SOFC-MP 2D User Manual

BJ Koeppel   K Lai
MA Khaleel

May 2011

Pacific Northwest
NATIONAL LABORATORY

Proudly Operated by **Battelle** *Since 1965*

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor Battelle Memorial Institute, nor any of their employees, makes **any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights**. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or Battelle Memorial Institute. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

SOFC-MP 2D User Manual

BJ Koeppel   K Lai
MA Khaleel

May 2011

Pacific Northwest National Laboratory
Richland, Washington 99352

Summary

This report provides instructions for use of the two-dimensional solid oxide fuel cell multi-physics (2D SOFC-MP) modeling code developed at Pacific Northwest National Laboratory (PNNL). This research software package evaluates the electrochemical performance and temperature distribution of multi-cell co-flow and counter-flow solid oxide fuel cell (SOFC) stacks. These types of analyses are useful to stack designers to evaluate the effect of cell design, geometric parameters, material properties, electrochemical properties, thermal boundary conditions, and operating conditions on stack performance. This report briefly presents an overview of the code followed by detailed instructions and examples for installation, model pre-processing, usage, solution, and results post-processing with the software. Several demonstration cases are presented which highlight the types of engineering analyses that can be performed with the software.

Acknowledgements

Acronyms and Abbreviations

2D	two dimensional
3D	three dimensional
AR	aspect ratio
ΔT	temperature difference
GUI	graphical user interface
IC	interconnect
I-V	current-voltage
NETL	National Energy Technology Laboratory
OCR	On-cell reformation
PNNL	Pacific Northwest National Laboratory
SECA	Solid-State Energy Conversion Alliance
SOFC	solid oxide fuel cell
SOFC-MP	solid oxide fuel cell multi-physics
UA	air utilization
UF	fuel utilization

Contents

List of Figures

List of Tables

1.0 Introduction

Numerical modeling has played an important role in solid oxide fuel cell (SOFC) development within the Solid-State Energy Conversion Alliance (SECA) program. Modeling of stacks provides insights to SOFC design, materials, and operation which can help to reduce the required number of costly experimental studies. PNNL developed the SOFC-MP (Solid Oxide Fuel Cell Multi-Physics) model to evaluate the flow, electrochemical, thermal, and structural performance of planar cells (Khaleel et al. 2004). This model operates on the full three-dimensional (3D) geometry of the stack using a finite element framework. The modeling approach was later adapted to evaluate a simpler representation of tall co/counter-flow stack geometries (Lai et al. 2010). This model has sufficiently fast solution times so that it can be used by the fuel cell designer to quickly evaluate different operating scenarios for multi-cell stacks. After a brief overview of the model capabilities, this document presents detailed instructions and demonstrations for the practical use of this code to evaluate SOFC stacks.

2.0 Model Overview

SOFC-MP 2D software is a quasi-two dimensional (2D) numerical model for the efficient computation of the current density, species concentration, and temperature distributions in planar symmetric solid oxide fuel cell stacks. It assumes fully developed steady flow of the fuel and oxidant through a multi-cell SOFC stack. The brief overview of the model capabilities in this document should be supplemented by the detailed discussions of the algorithms and capabilities provided in Lai et al. (2010).

2.1 Capabilities

The modeling code is designed to provide the following simulation capabilities:

- Co- or counter-flow geometry
- Mixed fuel compositions containing H_2, H_2O, CO, CO_2, CH_4, and N_2
- User-defined electrochemistry and methane reforming models
- Analysis of large area cells
- Analysis of multi-cell tall stacks
- Adiabatic or radiation/convection thermal boundary conditions

2.2 Assumptions

The modeling approach has the following primary assumptions:

- The model domain includes only the active area of the cells (i.e. manifold and cell support frames are not explicitly included).
- Variation of in-plane cell quantities normal to the flow direction is negligible.
- The working voltage is uniform for each cell but varies along the stack height.
- The water-gas shift equation is in equilibrium for carbon-containing fuels.
- Fuel and inlet gas temperatures along the cell height are known.

2.3 Numerical Overview

SOFC-MP 2D solves multi-physics phenomena for a fully developed steady laminar flow in a multi-cell SOFC stack. The model solves the fully coupled governing equations for

electrochemistry, heat transfer, and fluid flow in a simplified 2D plane with user defined boundary conditions. The solution provides detailed distributions of the temperature field, current density, and species partial pressures for each cell in the stack.

The solution starts with an initial guess for the temperature field and cell voltage based on inlet air and fuel temperatures as well as the average cell voltage specified from the input file. It then performs four numerical steps in two iteration loops.

The model follows a control volume marching scheme along the fuel flow direction from the control volumes in the inlet area toward the outlet area. In each control volume, the air and fuel gas composition is assumed known from the previous control volume. The oxygen and hydrogen consumption rates are then calculated based on the current density computed from the user-specified current-voltage (I-V) relationship, the remaining species content will be calculated, and then the gas partial pressure is rebalanced to give the new fuel and air composition for the subsequent volume. Thermal equilibrium is required for each control volume in the mesh and thus a matrix equation is created to solve the temperature distribution. The coefficients in the matrix equation depend on the current density, partial pressures, and temperature fields; therefore the solution scheme is an iterative one. Solution convergence is considered achieved when the temperature difference at every control volume from two consecutive iteration steps is within the user preset tolerance (e.g., $0.1^{o}C$). The calculation of temperature distribution for a given cell voltage distribution constitutes the inner iteration loop for the model.

