations

\[
\text{FinTypePRI} = \text{FinChoice.FinType} ;
\]
\[
\text{FinTypePRI} = \text{Colburn.FinType} ;
\]
\[
\text{FrontalArea} = \text{LengthHX*HeightHX} ;
\]
\[
\text{NoPlates} = (\text{HeightHX} - \text{FinChoice.Spacing\_b}(1) - 2*\text{PlateThickness})
\]
\[
/(\text{FinChoice.Spacing\_b}(1) + \text{FinChoice.Spacing\_b}(2) + 2*\text{PlateThickness}) ;
\]
\[
\text{Volume}(1) = \text{LengthHX}(1)*\text{LengthHX}(2)*\text{FinChoice.Spacing\_b}(1)*(\text{NoPlates} + 1) ;
\]
\[
\text{Volume}(2) = \text{LengthHX}(1)*\text{LengthHX}(2)*\text{FinChoice.Spacing\_b}(2)*\text{NoPlates} ;
\]
\[
\text{FinVolume} = \text{LengthHX}(1)*\text{LengthHX}(2)*\text{FinChoice.FinThickness}\text{NoPlates} \times (1 + \text{FinChoice.NoFinL}*(\text{FinChoice.Spacing\_b} - \text{FinChoice.FinThickness})) ;
\]
\[
\text{PlateVolume} = 2*(\text{NoPlates} + 1)*\text{LengthHX}(1)*\text{LengthHX}(2)*\text{PlateThickness} ;
\]
\[
\text{FinMass} = \text{MaterialDensity}\times\text{FinVolume} ;
\]
\[
\text{PlateMass} = \text{MaterialDensity}\times\text{PlateVolume} ;
\]
\[
\text{TotalMass} = \text{FinMass}(1) + \text{FinMass}(2) + \text{PlateMass} ;
\]
\[
\text{HeatTransferArea} = \text{FinChoice.Beta}\times\text{Volume} ;
\]
\[
\text{FreeFlowArea} = \text{FinChoice.Dhydraulic}\times\text{HeatTransferArea} / (4*\text{LengthHX}) ;
\]
\[
m = \sqrt{2\times\text{HTC}/(\text{K}\times\text{FinChoice.FinThickness})} ;
\]
\[
\text{FinLength} = \text{FinChoice.Spacing\_b}/2 - \text{FinChoice.FinThickness} ;
\]
\[
\text{N\_fin} = \text{TANH}(m\times\text{FinLength})/ (m\times\text{FinLength}) ;
\]
\[ N_{overall} = 1 - \text{FinChoice.AreaRatio} \times (1 - N_{fin}) ; \]

# Heat Transfer Calculations for the Compact Plate-Fin Heat Exchanger

\[ \text{MolarFlow}(1) = \text{MolesReformate} ; \]
\[ \text{MolarFlow}(2) = \text{MolesCombMix} ; \]
\[ G = \frac{\text{MolarFlow}}{\text{FreeFlowArea}} ; \]
\[ \text{Reynolds} = G \times \text{FinChoice.Dhydraulic} / \text{Viscosity} ; \]
\[ \text{Colburn.RE} = \log(\text{Reynolds}) ; \]
\[ \text{HTC} = \text{Colburn.FactorJ} \times G \times \text{CP}(\text{Viscosity} \times \text{CP}/\text{Conductivity})^{(-2/3)} ; \]
\[ \text{Cmin} = \min(\text{MolesReformate} \times \text{CP}(1), \text{MolesCombMix} \times \text{CP}(2)) ; \]
\[ \text{Cmax} = \max(\text{MolesReformate} \times \text{CP}(1), \text{MolesCombMix} \times \text{CP}(2)) ; \]
\[ \text{Cratio} = \frac{\text{Cmin}}{\text{Cmax}} ; \]
\[ \text{UA} = \frac{1}{(1/(N_{overall}(1) \times \text{HeatTransferArea}(1) \times \text{HTC}(1)) + 1/(N_{overall}(2) \times \text{HeatTransferArea}(2) \times \text{HTC}(2)))} ; \]

\[ \text{NTU} = \frac{\text{UA}}{\text{Cmin}} ; \]
\[ \text{Effectiveness} = 1 - \exp((1/\text{Cratio}) \times (\text{NTU}^{0.22}) \times (\exp(-\text{Cratio} \times \text{NTU}^{0.78}) - 1)) ; \]
\[ m\text{CP}_\text{HOT} = \text{MolesReformate} \times \text{CP}(1) ; \]
\[ m\text{CP}_\text{COLD} = \text{MolesCombMix} \times \text{CP}(2) ; \]
\[ T_{\text{Hot}_\text{IN}} = T_{\text{reformate}_\text{IN}} ; \]
\[ T_{\text{Hot}_\text{OUT}} = T_{\text{reformate}_\text{OUT}} ; \]
\[ T_{\text{Cold}_\text{OUT}} = T_{\text{combMix}_\text{OUT}} ; \]
\[ T_{\text{Cold}_\text{IN}} = T_{\text{combMix}_\text{IN}} ; \]

FOR \( k:= 1 \) TO \( KK \) DO
FOR \( i:= 1 \) TO \( NN \) DO
\[ \frac{1}{(KK \times NN)} \times \text{TotalMass} \times \text{Cp}_\text{metal} \times ST_{\text{Metal}}(i,k) = Q_{\text{Hot}_\text{Metal}}(i,k) - Q_{\text{Metal}_\text{Cold}}(i,k) ; \]
\[ Q_{\text{Hot}_\text{Metal}}(i,k) = 1/(KK \times NN) \times \text{HTC}(1) \times \text{HeatTransferArea}(1) \times (T_{\text{avg}_\text{Hot}}(i,k) - T_{\text{Metal}}(i,k)) ; \]
\[ Q_{\text{Hot}_\text{Metal}}(i,k) = 1/(NN) \times \text{CP}(1) \times \text{MolarFlow}(1) \times (T_{\text{Hot}_\text{IN}}(i,k) - T_{\text{Hot}_\text{OUT}}(i,k)) ; \]
\[ Q_{\text{Metal}_\text{Cold}}(i,k) = 1/(KK \times NN) \times \text{HTC}(2) \times \text{HeatTransferArea}(2) \times (T_{\text{Metal}}(i,k) - T_{\text{Cold}_\text{Cold}}(i,k)) ; \]
\[ Q_{\text{Metal}_\text{Cold}}(i,k) = 1/(KK) \times \text{CP}(2) \times \text{MolarFlow}(2) \times (T_{\text{Cold}_\text{OUT}}(i,k) - T_{\text{Cold}_\text{IN}}(i,k)) ; \]
\[ T_{\text{Hot}_\text{IN}}(i,k+1) = T_{\text{Hot}_\text{OUT}}(i,k) ; \]
\[ T_{\text{Cold}_\text{IN}}(i+1,k) = T_{\text{Cold}_\text{OUT}}(i,k) ; \]
\[ T_{\text{avg}_\text{Hot}}(i,k) = (T_{\text{Hot}_\text{IN}}(i,k) + T_{\text{Hot}_\text{OUT}}(i,k)) / 2 ; \]
\[ T_{\text{avg}_\text{Cold}}(i,k) = (T_{\text{Cold}_\text{IN}}(i,k) + T_{\text{Cold}_\text{OUT}}(i,k)) / 2 ; \]
END
END

\[ T_{\text{reformate}_\text{OUT}} = \Sigma(T_{\text{Hot}_\text{OUT}}(i,KK+1)) / (NN) ; \]
# hot stream
\[ T_{\text{combMix}_\text{OUT}} = \Sigma(T_{\text{Cold}_\text{OUT}}(NN+1,i)) / (KK) ; \]
# cold stream

\section*{B.6 Modeling the Reformer Mixer}

\# ==============================================================
\# Model of the Reformer Mixer
\# ==============================================================

\textbf{PARAMETER}
\[
\begin{align*}
\text{NoComp} & \quad \text{AS INTEGER} \\
\text{Tstandard} & \quad \text{AS REAL} \\
a, b, c, d & \quad \text{AS ARRAY (NoComp) OF REAL} \\
\text{Hformation} & \quad \text{AS ARRAY (NoComp) OF REAL}
\end{align*}
\]

\textbf{VARIABLE}
\[
\begin{align*}
\text{FlowComp}_3 & \quad \text{AS ARRAY (NoComp) OF General}
\end{align*}
\]
Y_2, Y_1, Y_3 AS ARRAY (NoComp) OF General
FlowRate_2, FlowRate_1, FlowRate_3 AS General
EnthalpyMix_2, EnthalpyMix_1, EnthalpyMix_3 AS General
Temp_3 AS General
Ho AS ARRAY (NoComp) OF General
Hcomp_3, HcompTotal_3 AS ARRAY (NoComp) OF General

SET
NoComp := 7;
Tstandard := 273.15 + 25;
a := [104.0, 180.0, 62.8, -55.6, 79.5, 10.3, 72.0];
b := [-77.8, -85.4, -22.6, 30.5, -26.3, 5.4, -26.9];
c := [20.1, 15.6, 4.6, -1.96, 4.23, -0.18, 5.19];
d := [-1.3, -0.858, -0.272, 0.0, -0.197, 0.0, -0.298];
Hformation := [-74900, -242000, -110600, -393800, 0.0, 0.0, 0.0]; # KJ/Kmol

EQUATION
# Specification of the component mole fractions at the mixer exit
FOR i:=1 TO 7 Do
  FlowComp_3(i) = FlowRate_1*Y_1(i) + FlowRate_2*Y_2(i); # MolesREF are the ones that comes from the reformer
END
FlowRate_3 = SIGMA(FlowComp_3);
Y_3 = FlowComp_3 / FlowRate_3;
# Energy balance on the Combustion Mixer
FlowRate_2*EnthalpyMix_2 + FlowRate_1*EnthalpyMix_1 - FlowRate_3*EnthalpyMix_3 = 0;
Ho = a*Tstandard + (4/5)*b*Tstandard^(5/4) + (2/3)*c*Tstandard^(3/2) +
    (4/7)*d*Tstandard^(7/4);
FOR i := 1 TO NoComp DO
  Hcomp_3(i) = a(i)*Temp_3 + (4/5)*b(i)*Temp_3^(5/4) +
              (2/3)*c(i)*Temp_3^(3/2) + (4/7)*d(i)*Temp_3^(7/4);
  HcompTotal_3(i) = Hformation(i) + Hcomp_3(i) - Ho(i);
END
EnthalpyMix_3 = sigma(Y_3(1:NoComp)*HcompTotal_3(1:NoComp));

B.7 Modeling the Combustion Mixer
# =======================================================================
#                       Model of the Combustion Mixer
# =======================================================================
PARAMETER
NoComp AS INTEGER
UtilizationH2 AS REAL
Tstandard AS REAL
a, b, c, d AS ARRAY (NoComp) OF REAL
Hformation AS ARRAY (NoComp) OF REAL

UNIT
CH4_new AS CpEvaluator_1
Anode AS CpEvaluator_1
Air AS CpEvaluator_1

5/6/2006
VARIABLE
AirToFuelRatio AS General
FlowRate_CH4_new, FlowRate_Air, FlowRate_Anode AS General
EnthalpyMix_CH4_new, EnthalpyMix_Air, EnthalpyMix_Anode AS General
Ho AS ARRAY (NoComp) OF General
Y_CH4_new AS ARRAY (NoComp) OF General
Y_Anode AS ARRAY (NoComp) OF General
Y_Air AS ARRAY (NoComp) OF General
Y_burner AS ARRAY (NoComp) OF General
FlowRate_Burner AS General
FlowComp_Burner AS ARRAY (NoComp) OF General
Temp_Burner AS General
Temp_Burner_1 AS General
T_CH4_new AS General
T_Anode AS General
T_Air AS General
Cp_CH4_new AS General
Cp_Anode AS General
Cp_Air AS General
Cp_burner AS General

SET
NoComp := 7;
Tstandard := 273.15 + 25;
a := [104.0, 180.0, 62.8, -55.6, 79.5, 10.3, 72.0];
b := [-77.8, -85.4, -22.6, 30.5, -26.3, 5.4, -26.9];
c := [20.1, 15.6, 4.6, -1.96, 4.23, -0.18, 5.19];
d := [-1.3, -0.858, -0.272, 0.0, -0.197, 0.0, -0.298];
Hformation := [-74900, -242000, -110600, -393800, 0.0, 0.0, 0.0]; # KJ/Kmol
UtilizationH2 := 0.85;

EQUATION
# Specification of the component mole fractions at the exit of the Combustion Mixer
AirToFuelRatio = 4;
FOR i:=1 TO 7 Do
  FlowComp_Burner(i) = FlowRate_CH4_new*Y_CH4_new(i) + FlowRate_Anode*Y_Anode(i) + FlowRate_Air*Y_Air(i);
END
FlowRate_Burner = SIGMA(FlowComp_Burner);
Y_Burner = FlowComp_Burner / FlowRate_Burner;

# Energy balance on the Combustion Mixer
CH4_new.Temperature = T_CH4_new;
CH4_new.Ycomp = Y_CH4_new;
Anode.Temperature = T_Anode;
Anode.Ycomp = Y_Anode;
Air.Temperature = T_Air;
Air.Ycomp = Y_Air;
Cp_CH4_new = CH4_new.CP;
Cp_Anode = Anode.CP;
Cp_Air = Air.CP;
Cp_burner = (Cp_CH4_new*FlowRate_CH4_new+Cp_Anode*FlowRate_Anode+
Cp_Air*FlowRate_Air)/(FlowRate_Burner);

### This is a great approximation which introduces little error ans speeds up the # code

FlowRate_CH4_new*Cp_CH4_new*T_CH4_new + FlowRate_Anode*Cp_Anode*T_Anode + FlowRate_Air*Cp_Air*T_Air - FlowRate_Burner*Cp_burner*Temp_Burner = 0;

Temp_Burner_1 = Temp_Burner;
Ho = a*Tstandard + (4/5)*b*Tstandard^(5/4) + (2/3)*c*Tstandard^(3/2) + (4/7)*d*Tstandard^(7/4);

## B.8 Modeling the Combustion Chamber

# Model of the Combustion Chamber
# - Combustion reactions taking place inside the combustion chamber
# - CH4 + 2 O2 --> CO2 + 2 H2O
# - H2 + 1/2 O2 --> H2O
# - Total Reaction
# - CH4 + H2 + 5/2 O2 --> CO2 + 3H2O
# - CH4 + H2 + CO + 3 O2 --> 2 CO2 + 3H20
#
# - Assumptions
#  i) Steady State Conditions
#  ii) Complete Combustion (all carbon and hydrogen converted)
#  iii) Adiabatic reactor
#  StoiCoeff_BURNER := [-1, 3, 0, 1, -1, -2.5, 0];
#  CH4 + 2 O2 --> CO2 + 2 H2O
#  H2 + 1/2 O2 --> H2O
#
# ==============================================================================  

PARAMETER
NoComp AS INTEGER
StoiCoeff_BURNER AS ARRAY(NoComp) OF REAL
Pambient AS REAL
P_reactor AS REAL
Tstandard AS REAL
a, b, c, d AS ARRAY (NoComp) OF REAL
Hformation AS ARRAY (NoComp) OF REAL

VARIABLE
FlowRate_out, FlowRate_in AS General
EnthalpyMix_out, EnthalpyMix_in AS General
F_BURNER_out AS ARRAY (NoComp) OF General
Y_BURNER_out, Y_BURNER_in AS ARRAY (NoComp) OF General
Ho, Hcomp, HcompTotal AS ARRAY (NoComp) OF General
T_design_Burner AS General
MolesCombMixer AS ARRAY (NoComp) OF General

SET
NoComp := 7;
StoiCoeff_BURNER := [-.1, .3, -.1, .2, -.1, -.3, .0];
Pambient := 101325;
P_reactor := 300000;
Tstandard := 273.15 + 25;
a := [104.0, 180.0, 62.8, -55.6, 79.5, 10.3, 72.0];
b := [-77.8, -85.4, -22.6, 30.5, -26.3, 5.4, -26.9];
c := [20.1, 15.6, 4.6, -1.96, 4.23, -0.18, 5.19];
d := [-1.3, -0.858, -0.272, 0.0, -0.197, 0.0, -0.298];
Hformation := [-74900, -242000, -110600, -393800, 0.0, 0.0, 0.0]; # KJ/ Kmol

EQUATION
# Energy balance on the Burner
FlowRate_out*EnthalpyMix_out - 0.98*FlowRate_in*EnthalpyMix_in = 0;
# Specifications of the constituents' moles at the exit of the burner
#Calculation of the flow rate at the outlet of BURNER
MolesCombMixer = FlowRate_in * Y_BURNER_in;
# Specifications of the constituents' moles at the exit of the burner
#       CH4 +  2   O2   -->  CO2 + 2 H2O
#       H2  +  1/2 O2   -->  H2O
#       CO + 1/2 O2    -->  CO2
#       CH4 + H2 + CO + 3 O2  -->  2 CO2 + 3H2O
F_BURNER_out(1) = 0;
F_BURNER_out(2) = MolesCombMixer(2) + 2*MolesCombMixer(1) + MolesCombMixer(5);
F_BURNER_out(3) = 0;
F_BURNER_out(4) = MolesCombMixer(4) + MolesCombMixer(1) + MolesCombMixer(3);
F_BURNER_out(5) = 0;
F_BURNER_out(6) = MolesCombMixer(6) - 2*MolesCombMixer(1) - 0.5*MolesCombMixer(5)- 0.5*MolesCombMixer(3);
F_BURNER_out(7) = MolesCombMixer(7);
FlowRate_out = FlowRate_in*(1-0.5*Y_BURNER_in(3)-0.5*Y_BURNER_in(5));
Y_BURNER_out(1) = 0;
Y_BURNER_out(2) = FlowRate_in/FlowRate_out*(Y_BURNER_in(2)+2*Y_BURNER_in(1)+Y_BURNER_in(5));
Y_BURNER_out(3) = 0;
Y_BURNER_out(4) = FlowRate_in/FlowRate_out*(Y_BURNER_in(4)+Y_BURNER_in(3)+Y_BURNER_in(1));
Y_BURNER_out(5) = 0;
Y_BURNER_out(6) = FlowRate_in/FlowRate_out*(Y_BURNER_in(6)+Y_BURNER_in(3)-2*Y_BURNER_in(1)-0.5*Y_BURNER_in(5));
Y_BURNER_out(7) = FlowRate_in/FlowRate_out*Y_BURNER_in(7);
Ho  =  a*Tstandard + (4/5)*b*Tstandard^(5/4) + (2/3)*c*Tstandard^(3/2) +
(4/7)*d*Tstandard^(7/4);
FOR i := 1 TO 7 DO
Hcomp(i) = a(i)*abs(T_design_BURNER) +(4/5)*b(i)*abs(T_design_BURNER)^5/4
+ (2/3)*c(i)*abs(T_design_BURNER)^3/2
+ (4/7)*d(i)*abs(T_design_BURNER)^7/4;
END
HcompTotal(i) = Hformation(i) + Hcomp(i) - Ho(i);
END
EnthalpyMix_out = sigma(Y_BURNER_out(1:7)*HcompTotal(1:7));
B.9 Modeling the Compound Alternator

#PARAMETER

UNIT
map as comp_new_map
mot as motor
turb as turbine_alt
tank as Air_Tank

# UnitName AS UnitModelName

VARIABLE
P1,P2,P2_P1,P1s,P2s,Pamb,P2s_P1s as general
M1,M2,M as general
T1,Tm,T2,Tamb,Tavg as general
eff as general
cp_m,cp_air,cp_O2,cp_N2 as general
HA_1,HA_0 as general
N,Ncorr,R,Fm,gamma as general
V,Area_in,Area_surf1,D_in,Pi,L as general
Nusselt,Re,Pr as general
h_in,rho,vel as general
K_O2,K_N2,K as general
mu_O2,mu_N2,mu as general
power,P_rat,head as general
D_out,Area_surf2 as general
V_m as general
diff as general

Kv as general
Kb as general
Ka as general
e as general
P_tank_ref as general
m_ref as general
EE as general
volt as general
Pro as general
Pro_int as general
Bias as general
Wk_comp as general

minimum_output as general
maximum_output as general
Assintotic as general
volt_1 as general
volt_2 as general
dswitch as general
M_tur as general
M_mixer as general
scale_factor as general

SELECTOR

EQUATION
P1s = P2s/P2s_P1s;
#P2s = 3;
P2 = P2s;
P2s_P1s = P2s/1;
#P2_P1 = 2;
\[ P2_P1 = \frac{P2}{P1}; \]
\[ \text{Tamb} = 298; \]
\[ T1 = \text{Tamb}; \]
\[ Tavg = \frac{(T1+T2)}{2}; \]
\[ \text{Pamb} = 1; \]
\[ \text{gamma} = 1.4; \]
\[ R = 0.2998; \]
\[ M1*\sqrt{T1}/P1 = \text{map.xact}*\text{scale_factor}; \]
\[ \text{map.speed} = \text{Ncorr}; \]
\[ \text{Ncorr} = \frac{N}{\sqrt{T1}}; \]
\[ \text{map.yact} = P2_P1; \]
\[ \text{eff} = \text{map.eff}; \]
\[ \Pi = 3.141592; \]
\[ \text{Area.in} = \pi*D_in^2/4*2; \]
\[ \text{Area.surf1} = \pi*D_in*L*2; \]
\[ \text{Area.surf2} = \pi*D_out*L*2; \]
\[ L = 0.0975; \]
\[ D_in = 0.0975/2; \]
\[ D_out = 0.12/2; \]
\[ V_m = \pi*(D_out-D_in)^2*L/4; \]
\[ V = \pi*D_in^2*L/4; \]
\[ F_m = 1.4; \]
\[ HA_0 = 0.16457*\text{Area.surf2}; \]
\[ HA_1 = H_in*\text{Area.surf1}; \]
\[ M = 7850*V_m; \]
\[ T2 = \left( T1 \cdot (1-HA_1/(2*M2*cp_air)+1/eff*((P2_P1)^((gamma-1)/gamma)-1)) + HA_1*Tm/(M2*cp_air) \right) / (1+HA_1/(2*M2*cp_air)); \]
\[ \text{power} = M2*cp_air*T1/eff*((P2_P1)^((gamma-1)/gamma)-1); \]
\[ \text{Wk_comp} = M2/29*31* T1/eff*(P2_P1^((\gamma - 1)/ \gamma) - 1); \]
\[ 0 = \text{Area.in}/L*((P2-P1)-(P2s-P1s)); \]
\[ 0 = R*T2/V \cdot (M2-M1) \cdot \text{Fm}; \]
\[ M*cp_m*$Tm = HA_1*(T1+T2)/2-Tm)-HA_0*(Tm-Tamb); \]
\[ \text{diff} = M2-M1; \]
\[ \text{Nusselt} = h_in *D_in/K; \]
\[ \text{Re} = \rho * V * D_in/mu; \]
\[ \text{Pr} = cp_air * mu/K; \]
\[ cp_02 = (29.342+(-3.5395)*10^(-3)*Tavg+(1.0076)*10^(-5)*Tavg^2+(-4.3116)*10^(-9)*Tavg^3+2.5935*10^(-13)*Tavg^4); \]
\[ cp_n2 = (29.342+(-8.8999)*10^(-3)*Tavg+3.8083*10^(-5)*Tavg^2+(-3.2629)*10^(-8)*Tavg^3+8.8607*10^(-12)*Tavg^4); \]
\[ K_02 = 0.00121+8.6157*10^(-5)*Tavg-1.3346*10^(-8)*Tavg^2; \]
\[ K_n2 = 0.00309+7.5930*10^(-5)*Tavg-1.1014*10^(-8)*Tavg^2; \]
\[ mu_02 = 44.224+5.62*10^(-1)*Tavg-1.13*10^(-4)*Tavg^2; \]
\[ mu_n2 = 42.606+4.75*10^(-1)*Tavg-9.88*10^(-5)*Tavg^2; \]
\[ \text{mu_air} = (0.79*cp_n2+0.21*cp_02)/28.96; \]
\[ K = 6.906*10^(-4); \]
\[ \text{mu} = 1.827*10^(-5); \]
\[ \text{vel} = (M2+M1)/2/rho/area_in; \]
\[ \text{rho} = P1*100/R/T2; \]
\[ \text{head} = R*T1*gamma/(gamma-1))*(P_rat^(gamma/(gamma-1))-1); \]
\[ P_rat = 3.2; \]
N = mot.speed1;
turb.N = mot.speed1;

$M_tur = -1*M_tur + 1*M_mixer;
turb.e_1 = M_tur - turb.M1;

if power > turb.power then
  mot.pow_1 = (power-turb.power)*1000;
else
  mot.pow_1 = 0;
end

Tank.F_Compressor = m2/29; #check this out
Tank.T_in = T2;

Assintotic = 1;
$EE = 0;
volt_1 = volt_2;
$volt_2 = -5*volt_2 + 5*volt;

{ CASE Assint OF
  WHEN Low_bound:
    Assintotic = 1;
    SWITCH TO High_bound IF (volt > (minimum_output));
  WHEN High_bound:
    Assintotic = maximum_output + dswitch;
    SWITCH TO Low_bound IF (volt < (minimum_output));
END

CASE StopIntegrator_1 OF
  WHEN inactive_1:
    $EE = E;
volt_1 = volt_2;
$volt_2 = -5*volt_2 + 5*volt;

    SWITCH TO active_1 IF ((volt < (minimum_output - dswitch)) OR
                             (volt > (maximum_output + dswitch)));
  WHEN active_1:
    $EE = 0;
volt_1 = volt_2;
$volt_2 = -5*volt_2 + 5*Assintotic;

    SWITCH TO inactive_1 IF ((volt > minimum_output) AND
                              (volt < maximum_output));
END #CASE
}
dswitch = 1;
C. PLANAR SOFC MODELING

C.1 One Dimensional Model

function [Power, Anode_Comp, Anode_Flow, Cathode_Comp, Cathode_Flow, Vout, FU, T, h, current_density, Qout] = fcn(constants, inputs, time)
% This block supports an embeddable subset of the MATLAB language.
% See the help menu for details.

% define variables in constants and inputs streams

length_local = (constants(1));
width = (constants(2));
cells = (constants(3));
stacks = (constants(4));
total_cells = cells*stacks;
nsteps = 25;
Air_Flowin = (inputs(1))/total_cells; % mol/s for individual cell
Fuel_Flowin = (inputs(2))/total_cells; % mol/s for individual cell
Air_Temp = (inputs(3)); % CH4, H2O, CO, CO2, H2, O2, N2 (everything but O2 and N2 == 0)
Fuel_Temp = (inputs(4)); % CH4, H2O, CO, CO2, H2, O2, N2 (O2 and N2 == 0)
nO2in = (inputs(10))*Air_Flowin;
nN2in = (inputs(11))*Air_Flowin;
nCH4in = (inputs(12))*Fuel_Flowin;
nH2Oin = (inputs(13))*Fuel_Flowin;
nCOin = (inputs(14))*Fuel_Flowin;
nCO2in = (inputs(15))*Fuel_Flowin;
nH2in = (inputs(16))*Fuel_Flowin;
nN2inert = (inputs(18))*Fuel_Flowin; % mol/s
Iin = (inputs(19))/stacks;
Tinf = (inputs(20));
sim_time = time;

% misc. variables/values

To = ((Air_Temp*Air_Flowin)+(Fuel_Temp*Fuel_Flowin))/(Air_Flowin+Fuel_Flowin);
k = (1.534E-02*To + 8.968)*0.5*1.1; % W/m-K, assumes porosity of 0.55
Cp = 1.854E-01*To + 4.251E+02; % J/kg-K
rho = 4083*1.1; % kg/m^3, assumes porosity of 0.55
nsteps = 25; % if this is changed, the output dimensions for this function m
thick = .00194936;
mair = Air_Flowin*(inputs(10)*32+inputs(11)*28)/1000; % mass flow air kg/s
mfuel = Fuel_Flowin*(inputs(12)*16+inputs(13)*18+inputs(14)*28+inputs(15)*44+inputs(16)*2)/1000; % mass flow fuel kg/s
Cpair = 1160; % J/kg-K specific heat of air stream
Cpfuel = 2600; % J/kg-K specific heat of fuel stream
sim_time = time;
%===============================================================================
% The first step is to determine the maximum allowable dt for stability
% If the current simulation time is less than dt since the last time evaluated
% it will be used for calculations. Otherwise, the time interval will be
% broken into smaller parts as dictated by max dt for stability.
%===============================================================================
max_dt = 0.5*Cp*rho*(length_local/nsteps)^2/k;

persistent tprev % time of previous successful simulation
if isempty (tprev)
tprev = 0;
dt = 0;
elseif ((sim_time-tprev) > max_dt)
dt = ((sim_time-tprev))/(round(((sim_time-tprev)/max_dt)+.5));
elseif ((sim_time-tprev)> 0)
dt = (sim_time-tprev);
else
dt = 0;
end

t_tracker = tprev+dt;

I = Iin;
stepsize = length_local/nsteps;
h = stepsize;
alpha = k*dt/(rho*Cp*stepsize^2);
V = thick*width*stepszie;

U = 10; %W/m^2-K heat coefficient to account for heat losses at the stack ends

persistent Q %from Sanjaya's model
persistent A
persistent Ti
persistent dHo
persistent nO2i
persistent nN2i
persistent nCH4i
persistent nH2Oi
persistent nCOi
persistent nCO2i
persistent nH2i
persistent pO2
persistent pCH4
persistent pCO
persistent pH2
persistent dH
persistent Etn
persistent dGo
persistent dG
persistent En
persistent ASR
persistent beta
persistent Vopn
persistent j
persistent dGoshift
persistent Kp
persistent t5
persistent t6
persistent t8
persistent t17
persistent t26
persistent t27
persistent t29
persistent t36
persistent x
persistent Hshift
%declaration of variable dimensions
if isempty(Ti)
Q = zeros(nsteps,1); %from Sanjaya's model
A = eye(nsteps);
Ti = zeros(nsteps,1);
dHo = zeros(nsteps,1);
nO2i = zeros(nsteps,1);
nN2i = zeros(nsteps,1);
nCH4i = zeros(nsteps,1);
nH2Oi = zeros(nsteps,1);
nCOi = zeros(nsteps,1);
nCO2i = zeros(nsteps,1);
nH2i = zeros(nsteps,1);
pO2 = zeros(nsteps,1);
pCH4 = zeros(nsteps,1);
pCO = zeros(nsteps,1);
pH2 = zeros(nsteps,1);
dH = zeros(nsteps,1);
Etn = zeros(nsteps,1);
dGo = zeros(nsteps,1);
dG = zeros(nsteps,1);
En = zeros(nsteps,1);
ASR = zeros(nsteps,1);
beta = zeros(nsteps,1);
Vopn = 0;
j = zeros(nsteps,1);
dGoshift = zeros(nsteps,1);
Kp = zeros(nsteps,1);
t5 = zeros(nsteps,1);
t6 = zeros(nsteps,1);
t8 = zeros(nsteps,1);
t17 = zeros(nsteps,1);
t26 = zeros(nsteps,1);
t27 = zeros(nsteps,1);
t29 = zeros(nsteps,1);
t36 = zeros(nsteps,1);
x = zeros(nsteps,1);
Hshift = zeros(nsteps,1);

%Declaration of initial conditions
for n=1:nsteps
    Ti(n,1) = To;
    nO2i(n,1) = nO2in;
    nN2i(n,1) = nN2in;
    nCH4i(n,1) = nCH4in;
    nH2Oi(n,1) = nH2Oin;
    nCOi(n,1) = nCOin;
    nCO2i(n,1) = nCO2in;
    nH2i(n,1) = nH2in;
end

%This is the case where t=0 and the initial values will be returned for everthing
%This will also return the OCV for the stack voltage since current is assumed to be 0.
for n=1:nsteps
    j(n,1) = 0; %set to zero because I(t=0) = 0
    %shift equilibrium calculations
    dGoshift(n,1) = -39.381e3+40.81*Ti(n,1)-4.5e-3*Ti(n,1)^2;
    Kp(n,1) = exp(-dGoshift(n,1)/(8.314*Ti(n,1)));
    Hshift(n,1) = -(47.1e3-22.8*Ti(n,1)+7.63e-3*Ti(n,1)^2);
    t5(n,1) = Kp(n,1)^2;
    t6(n,1) = nCOi(n,1)^2;
    t8(n,1) = nCOi(n,1)*nH2Oi(n,1);
    t17(n,1) = nH2Oi(n,1)^2;
    t26(n,1) = nCO2i(n,1)^2;
    t27(n,1) = nCO2i(n,1)*nH2i(n,1);
    t29(n,1) = nH2i(n,1)^2;
    t36(n,1) = sqrt(t5(n,1)*t6(n,1)-2*t5(n,1)*t8(n,1)+2*Kp(n,1)*nCOi(n,1)*nCO2i(n,1)...
 +2*Kp(n,1)*nCOi(n,1)*nH2i(n,1)+t5(n,1)*t17(n,1)+2*Kp(n,1)*nH2Oi(n,1)*nCO2i(n,1)...

5/6/2006 224
\[ +2K_p(n,1) \cdot nH_2O_i(n,1) \cdot nH_2i(n,1) + t_{26}(n,1) - 2t_{27}(n,1) + t_{29}(n,1) + 4K_p(n,1) \cdot t_{27}(n,1) \ldots \\
+4K_p(n,1) \cdot t_{28}(n,1); \]
\[ x(n,1) = \frac{1}{(K_p(n,1) - 1) \cdot nCO_i(n,1)}; \]
\[ nH_2i(n,1) = nH_2i(n,1) + x(n,1); \]
\[ nCO_i(n,1) = nCO_i(n,1) - x(n,1); \]
\[ nCO2i(n,1) = nCO2i(n,1) + x(n,1); \]
\[ nH2Oi(n,1) = nH2Oi(n,1) - x(n,1); \]
\[ nH_2O(n,1) = \frac{1}{(K_p(n,1) - 1)^2} \cdot \left( K_p(n,1) \cdot nCO_i(n,1) + K_p(n,1) \cdot nH_2O_i(n,1) + nCO2i(n,1) + nH_2i(n,1) - t_{36}(n,1) \right) / 2; \]
\[ \text{% adjust compositions to equilibrium as well as temperature} \]
\[ nH_2i(n,1) = nH_2i(n,1) + x(n,1); \]
\[ nCO_i(n,1) = nCO_i(n,1) - x(n,1); \]
\[ nCO2i(n,1) = nCO2i(n,1) + x(n,1); \]
\[ nH2Oi(n,1) = nH2Oi(n,1) - x(n,1); \]
\[ dH(n,1) = \left( -235.36 - 0.026522 \cdot T_i(n,1) + 0.000012144 \cdot T_i(n,1) \cdot T_i(n,1) / 2 \right) \cdot 1000; \text{ % for H2} \]
\[ pO_2(n,1) = (nO_2i(n,1) / (nO_2i(n,1) + nN_2i(n,1))); \]
\[ E_{t,n}(n,1) = -\frac{dH(n,1)}{2 \cdot 96485}; \]
\[ dG(n,1) = \left( -241 + 3.52e-2 \cdot T_i(n,1) + 1.97e-5 \cdot T_i(n,1) \cdot T_i(n,1) / 2 - 8.28e-9 \cdot T_i(n,1) \cdot T_i(n,1) / 3 + 1.39e-12 \cdot T_i(n,1) \cdot T_i(n,1) / 4 \right) \cdot 1000; \]
\[ dG(n,1) = dG(n,1) + 8.314 \cdot T_i(n,1) \cdot \log(nH_2O_i(n,1) / (nH_2i(n,1) / \sqrt{pO_2(n,1)})); \]
\[ E_{n,n}(n,1) = -\frac{dG(n,1)}{2 \cdot 96485}; \]
\[ ASR(n,1) = (8.39355e-4 \cdot \exp(8032.32 / \left( T_i(n,1) \right))) / \left( 100^2 \right); \text{ % Temp dependent, experimental fitted data} \]
\[ ASR(n,1) = (1.5261e-5 \cdot \exp((11156) / \left( T_i(n,1) \right))) / \left( 100^2 \right); \text{ % Temp dependent, Based on Ceramatec data} \]
\end{verbatim}

\% Return initial condition outputs
\begin{verbatim}
\end{verbatim}

\begin{verbatim}
\text{% resolve for Vopn (secant method)}
\text{flag = 0;}
\text{Vopmax = En(round(nsteps/2),1);}
\text{Vopmin = 0;}
\text{Imin = 0;}
\text{Imax = 0;}
\text{for n = 1:1:nsteps}
\text{Imax = Imax + width*En(n,1)/ASR(n,1);}
\text{end}
\text{slope = -(Vopmax-Vopmin)/(Imax-Imin);}
\text{Vopn = slope*(Iin - Imin) + Vopmax;}
\text{while flag == 0}
\text{Io = 0;}
\text{for n = 1:1:nsteps}
\text{Io = Io + width*(En(n,1)-Vopn)/(ASR(n,1));}
\text{end}
\text{if Iin == 0}
\text{Vopn = En(1,1);}
\text{flag = 1;}
\text{elseif(I - Io) > 0.001}
\text{Vopmax = Vopn;}
\text{Vopmin = Vopn;}
\text{Imax = Io;}
\end{verbatim}
elseif (I - Io) < -0.001
    Vopmin = Vopn;
    Imax = Io;
else
    flag = 1;
end
slope = -(Vopmax-Vopmin)/(Imax-Imin);
Vopn = slope*(Iin - Imin) + Vopmax;
end

% return unchanged anode and cathode streams
Anode_Flow = (nCH4i(nsteps,1) + nH2Oi(nsteps,1) + nCOi(nsteps,1) + nCO2i(nsteps,1) + nH2i(nsteps,1) + nN2inert)*total_cells;
xCH4 = (nCH4i(nsteps,1)*total_cells)/Anode_Flow;
xH2O = (nH2Oi(nsteps,1)*total_cells)/Anode_Flow;
xCO = (nCOi(nsteps,1)*total_cells)/Anode_Flow;
xCO2 = (nCO2i(nsteps,1)*total_cells)/Anode_Flow;
xH2 = (nH2i(nsteps,1)*total_cells)/Anode_Flow;
xN2inert = (nN2inert*total_cells)/Anode_Flow;
Anode_Comp = [xCH4;xH2O;xCO;xCO2;xH2;0;xN2inert];

Cathode_Flow = (nO2i(nsteps,1) + nN2i(nsteps,1))*total_cells;
xO2 = (nO2i(nsteps,1)*total_cells)/Cathode_Flow;
xN2 = (nN2i(nsteps,1)*total_cells)/Cathode_Flow;
Cathode_Comp = [0;0;0;0;0;xO2;xN2];
else
    % calculate component data from final value of Vop from last time step
    for n = 1:nsteps
        if Iin == 0
            j(n,1) = 0;
        else
            j(n,1) = (En(n,1)-Vopn)/ASR(n,1);
        end
        if n == 1
            nH2Oi(n,1) = nH2Oin + j(n,1)*stepsize*width/(2*96485);
            nH2i(n,1) = nH2in - j(n,1)*stepsize*width/(2*96485);
            nO2i(n,1) = nO2in - (1/2)*j(n,1)*stepsize*width/(2*96485);
            pO2(n,1) = nO2i(n,1)/(nO2i(n,1)+nN2i(n,1));
        else
            nH2Oi(n,1) = nH2Oi(n-1,1) + j(n,1)*stepsize*width/(2*96485);
            nH2i(n,1) = nH2i(n-1,1) - j(n,1)*stepsize*width/(2*96485);
            nO2i(n,1) = nO2i(n-1,1) - (1/2)*j(n,1)*stepsize*width/(2*96485);
            pO2(n,1) = nO2i(n,1)/(nO2i(n,1)+nN2i(n,1));
        end
    end
    % shift reaction
    dGoshift(n,1) = -39.381e3+40.81*Ti(n,1)-4.5e-3*Ti(n,1)^2;
    Kp(n,1) = exp(-dGoshift(n,1)/(8.314*Ti(n,1)));
    t5(n,1) = Kp(n,1)^2;
    t6(n,1) = nCOi(n,1)^2;
    t8(n,1) = nCOi(n,1)*nH2o1i(n,1);
    t17(n,1) = nH2o1i(n,1)^2;
    t26(n,1) = nCO2i(n,1)^2;
    t27(n,1) = nCO2i(n,1)*nH2i(n,1);
    t29(n,1) = nH2i(n,1)^2;
    t36(n,1) = sqrt(t5(n,1)*t6(n,1)-
        2*t5(n,1)*t8(n,1)+2*Kp(n,1)*nCOi(n,1)*nCO2i(n,1))... +2*Kp(n,1)*nCOi(n,1)*nH2i(n,1)+t5(n,1)*t17(n,1)+2*Kp(n,1)*nH2o1i(n,1)*nCO2i(n,1)... +2*Kp(n,1)*nH2o1i(n,1)*nH2i(n,1)+t26(n,1)-
    2*t27(n,1)+t29(n,1)+4*Kp(n,1)*t27(n,1)... +4*Kp(n,1)*t8(n,1));
\(x(n,1) = 1/(Kp(n,1)-1)\times(Kp(n,1)*nCOi(n,1)+Kp(n,1)*nH2Oi(n,1)+nCO2i(n,1)+nH2i(n,1)-t36(n,1))/2;\)

%adjust compositions to equilibrium
\[nH2i(n,1) = nH2i(n,1) + x(n,1);\]
\[nCOi(n,1) = nCOi(n,1) - x(n,1);\]
\[nCO2i(n,1) = nCO2i(n,1) + x(n,1);\]
\[nH2Oi(n,1) = nH2Oi(n,1) - x(n,1);\]
\[nH2O(n,1) = nH2O(n,1) - x(n,1);\]

end

%Write out component data from last successful time step
Anode_Flow = (nCH4i(nsteps,1) + nH2Oi(nsteps,1) + nCOi(nsteps,1) + nCO2i(nsteps,1) + nH2i(nsteps,1) + nN2inert)*total_cells;
\[xCH4 = (nCH4i(nsteps,1)*total_cells)/Anode_Flow;\]
\[xH2O = (nH2Oi(nsteps,1)*total_cells)/Anode_Flow;\]
\[xCO = (nCOi(nsteps,1)*total_cells)/Anode_Flow;\]
\[xCO2 = (nCO2i(nsteps,1)*total_cells)/Anode_Flow;\]
\[xH2 = (nH2i(nsteps,1)*total_cells)/Anode_Flow;\]
\[xN2inert = (nN2inert*total_cells)/Anode_Flow;\]
Anode_Comp = [xCH4; xH2O; xCO; xCO2; xH2; 0; 0];

Cathode_Flow = (nO2i(nsteps,1) + nN2i(nsteps,1))*total_cells;
\[xO2 = (nO2i(nsteps,1)*total_cells)/Cathode_Flow;\]
\[xN2 = (nN2i(nsteps,1)*total_cells)/Cathode_Flow;\]
Cathode_Comp = [0; 0; 0; 0; xO2; xN2];
while (t_tracker <= sim_time)

%set up solution matrix
for n = 1:nsteps
if (n == 1)
\[A(n,n) = (1-alpha) - mair*Cpair*dt/(rho*V*Cp) - mfuel*Cpfuel*dt/(rho*V*Cp);\]
\[A(n, n+1) = (alpha);\]
\[beta(n,1) = mair*Cpair*Air_Temp*dt/(rho*V*Cp) + mfuel*Cpfuel*Fuel_Temp*dt/(rho*V*Cp)...-Hshift(n,1)*x(n,1)*dt/(V*rho*Cp) - U*stepsize*width*(Ti(n,1)-(Tinf))*dt/(V*rho*Cp);\]
elseif (n == nsteps)
\[A(n, n-1) = (alpha) + mair*Cpair*dt/(rho*V*Cp) + mfuel*Cpfuel*dt/(rho*V*Cp);\]
\[A(n, n) = (1-2*alpha) - mair*Cpair*dt/(rho*V*Cp) - mfuel*Cpfuel*dt/(rho*V*Cp);\]
\[beta(n,1) = -(5.67051e-8*0.8)*dt/(rho*stepsize*Cp)*(Ti(n,1)^4-(Tinf)^4)...-Hshift(n,1)*x(n,1)*dt/(V*rho*Cp) - U*stepsize*width*(Ti(n,1)-(Tinf))*dt/(V*rho*Cp);\]
else
\[Q(n,1) = (Etn(n,1)-En(n,1)+j(n,1)*ASR(n,1));%from Sanjaya's model(heat rate)\]
\[A(n, n-1) = (alpha) + mair*Cpair*dt/(rho*V*Cp) + mfuel*Cpfuel*dt/(rho*V*Cp);\]
\[A(n, n) = (1-2*alpha) - mair*Cpair*dt/(rho*V*Cp) - mfuel*Cpfuel*dt/(rho*V*Cp);\]
\[A(n, n+1) = (alpha);\]
\[beta(n,1) = j(n,1)*dt/(rho*Cp*thick)*(Etn(n,1) - En(n,1)+j(n,1)*ASR(n,1))...-Hshift(n,1)*x(n,1)*dt/(V*rho*Cp) - U*stepsize*width*(Ti(n,1)-(Tinf))*dt/(V*rho*Cp);\]
end
end

%Solve for new temp(x) then update temp dependent variables
Ti = A*Ti + beta;
for n=1:1:nsteps
\begin{verbatim}

\text{dH(n,1) = (-235.36-0.026522*Ti(n,1)+0.000012144*Ti(n,1)^2)*1000;}
\text{Etn(n,1) = -(dH(n,1)/(2*96485));}
\text{dGo(n,1) = (-241 +3.52e-2*Ti(n,1)+1.97e-5*Ti(n,1)^2-8.28e-9*Ti(n,1)^3+1.39e-12*Ti(n,1)^4)*1000;}
\text{dG(n,1) = dGo(n,1)+8.314*Ti(n,1)*log(nH2Oi(n,1)/(nH2i(n,1)*sqrt(pO2(n,1))));
En(n,1) = -(dG(n,1)/(2*96485));
ASR(n,1) = (8.39355e-4*exp(8032.32/(Ti(n,1))))/(100^2);}%Temp dependent, experimental fitted data
%ASR(n,1) = (1.5261e-5*exp((11156)/(Ti(n,1))))/(100^2);%Temp dependent, Based on Ceramatec data
end
%Solve for Vopn (secant method)
flag = 0;
Vopmax = En(round(nsteps/2),1);
Vopmin = 0;
Imin = 0;
Imax = 0;
for n = 1:1:nsteps
  Imax = Imax + stepsize*width*En(n,1)/ASR(n,1);
end
slope = -(Vopmax-Vopmin)/(Imax-Imin);
Vopn = slope*(Iin - Imin) + Vopmax;
while flag == 0
  Io = 0;
  for n = 1:1:nsteps
    Io = Io + stepsize*width*(En(n,1)-Vopn)/(ASR(n,1));
  end
  if Iin == 0
    Vopn = En(1,1);
    flag = 1;
  elseif(I - Io) > 0.001
    Vopmax = Vopn;
    Imin = Io;
  elseif (I - Io) < -0.001
    Vopmin = Vopn;
    Imax = Io;
  else
    flag = 1;
  end
  slope = -(Vopmax-Vopmin)/(Imax-Imin);
  Vopn = slope*(Iin - Imin) + Vopmax;
end
if Iin == 0
  j(1,1) = 0;
else
  j(1,1) = (En(1,1)-Vopn)/ASR(1,1);
end
for n = 1:1:nsteps
  if Iin == 0
    j(n,1) = 0;
  else
    j(n,1) = (En(n,1)-Vopn)/ASR(n,1);
  end
  if n == 1
    nO2i(n,1) = nO2in - (1/2)*j(n,1)*stepsize*width/(2*96485);
    pO2(n,1) = nO2i(n,1)/((nO2i(n,1)+nN2i(n,1)));
  nH2i(n,1) = nH2in - j(n,1)*stepsize*width/(2*96485);
    nH2Oi(n,1) = nH2Oin + j(n,1)*stepsize*width/(2*96485);
  else
    nO2i(n,1) = nO2i(n-1,1) - (1/2)*j(n,1)*stepsize*width/(2*96485);
    pO2(n,1) = nO2i(n,1)/((nO2i(n,1)+nN2i(n,1)));
end
\end{verbatim}
\[ n_{H_2}(n,1) = n_{H_2}(n-1,1) - j(n,1) \text{stepsize}\text{width}/(2*96485); \]
\[ n_{H_2O}(n,1) = n_{H_2O}(n-1,1) + j(n,1) \text{stepsize}\text{width}/(2*96485); \]

%shift equilibrium calculations
\[ dG_{shift}(n,1) = -39.381e3 + 40.81T(n,1) - 4.5e-3T(n,1)^2; \]
\[ K_p(n,1) = \exp(-dG_{shift}(n,1)/(8.314T(n,1)))); \]
\[ t5(n,1) = K_p(n,1)\text{^2}; \]
\[ t6(n,1) = n_{CO(i)}(n,1)\text{^2}; \]
\[ t8(n,1) = n_{CO(i)}(n,1)*n_{H_2O}(n,1); \]
\[ t17(n,1) = n_{H_2O}(n,1)\text{^2}; \]
\[ t26(n,1) = n_{CO2(i)}(n,1)\text{^2}; \]
\[ t27(n,1) = n_{CO2(i)}(n,1)*n_{H_2}(n,1); \]
\[ t29(n,1) = n_{H_2}(n,1)\text{^2}; \]
\[ t36(n,1) = \sqrt{(t5(n,1)*t6(n,1)-2*t5(n,1)*t8(n,1)+2*K_p(n,1)*n_{CO(i)}(n,1)\text{*n_{CO2(i)}(n,1)}...+2*K_p(n,1)*n_{H_2O}(n,1)\text{*n_{H_2}(n,1)\text{+t26(n,1)-}...2*t27(n,1)+t29(n,1)+4*K_p(n,1)*t27(n,1)\text{)}...+4*K_p(n,1)\text{*t8(n,1))}}; \]
\[ x(n,1) = \frac{1}{K_p(n,1)-1}(K_p(n,1)*n_{CO(i)}(n,1)+K_p(n,1)*n_{H_2O}(n,1)+n_{CO2(i)}(n,1)+n_{H_2}(n,1)-t36(n,1))/2; \]
%adjust compositions to equilibrium
\[ n_{H_2}(n,1) = n_{H_2}(n,1) + x(n,1); \]
\[ n_{CO}(n,1) = n_{CO}(n,1) - x(n,1); \]
\[ n_{CO2}(n,1) = n_{CO2}(n,1) + x(n,1); \]
\[ n_{H_2O}(n,1) = n_{H_2O}(n,1) - x(n,1); \]

%Results returned to Simulink simulation (only sim_time reported)
\[ F_U = (n_{H_2in}-n_{H_2i}(n_{steps,1}))/n_{H_2in}; \] %from Sanjaya's model
\[ \text{current}\_density = j; \] %from Sanjaya's model
\[ T = T_i; \]
\[ \text{Vop} = \text{Vopn}; \] %Operating voltage for a single cell
\[ \text{Vstk} = \text{Vop}\text{*cells}; \]
\[ \text{Im} = \text{stacks}\text{*I}; \]
\[ \text{Vout} = \text{Vstk}; \]
\[ \text{Power} = \text{Vout}\text{*Im}; \]
\[ \text{Qout} = \text{Q}; \] %from Sanjaya's model
\[ \text{time} \text{is recorded for next calculation} \]
\[ \text{tprev} = \text{sim}\_\text{time}; \]

\section*{C.2 Two Dimensional Model}

\begin{verbatim}
function \[\text{[Power, Anode_Comp, Anode_Flow, Cathode_Comp, Cathode_Flow, Vout, ji, T, FU, h]} = \text{fcn}(\text{constants, inputs, time})\]
% This block supports an embeddable subset of the MATLAB language.

%define variables in constants and inputs streams
\end{verbatim}
nsteps = 30; %number of individual steps evaluated along each cell side  
activesteps = 24; %number of individual steps along each electrolyte side  
n_total = 900; %number of finite volume elements throughout model  
Air_Flowin = (inputs(1))/total_cells; %mol/s for individual cell  
Fuel_Flowin = (inputs(2))/total_cells; %mol/s for individual cell  
Tair = (inputs(3)); %CH4, H2O, CO, CO2, H2, O2, N2 (everything but O2 and N2 == 0,  
need to add steam)  
Tfuel = (inputs(4)); %CH4, H2O, CO, CO2, H2, O2, N2 (O2 and N2 == 0)  
nO2in = (inputs(10))*Air_Flowin/activesteps; %mol/s  
nN2in = (inputs(11))*Air_Flowin/activesteps; %mol/s  
nCH4in = (inputs(12))*Fuel_Flowin/activesteps; %mol/s  
nH2Oin = (inputs(13))*Fuel_Flowin/activesteps; %mol/s  
nCOin = (inputs(14))*Fuel_Flowin/activesteps; %mol/s  
nCO2in = (inputs(15))*Fuel_Flowin/activesteps; %mol/s  
nH2in = (inputs(16))*Fuel_Flowin/activesteps; %mol/s  
nN2inert = (inputs(18))*Fuel_Flowin/activesteps; %mol/s  
Iin = (inputs(19))/stacks; %Current (A)  
Tinf = (inputs(20));  
sim_time = time; %simulation time  

%misc. variables/values  
To = ((Tair*Air_Flowin)+ (Tfuel*Fuel_Flowin))/(Air_Flowin+Fuel_Flowin); %Initial  
Temperature (K)  
%Temperature of surrounding environment (for radiation calculation)  
k = (1.534E-02*To + 8.968)*0.5; %W/m-K thermal conductivity of fuel cell (assumes an  
overall porosity of 0.5)  
Cp = 1.854E-01*To + 4.251E+02; %J/kg-K specific heat of fuel cell  
rho = 4083*1.0; %kg/m^3 density of fuel cell, assumes porosity of 0.5  
V = stepsize^2*thick; %note that each side of fuel cell must be same length  
sim_time = time;  

%Refine value later to depend on composition and temp vs. just a constant  
MWair = (inputs(10)*32 + inputs(11)*28)/1000; %kg/mol molecular weight of air  
mair = Air_Flowin*MWair/activesteps; %kg/s mass flow rate of air in each channel of a  
single fuel cell  
MWfuel = (inputs(12)*16+inputs(13)*18+inputs(14)*28+inputs(15)*44+inputs(16)*2)/1000;  
%kg/mol molecular weight of fuel  
mfuel = Fuel_Flowin*MWfuel/activesteps; %kg/s mass flow rate of fuel in each channel  
of a single fuel cell  
Cpair = 1160; %J/kg-K specific heat of air stream  
Cpfuel = 2600; %J/kg-K specific heat of fuel stream  

%The first step is to determine the maximum allowable dt for stability  
%If the current simulation time is less than dt since the last time evaluated  
%it will be used for calculations. Otherwise, the time interval will be  
%broken into smaller parts as dictated by max dt for stability.  

alpha = k/(rho*Cp);  
max_dt = 0.25*(stepsize)^2/alpha; %maximum allowable time step for stability  
persistent tprev %time of previous successful simulation  
if isempty (tprev)  
    tprev = 0;  
else  
    dt = (sim_time-tprev)/(round(((sim_time-tprev)/max_dt)+.5));  
else  
    dt = (sim_time-tprev);  
end  

5/6/2006
dt = 0;
end
t_tracker = tprev+dt;
I = Iin;
U = 7;  %W/m^2-K heat coefficient to account for heat losses at the stack ends

Fo = alpha*dt/stepsiz^2;
persistent A %define variables so that their values are carried over from time step to
time step
persistent Ti
persistent Tgradient
persistent dHo
persistent nO2i
persistent nN2i
persistent nCH4i
persistent nH2Oi
persistent nCOi
persistent nCO2i
persistent nH2i
persistent pO2
persistent dH
persistent Etn
persistent dGo
persistent dG
persistent En
persistent ASR
persistent beta
persistent q
persistent Vopn
persistent j
persistent dGoshift
persistent Kp
persistent t5
persistent t6
persistent t8
persistent t17
persistent t26
persistent t27
persistent t29
persistent t36
persistent x
persistent Hshift
persistent Tmat
%declaration of variable dimensions
if isempty(Ti)
    A = zeros(n_total,5);
    T_i = zeros(n_total,1);
    Tgradient = zeros(nsteps,nsteps);
    TgradientS = zeros(n_total,1);
    dHo = zeros(n_total,1);
    nO2i = zeros(n_total,1);
    nN2i = zeros(n_total,1);
    nCH4i = zeros(n_total,1);
    nH2Oi = zeros(n_total,1);
    nCOi = zeros(n_total,1);
    nCO2i = zeros(n_total,1);
    nH2i = zeros(n_total,1);
    pO2 = zeros(n_total,1);
    dH = zeros(n_total,1);
    Etn = zeros(n_total,1);
    dGo = zeros(n_total,1);
    dG = zeros(n_total,1);
    En = zeros(n_total,1);
\begin{verbatim}
ASR = zeros(n_total,1);
beta = zeros(n_total,1);
q = zeros(n_total,1);
Vopn = 0;
j = zeros(n_total,1);
dGoshift = zeros(n_total,1);
Kp = zeros(n_total,1);
t5 = zeros(n_total,1);
t6 = zeros(n_total,1);
t8 = zeros(n_total,1);
t17 = zeros(n_total,1);
t26 = zeros(n_total,1);
t27 = zeros(n_total,1);
t29 = zeros(n_total,1);
t36 = zeros(n_total,1);
x = zeros(n_total,1);
Hshift = zeros(n_total,1);
Tmat = zeros(nsteps, nsteps);
end

%Declaration of initial conditions (temperature and flow composition)
for n=1:n_total
    Ti(n,1) = To;
    if ((n <= 3)||(n>=28&&n<=33)||(n>=58&&n<=63)||(n>=88&&n<=90)||
        (n>=811&&n<=813)||(n>=838&&n<=843)||(n>=868&&n<=873)||(n>=898&&n<=900))
        %corners where separation ribs meet
        nO2i(n,1) = 0;
nN2i(n,1) = 0;
nCH4i(n,1) = 0;
nH2Oi(n,1) = 0;
nCOi(n,1) = 0;
nCO2i(n,1) = 0;
nH2i(n,1) = 0;
    elseif ((n>=4&&n<=27)||(n>=34&&n<=57)||(n>=64&&n<=87)||(n>=814&&n<=837)||
        (n>=844&&n<=867)||(n>=874&&n<=897)) %fuel stream inlet (no air)
        nO2i(n,1) = 0;
nN2i(n,1) = 0;
nCH4i(n,1) = nCH4in;
nH2Oi(n,1) = nH2Oin;
nCOi(n,1) = nCOin;
nCO2i(n,1) = nCO2in;
        nH2i(n,1) = nH2in;
    elseif ((n>=91&&n<=93)||(n>=118&&n<=123)||(n>=148&&n<=153)||
        (n>=178&&n<=183)||(n>=208&&n<=213)||(n>=238&&n<=243)||
        (n>=268&&n<=273)||(n>=298&&n<=303)||(n>=328&&n<=333)||
        (n>=358&&n<=363)||(n>=388&&n<=393)||(n>=418&&n<=423)||
        (n>=448&&n<=453)||(n>=478&&n<=483)||(n>=508&&n<=513)||
        (n>=538&&n<=543)||(n>=568&&n<=573)||(n>=598&&n<=603)||
        (n>=628&&n<=633)||(n>=658&&n<=663)||(n>=688&&n<=693)||
        (n>=718&&n<=723)||(n>=748&&n<=753)||(n>=778&&n<=783))
        %air stream inlet (no fuel)
        nO2i(n,1) = nO2in;
nN2i(n,1) = nN2in;
nCH4i(n,1) = 0;
nH2Oi(n,1) = 0;
nCOi(n,1) = 0;
nCO2i(n,1) = 0;
        nH2i(n,1) = 0;
        pO2(n,1) = nO2i(n,1)/(nO2i(n,1)+nN2i(n,1));
    else %active area
        nO2i(n,1) = nO2in;
nN2i(n,1) = nN2in;
nCH4i(n,1) = nCH4in;
nH2Oi(n,1) = nH2Oin;
nCOi(n,1) = nCOin;

end
\end{verbatim}
nCO2i(n,1) = nCO2in;
nH2i(n,1) = nH2in;
pO2(n,1) = nO2i(n,1)/(nO2i(n,1)+nN2i(n,1));
end
end
%This is the case where t=0 and the initial values will be returned for everthing
%This will also return the OCV for the stack voltage since current is assumed to be
0.
for l = 1:30
    for m = 1:24
        j(n,1) = 0;
        dGoshaft(n,1) = -39.381e3+40.81*Ti(n,1)-4.5e-3*Ti(n,1)^2;
        Kp(n,1) = exp(-dGoshaft(n,1)/(8.314*Ti(n,1)));
        Hshift(n,1) = -(47.1e3-22.8*Ti(n,1)+7.63e-3*Ti(n,1)^2);
        t5(n,1) = Kp(n,1)^2;
        t6(n,1) = nCOi(n,1)^2;
        t8(n,1) = nCOi(n,1)*nH2Oi(n,1);
        t17(n,1) = nH2Oi(n,1)^2;
        t26(n,1) = nCO2i(n,1)^2;
        t27(n,1) = nCO2i(n,1)*nH2i(n,1);
        t29(n,1) = nH2i(n,1)^2;
        t36(n,1) = sqrt(t5(n,1)*t6(n,1)-2*t5(n,1)*t8(n,1)+2*Kp(n,1)*nCOi(n,1)*
                        nCO2i(n,1) +2*Kp(n,1)*nCOi(n,1)*nH2i(n,1)+t5(n,1)*
                        t17(n,1)+2*Kp(n,1)*nH2Oi(n,1)*nCO2i(n,1) +2*Kp(n,1)*nH2Oi(n,1)*
                        nH2i(n,1)+t26(n,1)+2*t27(n,1)+t29(n,1)+4*Kp(n,1)*t27(n,1)
                        +4*Kp(n,1)*t8(n,1));
        x(n,1) = 1/(Kp(n,1)-1) * (Kp(n,1)*nCOi(n,1)+Kp(n,1)*nH2Oi(n,1) + nCO2i(n,1)+
                        nH2i(n,1)-t36(n,1))/2;
        %adjust compositions to shift equilibrium
        nH2i(n,1) = nH2i(n,1) + x(n,1);
        nCOi(n,1) = nCOi(n,1) - x(n,1);
        nCO2i(n,1) = nCO2i(n,1) + x(n,1);
        nH2Oi(n,1) = nH2Oi(n,1) - x(n,1);
        if (l>3&&l<28)
            dH(n,1) = (-235.36-0.026522*Ti(n,1)+0.000012144*Ti(n,1)^2)*1000; %for H2
            Etn(n,1) = -(dH(n,1)/(2*96485));
            dGo(n,1) = (-241 + 3.52e-2*Ti(n,1)+1.97e-5*Ti(n,1)^2-8.28e-9*Ti(n,1)^3+
                        1.39e-12*Ti(n,1)^4)*1000;
            dG(n,1) = dGo(n,1)+8.314*Ti(n,1)*log(nH2Oi(n,1)/(nH2i(n,1)*sqrt(pO2(n,1))));
            En(n,1) = -(dG(n,1)/(2*96485));
            %ASR Equations************
            ASR(n,1) = (8.39355e-4*exp(8032.32/(Ti(n,1))))/(100^2); %Temp dependent
        end
    end
end
%Return initial condition outputs
Vopn = En(round(nsteps*nsteps/2+nsteps/2),1);
flowCH4 = 0;
flowH2O = 0;
flowCO = 0;
flowCO2 = 0;
flowH2 = 0;
flowO2 = 0;
flowN2 = 0;
flowN2inert = 0;
for n = 874:1:897
    flowCH4 = flowCH4 + nCH4i(n,1);
    flowH2O = flowH2O + nH2Oi(n,1);
    flowCO2 = flowCO2 + nCO2i(n,1);
    flowCO = flowCO + nCOi(n,1);
flowH2 = flowH2 + nH2i(n,1);
flowN2inert = flowN2inert + nN2inert;
end
Anode_Flow = (flowCH4 + flowH2O + flowCO + flowCO2 + flowH2 + flowN2inert)*
total_cells;
xCH4  = (flowCH4*total_cells)/Anode_Flow;
xH2O = (flowH2O*total_cells)/Anode_Flow;
xCO  = (flowCO*total_cells)/Anode_Flow;
xCO2 = (flowCO2*total_cells)/Anode_Flow;
xH2  = (flowH2*total_cells)/Anode_Flow;
xN2inert = (flowN2inert*total_cells)/Anode_Flow;
Anode_Comp = [xCH4;xH2O;xCO;xCO2;xH2;0;xN2inert];
for n = 120:30:810
  flowO2 = flowO2 + nO2i(n,1);
  flowN2 = flowN2 + nN2i(n,1);
end
Cathode_Flow = (flowO2 + flowN2)*total_cells;
xO2 = (flowO2*total_cells)/Cathode_Flow;
xN2 = (flowN2*total_cells)/Cathode_Flow;
Cathode_Comp = [0;0;0;0;0;xO2;xN2];
else
  if (dt == 0) %resolve for Vopn (secant method)
    flag   = 0;
    Vopmax = En(round(nsteps*nsteps/2+nsteps/2),1);
    Vopmin = 0;
    Imin   = 0;
    Imax   = 0;
    for l = 1:24
      for m = 1:24
        n = 63 + l*(30) + m;
        Imax = Imax + stepsize^2*En(n,1)/ASR(n,1);
      end
    end
    slope = -(Vopmax-Vopmin)/(Imax-Imin);
    Vopn  = slope*(Iin - Imin) + Vopmax;
    while flag == 0
      Io = 0;
      for l = 1:24
        for m = 1:24
          n = 63 + l*(30) + m;
          Io = Io + stepsize^2*(En(n,1)-Vopn)/(ASR(n,1));
        end
      end
      if Iin == 0
        Vopn   = En(round(nsteps*nsteps/2+nsteps/2),1);
        flag   = 1;
      elseif(I - Io) > 0.001
        Vopmax = Vopn;
        Imin   = Io;
        slope = -(Vopmax-Vopmin)/(Imax-Imin);
        Vopn = slope*(Iin - Imin) + Vopmax;
      elseif (I - Io) < -0.001
        Vopmin = Vopn;
        Imax   = Io;
        slope = -(Vopmax-Vopmin)/(Imax-Imin);
        Vopn = slope*(Iin - Imin) + Vopmax;
      else
        flag   = 1;
      end
    end
  end
  if flag == 0
    Vopn = En(round(nsteps*nsteps/2+nsteps/2),1);
  end
end
%return unchanged anode and cathode streams
flowCH4 = 0;
flowH2O = 0;
flowCO = 0;
flowCO2 = 0;
flowH2 = 0;
flowO2 = 0;
flowN2 = 0;
flowN2inert = 0;
for n = 874:1:897
    flowCH4 = flowCH4 + nCH4i(n,1);
    flowH2O = flowH2O + nH2Oi(n,1);
    flowCO2 = flowCO2 + nCO2i(n,1);
    flowCO = flowCO + nCOi(n,1);
    flowH2 = flowH2 + nH2i(n,1);
    flowN2inert = flowN2inert + nN2inert;
end
Anode_Flow = (flowCH4 + flowH2O + flowCO + flowCO2 + flowH2 + flowN2inert)*total_cells;
xCH4  = (flowCH4*total_cells)/Anode_Flow;
xH2O = (flowH2O*total_cells)/Anode_Flow;
xCO = (flowCO*total_cells)/Anode_Flow;
xCO2 = (flowCO2*total_cells)/Anode_Flow;
xH2 = (flowH2*total_cells)/Anode_Flow;
xN2inert = (flowN2inert*total_cells)/Anode_Flow;
Anode_Comp = [xCH4;xH2O;xCO;xCO2;xH2;0;xN2inert];
for n =120:30:810
    flowO2 = flowO2 + nO2i(n,1);
    flowN2 = flowN2 + nN2i(n,1);
end
Cathode_Flow = (flowO2 + flowN2)*total_cells;
xO2 = (flowO2*total_cells)/Cathode_Flow;
xN2 = (flowN2*total_cells)/Cathode_Flow;
Cathode_Comp = [0;0;0;0;0;xO2;xN2];
else %calculate component data from final value of Vop from last time step
    for l = 1:24
        for m = 1:24
            n = 63 + l*(30) + m;
            if Iin ==0
                j(n,1) = 0;
            else
                j(n,1) = (En(n,1)-Vopn)/ASR(n,1);
            end
        end
    end
    nO2o = nO2i;
    nN2o = nN2i;
    nCH4o = nCH4i;
    nH2Oo = nH2Oi;
    nCOo = nCOi;
    nCO2o = nCO2i;
    nH2o = nH2i;
    for n = 1:n_total
        if (n <= 3)||(n>=28&&n<=33)||(n>=58&&n<=63)||(n>=88&&n<=90)||(n>=811&&n<=813)||(n>=838&&n<=843)||(n>=868&&n<=873)||(n>=898&&n<=900)) %corners where separation ribs meet
            nCH4i(n,1) = 0;
            nH2Oi(n,1) = 0;
            nCOi(n,1) = 0;
            nCO2i(n,1) = 0;
            nH2i(n,1) = 0;
            nO2i(n,1) = 0;
            nN2i(n,1) = 0;
        elseif (n>3 && n<28)
            nCH4i(n,1) = nCH4in;
nH2Oi(n,1) = nH2Oin;
nCOi(n,1) = nCOin;
nCO2i(n,1) = nCO2in;
nH2i(n,1) = nH2in;

elseif
(n==91 || n==121 || n==151 || n==181 || n==211 || n==241 || n==271 || n==301 || n==331 || n==361
|| n==391 || n==421 || ... || n==451 || n==481 || n==511 || n==541 || n==571 || n==601 || n==631
|| n==661 || n==691 || n==721 || n==751 || n==781)
nO2i(n,1) = nO2in;
nN2i(n,1) = nN2in;
else
nCH4i(n,1) = nCH4o(n-30,1);
nH2Oi(n,1) = nH2Oo(n-30,1) + j(n,1)*steptime^2/(2*96485);
nCOi(n,1) = nCOo(n-30,1);
nCO2i(n,1) = nCO2o(n-30,1);
nH2i(n,1) = nH2o(n-30,1) - j(n,1)*steptime^2/(2*96485);
nO2i(n,1) = nO2o(n-1,1) - (1/2)*j(n,1)*steptime^2/(2*96485);
nN2i(n,1) = nN2o(n-1,1);
if nO2i(n,1) == 0;
pO2(n,1) = 0;
else
pO2(n,1) = nO2i(n,1)/(nO2i(n,1)+nN2i(n,1));
end
end
end
for l = 1:30
for m = 1:24
n = 3 + (l-1)*(30) + m;
dGoshift(n,1) = -30.381e3+40.81*Ti(n,1)-4.5e-3*Ti(n,1)^2;
Hshift(n,1) = -(47.1e3-22.8*Ti(n,1)+7.63e-3*Ti(n,1)^2);
Kp(n,1) = exp(-dGoshift(n,1)/(8.314*Ti(n,1)));
t5(n,1) = Kp(n,1)^2;
t6(n,1) = nCOi(n,1)^2;
t8(n,1) = nCOi(n,1)*nH2Oi(n,1);
t17(n,1) = nH2O1i(n,1)^2;
t26(n,1) = nCO2i(n,1)^2;
t27(n,1) = nCO2i(n,1)*nH2i(n,1);
t29(n,1) = nH2i(n,1)^2;
t36(n,1) = sqrt(t5(n,1)*t6(n,1)-2*t5(n,1)*t8(n,1)+ 2*Kp(n,1)*
nCOi(n,1)*nCO2i(n,1)+2*Kp(n,1)*nCOi(n,1)*nH2i(n,1)+
t5(n,1)*t17(n,1)+2*Kp(n,1)*nH2O1i(n,1)*nCO2i(n,1)+2*Kp(n,1)*
nH2O1i(n,1)*nH2i(n,1)+t26(n,1)-2*t27(n,1)+t29(n,1)+
4*Kp(n,1)*t27(n,1)+4*Kp(n,1)*t8(n,1));
x(n,1) = 1/(Kp(n,1)-1)*Kp(n,1)*nCOi(n,1)+Kp(n,1)*nH2O1i(n,1)+
nCO2i(n,1)*nH2i(n,1)-t36(n,1))/2;

nH2(i,n,1) = nH21i(n,1) + x(n,1);
nCOi(n,1) = nCO1i(n,1) - x(n,1);
nCO2i(n,1) = nCO2i(n,1) + x(n,1);
nH2Oi(n,1) = nH2O1i(n,1) - x(n,1);
end
end
%Write out component data from last successful time step
flowCH4 = 0;
flowH2O = 0;
flowCO = 0;
flowCO2 = 0;
flowH2 = 0;
flowO2 = 0;
flowN2 = 0;
flowN2inert = 0;
for n = 874:1:897

5/6/2006
flowCH4 = flowCH4 + nCH4i(n,1);
flowH2O = flowH2O + nH2Oi(n,1);
flowCO2 = flowCO2 + nCO2i(n,1);
flowCO = flowCO + nCOi(n,1);
flowH2 = flowH2 + nH2i(n,1);
flowN2inert = flowN2inert + nN2inert;
end
Anode_Flow = (flowCH4 + flowH2O + flowCO + flowCO2 + flowH2 + flowN2inert) *total_cells;
xCH4  = (flowCH4*total_cells)/Anode_Flow;
xH2O = (flowH2O*total_cells)/Anode_Flow;
xCO  = (flowCO*total_cells)/Anode_Flow;
xCO2 = (flowCO2*total_cells)/Anode_Flow;
xH2 = (flowH2*total_cells)/Anode_Flow;
xN2inert = (flowN2inert*total_cells)/Anode_Flow;
Anode_Comp = [xCH4;xH2O;xCO;xCO2;xH2;0;xN2inert];
for n = 30:30:900
    flowO2 = flowO2 + nO2i(n,1);
    flowN2 = flowN2 + nN2i(n,1);
end
Cathode_Flow = (flowO2 + flowN2)*total_cells;
xO2 = (flowO2*total_cells)/Cathode_Flow;
xN2 = (flowN2*total_cells)/Cathode_Flow;
Cathode_Comp = [0;0;0;0;0;xO2;xN2];
while (t_tracker <= sim_time)
    for n = 1:n_total %set up temperature solution matrix
        if (n == 1) %corner between fuel and air inlets
            A(n, 1) = 0;
            A(n, 2) = 0;
            A(n, 3) = (1-2*Fo);
            A(n, 4) = (Fo);
            A(n, 5) = (Fo);
            beta(n,1) = -U*stepsize^2*(Ti(n,1)-(Tinf))*dt/(V*rho*Cp);
        elseif(n==2||n==3||n==28||n==29) %rib on fuel inlet side
            A(n, 1) = 0;
            A(n, 2) = (Fo);
            A(n, 3) = (1-3*Fo);
            A(n,4) = (Fo);
            A(n, 5) = (Fo);
            beta(n,1) = -U*stepsize^2*(Ti(n,1)-(Tinf))*dt/(V*rho*Cp);
        elseif (n > 3 && n < 28) %fuel inlet
            A(n, 1) = 0;
            A(n, 2) = (Fo);
            A(n, 3) = (1-3*Fo)-mfuel*Cpfuel*dt/(rho*V*Cp);
            A(n, 4) = (Fo);
            A(n, 5) = (Fo);
            beta(n,1) = mfuel*Cpfuel*Tfuel*dt/(rho*V*Cp) - Hshift(n,1)*x(n,1)*dt/(V*rho*Cp) - U*stepsize^2*(Ti(n,1)-(Tinf))*dt/(V*rho*Cp);
        elseif (n == 30); %corner between fuel inlet and air outlet
            A(n, 1) = 0;
            A(n, 2) = (Fo);
            A(n, 3) = (1-2*Fo);
            A(n, 4) = 0;
            A(n, 5) = (Fo);
            beta(n,1) = -sigma*epsilon*dt/(rho*stepsize*Cp)*(Ti(n,1)^4-(Tinf)^4) - U*stepsize^2*(Ti(n,1)-(Tinf))*dt/(V*rho*Cp);
        elseif ((n > 31 && n < 60)||(n > 61 && n < 90)||(n > 811 && n < 840)||(n > 841 && n < 870))
            A(n, 1) = (Fo) + mfuel*Cpfuel*dt/(rho*V*Cp);
            A(n, 2) = (Fo);
            A(n, 3) = (1-4*Fo) - mfuel*Cpfuel*dt/(rho*V*Cp);
            A(n, 4) = (Fo);
            beta(n,1) = -sigma*epsilon*dt/(rho*stepsize*Cp)*(Ti(n,1)^4-(Tinf)^4) - U*stepsize^2*(Ti(n,1)-(Tinf))*dt/(V*rho*Cp);
        elseif ((n > 61 && n < 90)||(n > 811 && n < 840))
            A(n, 1) = (Fo);
            A(n, 2) = (Fo);
        elseif ((n > 841 && n < 870))
            A(n, 1) = (Fo);
            A(n, 2) = (Fo);
        end
    end
end
%Fuel entrance and exit internal rib edge (fuel cell top and bottom)
elseif ((n > 31 && n < 60)||(n > 61 && n < 90)||(n > 811 && n < 840)||(n > 841 && n < 870))
    A(n, 1) = (Fo);
    A(n, 2) = (Fo);
    A(n, 3) = (1-4*Fo) - mfuel*Cpfuel*dt/(rho*V*Cp);
    A(n, 4) = (Fo);
    beta(n,1) = -sigma*epsilon*dt/(rho*stepsize*Cp)*(Ti(n,1)^4-(Tinf)^4) - U*stepsize^2*(Ti(n,1)-(Tinf))*dt/(V*rho*Cp);
end
5/6/2006 237
\[
A(n, 5) = (F_o);
\]
\[
\text{beta}(n, 1) = -H_{\text{shift}}(n, 1) \cdot x(n, 1) \cdot dt/(V \cdot \rho \cdot C_p) - U \cdot \text{stepsize}^2 \cdot (T_i(n, 1) - (T_{\text{inf}})) \cdot dt/(V \cdot \rho \cdot C_p);
\]
\[
\text{elseif (}(n>91 \& \& n<93) || (n>118 \& \& n<123) || (n=148 \& \& n=153) || (n>178 \& \& n<183) || (n>208 \& \& n<213) || (n>238 \& \& n<243) || (n>268 \& \& n<273) || (n>298 \& \& n<303) || (n>328 \& \& n=333) || (n>358 \& \& n<363) || (n>388 \& \& n<393) || (n=418 \& \& n=423) || (n>448 \& \& n<453) || (n>478 \& \& n<483) || (n>508 \& \& n<513) || (n>538 \& \& n<543) || (n>568 \& \& n<573) || (n>598 \& \& n<603) || (n>628 \& \& n<633) || (n>658 \& \& n<663) || (n>688 \& \& n<693) || (n>718 \& \& n<723) || (n>748 \& \& n<753) || (n>778 \& \& n<783)\]
\]
\%Air in internal rib (fuel cell left side)
\[
A(n, 1) = (F_o);
\]
\[
A(n, 2) = (F_o) + m_{\text{air}} \cdot C_{\text{pair}} \cdot dt/(\rho \cdot V \cdot C_p);
\]
\[
A(n, 3) = (1-4 \cdot F_o) - m_{\text{air}} \cdot C_{\text{pair}} \cdot dt/(\rho \cdot V \cdot C_p);
\]
\[
A(n, 4) = (F_o);
\]
\[
A(n, 5) = (F_o);
\]
\[
\text{beta}(n, 1) = -U \cdot \text{stepsize}^2 \cdot (T_i(n, 1) - (T_{\text{inf}})) \cdot dt/(V \cdot \rho \cdot C_p);
\]
\[
\text{elseif (}(n==59 || n==89 || n==119 || n==149 || n==179 || n==209 || n==239 || n==269 || n==299 || n==329 || n==359 || n==389 \& \& n=419 || ...
\]
\]
\[
A(n, 1) = (F_o);
\]
\[
A(n, 2) = (F_o) + m_{\text{air}} \cdot C_{\text{pair}} \cdot dt/(\rho \cdot \rho \cdot V \cdot C_p);
\]
\[
A(n, 3) = (1-4 \cdot F_o) - m_{\text{air}} \cdot C_{\text{pair}} \cdot dt/(\rho \cdot \rho \cdot V \cdot C_p);
\]
\[
A(n, 4) = (F_o);
\]
\[
A(n, 5) = (F_o);
\]
\[
\text{beta}(n, 1) = -U \cdot \text{stepsize}^2 \cdot (T_i(n, 1) - (T_{\text{inf}})) \cdot dt/(V \cdot \rho \cdot C_p);
\]
\[
\text{elseif (}(n==31 || n==61 || n==841 || n==811) \%Air entrance edge rib
\]
\[
A(n, 1) = (F_o);
\]
\[
A(n, 2) = 0;
\]
\[
A(n, 3) = (1-3 \cdot F_o);
\]
\[
A(n, 4) = (F_o);
\]
\[
A(n, 5) = (F_o);
\]
\[
\text{beta}(n, 1) = -U \cdot \text{stepsize}^2 \cdot (T_i(n, 1) - (T_{\text{inf}})) \cdot dt/(V \cdot \rho \cdot C_p);
\]
\[
\text{elseif (}(n==91 || n==121 || n==151 || n==181 || n==211 || n==241 || n==271 || n==301 || n==331 || n==361 || n==391 || ...
\]
\]
\[
A(n, 1) = (F_o); \%air entrance
\]
\[
A(n, 2) = 0;
\]
\[
A(n, 3) = (1-3 \cdot F_o) - m_{\text{air}} \cdot C_{\text{pair}} \cdot dt/(\rho \cdot \rho \cdot V \cdot C_p);
\]
\[
A(n, 4) = (F_o);
\]
\[
A(n, 5) = (F_o);
\]
\[
\text{beta}(n, 1) = m_{\text{air}} \cdot C_{\text{pair}} \cdot T_{\text{air}} \cdot dt/(\rho \cdot \rho \cdot \rho \cdot V \cdot C_p) - U \cdot \text{stepsize}^2 \cdot (T_i(n, 1) - (T_{\text{inf}})) \cdot dt/(V \cdot \rho \cdot C_p);
\]
\[
\text{elseif (}(n==60 || n==90 || n==870 || n==840) \%air exit edge rib
\]
\[
A(n, 1) = (F_o);
\]
\[
A(n, 2) = (F_o);
\]
\[
A(n, 3) = (1-3 \cdot F_o);
\]
\[
A(n, 4) = 0;
\]
\[ A(n, 5) = (F_0); \]
\[ \beta(n, 1) = -\sigma* \varepsilon*dt/(\rho*\text{stepsize}*C_p)*(T_i(n,1)^4-(T_{\infty})^4) - U*\text{stepsize}^2*(T_i(n,1)-(T_{\infty}))*dt/(V*rho*C_p); \]
\[ \text{elseif (n==120 || n==150 || n==210 || n==270 || n==300 || n==330 || n==360 || n==420 || n==450 || n==480 || n==510 || n==540 || n==570 || n==600 || n==630 || n==660 || n==690 || n==720 || n==750 || n==780 || n==810); %Air outlet} \]
\[ A(n, 1) = (F_0); \]
\[ A(n, 2) = (F_0) + m_{air}*C_{pair}*dt/(\rho*V*C_p); \]
\[ A(n, 3) = (1-3*F_0) - m_{air}*C_{pair}*dt/(\rho*V*C_p); \]
\[ A(n, 4) = 0; \]
\[ A(n, 5) = (F_0); \]
\[ \beta(n, 1) = -\sigma* \varepsilon*dt/(\rho*\text{stepsize}*C_p)*(T_i(n,1)^4-(T_{\infty})^4) - U*\text{stepsize}^2*(T_i(n,1)-(T_{\infty}))*dt/(V*rho*C_p); \]
\[ \text{elseif (n == 872 || n==873 || n==898 || n==899) %fuel exit rib} \]
\[ A(n, 1) = (F_0); \]
\[ A(n, 2) = (F_0); \]
\[ A(n, 3) = (1-3*F_0); \]
\[ A(n, 4) = (F_0); \]
\[ A(n, 5) = 0; \]
\[ \beta(n, 1) = -\sigma* \varepsilon*dt/(\rho*\text{stepsize}*C_p)*(T_i(n,1)^4-(T_{\infty})^4) - U*\text{stepsize}^2*(T_i(n,1)-(T_{\infty}))*dt/(V*rho*C_p); \]
\[ \text{elseif (n > 873 && n < 898) %Fuel exit edge} \]
\[ A(n, 1) = (F_0) + m_{fuel}*C_{pfuel}*dt/(\rho*V*C_p); \]
\[ A(n, 2) = (F_0); \]
\[ A(n, 3) = (1-3*F_0) - m_{fuel}*C_{pfuel}*dt/(\rho*V*C_p); \]
\[ A(n, 4) = (F_0); \]
\[ A(n, 5) = 0; \]
\[ \beta(n, 1) = -\sigma* \varepsilon*dt/(\rho*\text{stepsize}*C_p)*(T_i(n,1)^4-(T_{\infty})^4) - U*\text{stepsize}^2*(T_i(n,1)-(T_{\infty}))*dt/(V*rho*C_p); \]
\[ \text{elseif (n == 871) %corner between air inlet and fuel outlet} \]
\[ A(n, 1) = (F_0); \]
\[ A(n, 2) = 0; \]
\[ A(n, 3) = (1-2*F_0); \]
\[ A(n, 4) = (F_0); \]
\[ A(n, 5) = 0; \]
\[ \beta(n, 1) = -\sigma* \varepsilon*dt/(\rho*\text{stepsize}*C_p)*(T_i(n,1)^4-(T_{\infty})^4) - U*\text{stepsize}^2*(T_i(n,1)-(T_{\infty}))*dt/(V*rho*C_p); \]
\[ \text{elseif (n == 900) %corner between fuel and air outlets} \]
\[ A(n, 1) = (F_0) + m_{fuel}*C_{pfuel}*dt/(\rho*V*C_p); \]
\[ A(n, 2) = (F_0) + m_{air}*C_{pair}*dt/(\rho*V*C_p); \]
\[ A(n, 3) = (1-4*F_0) - m_{air}*C_{pair}*dt/(\rho*V*C_p) - m_{fuel}*C_{pfuel}*dt/(\rho*V*C_p); \]
\[ A(n, 4) = (F_0); \]
\[ A(n, 5) = 0; \]
\[ \beta(n, 1) = -2*\sigma* \varepsilon*dt/(\rho*\text{stepsize}*C_p)*(T_i(n,1)^4-(T_{\infty})^4) - U*\text{stepsize}^2*(T_i(n,1)-(T_{\infty}))*dt/(V*rho*C_p); \]
\[ \text{else %active region} \]
\[ A(n, 1) = (F_0) + m_{fuel}*C_{pfuel}*dt/(\rho*V*C_p); \]
\[ A(n, 2) = (F_0) + m_{air}*C_{pair}*dt/(\rho*V*C_p); \]
\[ A(n, 3) = (1-4*F_0) - m_{air}*C_{pair}*dt/(\rho*V*C_p) - m_{fuel}*C_{pfuel}*dt/(\rho*V*C_p); \]
\[ A(n, 4) = (F_0); \]
\[ A(n, 5) = (F_0); \]
\[ q(n, 1) = (E_{tn}(n,1)-E_{n}(n,1)+j(n,1)*ASR(n,1))*j(n,1)*\text{stepsize}^2; \]
\[ \beta(n, 1) = -\sigma*H_{shift}(n,1)*x(n,1)*dt/(V*rho*C_p) + q(n,1)*dt/(rho*C_p*V) - U*\text{stepsize}^2*(T_i(n,1)-(T_{\infty}))*dt/(V*rho*C_p); \]
\[ \text{end} \]

% Solve for new temp(x) then update temp dependent variables
\[ T_t = T_i; \]
for n=1:n_total
\[ \text{if (n==1)} \]

5/6/2006  239
Ti(n,1) = A(n,3)*Tt(n,1) + A(n,4)*Tt(n+1,1) + A(n,5)*Tt(n+30,1) +
beta(n,1);
elseif (n>1 && n<31)
    Ti(n,1) = A(n,2)*Tt(n-1,1) + A(n,3)*Tt(n,1) + A(n,4)*Tt(n+1,1) +
A(n,5)*Tt(n+30,1) + beta(n,1);
elseif (n>870 && n<900)
    Ti(n,1) = A(n,1)*Tt(n-30,1) + A(n,2)*Tt(n-1,1) + A(n,3)*Tt(n,1) +
A(n,4)*Tt(n+1,1) + beta(n,1);
elseif (n == 900)
    Ti(n,1) = A(n,1)*Tt(n-30,1) + A(n,2)*Tt(n-1,1) + A(n,3)*Tt(n,1) +
A(n,4)*Tt(n+1,1)+...
    A(n,5)*Tt(n+30,1) + beta(n,1);
end

%ASR
Equations*****************************************************************************
**
%ASR(n,1) = 0.0136*exp(3931.5/(Ti(n,1)))/(100^2); %Temp dependent, from
PNNL data
%ASR(n,1) = (55*1.5261e-5*exp(11156*.72/(Ti(n,1))))/(100^2); %Temp
dependent, from Ceramatec data
ASR(n,1) = (8.39355e-4*exp(8032.32/(Ti(n,1))))/(100^2); %Temp dependent,
experimental fitted data
%ASR
Equations*****************************************************************************
****
end
for l = 1:24
    for m = 1:24
        n = 63 + l*(30) + m;
        dH(n,1) = (-235.36-0.026522*Ti(n,1)+0.000012144*Ti(n,1)^2)*1000;
        Etn(n,1) = -(dH(n,1)/(2*96485));
        dGo(n,1) = (-241 +3.52e-2*Ti(n,1)+1.97e-5*Ti(n,1)^2-8.28e-
9*Ti(n,1)^3+1.39e-12*Ti(n,1)^4)*1000;
        dG(n,1) =
        dGo(n,1)+8.314*Ti(n,1)*log(nH2O1(n,1)/(nH2i(n,1)*sqrt(pO2(n,1))));
        En(n,1) = -(dG(n,1)/(2*96485));
    end
end
flag = 0; %Solve for Vopn (secant method)
Vopmax = En((nsteps*nsteps/2+nsteps/2),1);
Vopmin = 0;
Imin = 0;
Imax = 0;
for l = 1:24
    for m = 1:24
        n = 63 + l*(30) + m;
        Imax = Imax + stepsize^2*En(n,1)/ASR(n,1);
    end
end
slope = -(Vopmax-Vopmin)/(Imax-Imin);
Vopn = slope*(Iin - Imin) + Vopmax;
while flag == 0
    Io = 0;
    for l = 1:24
        for m = 1:24
            n = 63 + l*(30) + m;
            Io = Io + stepsize^2*(En(n,1)-Vopn)/(ASR(n,1));
        end
    end
    if Iin == 0

Vopn = En(round(nsteps*nsteps/2+nsteps/2),1);
flag = 1;
elseif(I - Io) > 0.001
    Vopmax = Vopn;
    Imax = Io;
    slope = -(Vopmax-Vopmin)/(Imax-Imin);
    Vopn = slope*(Iin - Imin) + Vopmax;
elseif (I - Io) < -0.001
    Vopmin = Vopn;
    Imax = Io;
    slope = -(Vopmax-Vopmin)/(Imax-Imin);
    Vopn = slope*(Iin - Imin) + Vopmax;
else
    flag = 1;
end
end
if (t_tracker + dt <= sim_time)  %meaning it will have to loop again so as to
    retain stability
    for l = 1:24
        for m = 1:24
            n = 63 + 1*(30) + m;
            if Iin ==0
                j(n,1) = 0;
            else
                j(n,1) = (En(n,1)-Vopn)/ASR(n,1);
            end
        end
    end
    nO2o = nO2i;
    nN2o = nN2i;
    nCH4o = nCH4i;
    nH2Oo = nH2Oi;
    nCOo = nCOi;
    nCO2o = nCO2i;
    nH2o = nH2i;
    for n = 1:n_total
        if ((n <= 3)||(n>38&&n<=63)||(n>88&&n<=90)||(n>=811&&n<=813)||(n>=838&&n<=843)
            nCH4i(n,1) = 0;
            nH2Oi(n,1) = 0;
            nCOi(n,1) = 0;
            nCO2i(n,1) = 0;
            nH2i(n,1) = 0;
            nO2i(n,1) = 0;
            nN2i(n,1) = 0;
        elseif (n>=38 && n<63)
            nCH4i(n,1) = nCH4in;
            nH2Oi(n,1) = nH2Oin;
            nCOi(n,1) = nCOin;
            nCO2i(n,1) = nCO2in;
        elseif (n>63 && n<=88)
            nCH4i(n,1) = nCH4in;
            nH2Oi(n,1) = nH2Oin;
            nCOi(n,1) = nCOin;
            nCO2i(n,1) = nCO2in;
        elseif (n>88 && n<=90)
            nCH4i(n,1) = nCH4in;
            nH2Oi(n,1) = nH2Oin;
            nCOi(n,1) = nCOin;
            nCO2i(n,1) = nCO2in;
        elseif (n>90 && n<=121)
            nCH4i(n,1) = nCH4o(n-30,1);
nH2O_i(n,1) = nH2O_o(n-30,1) + j(n,1)*stepsize^2/(2*96485);
nCO_i(n,1) = nCO_o(n-30,1);
nCO2_i(n,1) = nCO2_o(n-30,1);
nH2_i(n,1) = nH2_o(n-30,1);
if nO2_i(n,1) == 0;
pO2(n,1) = 0;
else
  pO2(n,1) = nO2_i(n,1)/(nO2_i(n,1)+nN2_i(n,1));
end
end

for l = 1:30
  for m = 1:24
    n = 3 + (l-1)*(30) + m;
    dGoshift(n,1) = -39.381e3+40.81*Ti(n,1)-4.5e-3*Ti(n,1)^2;
    Kp(n,1) = exp(-dGoshift(n,1)/(8.314*Ti(n,1)));
    Hshift(n,1) = -(47.1e3-22.8*Ti(n,1)+7.63e-3*Ti(n,1)^2);
    t5(n,1) = Kp(n,1)^2;
    t6(n,1) = nCO_i(n,1)^2;
    t8(n,1) = nCO_i(n,1)*nH2O_i(n,1);
    t17(n,1) = nH2O_i(n,1)^2;
    t26(n,1) = nCO2_i(n,1)^2;
    t27(n,1) = nCO2_i(n,1)*nH2_i(n,1);
    t29(n,1) = nH2i(n,1)^2;
    t36(n,1) = sqrt(t5(n,1)*t6(n,1)-
          2*t5(n,1)*t8(n,1)+2*Kp(n,1)*nCO_i(n,1)*nCO2_i(n,1)...+
          2*Kp(n,1)*nH2O_i(n,1)*nCO2_i(n,1)*nH2_i(n,1)+t26(n,1)-
          2*t27(n,1)+t29(n,1)+4*Kp(n,1)*t27(n,1)...
          +4*Kp(n,1)*t8(n,1));
    x(n,1) = 1/(Kp(n,1)-
1)*(Kp(n,1)*nCO_i(n,1)+Kp(n,1)*nH2O_i(n,1)+nCO2_i(n,1)+nH2i(n,1)-t36(n,1))/2;
    nH2i(n,1) = nH2i(n,1) + x(n,1);
    nCO_i(n,1) = nCO_i(n,1) - x(n,1);
    nCO2_i(n,1) = nCO2_i(n,1) + x(n,1);
    nH2O_i(n,1) = nH2O_i(n,1) - x(n,1);
  end
end

t_tracker = t_tracker + dt;
end
end

%Results returned to Simulink simulation (only sim_time reported)

FU = (inputs(16)*Fuel_Flowin-xH2*Anode_Flow)/(inputs(16)*Fuel_Flowin); %from Sanjaya's model
ji = j; %from Sanjaya's model

T = Ti; %surface temperature
Vop = Vopn; %operating voltage for a single cell
Vstk = Vop*cells; %operating voltage in a single stack
Im = stacks*I;
Vout = Vstk; %operating voltage for module
Power = Vout*Im; %module power output
%time is recorded for next calcualtion
tprev = sim_time;