For this given cell voltage distribution, the current for each cell in the stack is calculated by integrating the current density along the flow direction. Because all cells are connected in series in the same circuit, each cell must have the same total current. The difference of current in each cell indicates that the cell voltage must be redistributed. This voltage rebalance activity forms the outer loop iteration that converges when the current difference among cells is within the user-specified tolerance (e.g., 1% of the total current).

The model reaches the final solution when convergence criteria for both the inner temperature loop and the outer voltage-current loop are achieved. Further details of the model solution are provided in Lai et al (2010).

3.0 Installation of SOFC-MP 2D

The SOFC-MP code has been compiled for both the MS Windows and Linux environments.

3.1 Installation Compact Disk

A compact disk (CD) containing the installation files, software, demonstration problems, and documentation is available for use with this document.

3.2 Microsoft Windows Platform

System requirement: Windows XP or Windows 7 server, with minimum 1G RAM and 10G free space.
Third party software requirement: None.

Double click setup.exe or SOFC_MP.msi and follow the instructions. The default installation destination directory is C:\PNNL\SOFC_MP, but you are free to specify a different one. The installation procedure will copy the following files to the installed directory:

1. EC_IntegralModel.exe
2. libmmd.dll
3. libifcoremd.dll
4. ButlerVolmer.inp
5. trans.lib
6. thermo.lib

After installation, the installation directory should be added to the system **PATH** variable. Go to Windows System Properties -> Environment Variables and add the installed directory to the **PATH** variable. (Note: the default path to add is *C:\PNNL\SOFC_MP* unless changed by the user).

The installation compact disk (CD) provides a */Utilities* directory that users can also copy to the installation directory. In the directory, there are two batch files which will facilitate the simulation executions, and one Microsoft Excel spreadsheet which can be used for simulation result post processing if desired.

The installation disk also provides eighteen example cases for use with SOFC-MP 2D, each in its own directory, from */2Dcase01* to */2Dcase18*. The file *CaseDescriptions.txt* in the */Documents* directory provides the detailed descriptions of those eighteen cases. Copy all directories included with the installation disk to the installed directory if needed.

3.3   Linux Platform

On a Linux platform, the file *sofc.tar* contains all compressed files the SOFC-MP 2D model requires. Assuming $HOME/SOFC-MP as the installation directory, run the tar command:

```
$ tar –xvf sofc.tar
```

A few files will be uncompressed in directory $HOME/SOFC-MP:

- sofc – the main executable for SOFC-MP 2D
- trans.lib – a library of species transport properties
- thermo.lib – a library of species thermodynamic properties
- ButlerVolmer.inp – parameter file for electrochemistry calculations

The same tar command will also create eighteen sample directories under $HOME/SOFC-MP. The following library setting statement must be inserted in the Linux shell startup setting file (such as *.bashrc* depending on the user's operating system):

```
export LD_LIBRARY_PATH=/share/apps/gcc-
4.4.1/lib64:/share/apps/gcc-4.4.1/lib:$LD_LIBRARY_PATH
```

To run SOFC-MP 2D in a directory other than the installed directory, the same .bashrc file should contains the following PATH setting statement:

```
Export PATH=$HOME/SOFC_MP/bin:$PATH
```

4.0   Usage of SOFC-MP 2D

The SOFC-MP model was developed to quickly evaluate the sensitivity of stack performance to geometric and operational parameter changes. The model is useful for initial design of stacks to characterize the expected temperature field based on the electrochemical response and stack thermal boundary conditions. It is also useful for simulation of stack experiments to more fully understand observed trends during physical testing of actual stacks. The generation of the numerical model for a stack simulation is described in the following subsections.

4.1   Pre-Processing

4.1.1   Model Geometry

The model uses a simplified geometrical representation of the stack for the computations. This simplified geometry provides the benefits of numerical efficiency while being applicable to general planar stack designs. The model domain consists of the cell active area, where the geometry of the manifolds is not included and the fuel/oxidant inlet flows are assumed to be provided uniformly across each cell. The user provides the active cell width and length and indicates the flow orientation (co-flow or counter-flow). The thicknesses of the cell components are also necessary to account for the in-plane thermal heat transfer. The user provides the total cell thickness (anode + electrolyte + cathode), the thickness of a simple flat interconnect, and the thicknesses of the upper and lower load plates constraining the stack. The heights of the fuel and oxidant channels are also required. If a multi-cell stack is desired, the total number of cells is then input. These are the primary geometry parameters for the stack. If the model is to consider an insulation enclosure around the stack, the thickness of the insulation layer on each side is also required. If the model is to consider the thermal effects of manifold geometry, equivalent thermal links at the inlet and outlet of the stack can be used to include additional heat conduction between adjacent cells.

4.1.2   Operating Parameters

The operating parameters of the stack consist of the inlet fuel definition, inlet oxidant definition, and the solution target for the mode of electrical operation. For the fuel definition, the total molar flow rate, species molar fractions (consisting of H_2, H_2O, CO, CO_2, CH_4, and N_2 species), and inlet temperature is required. For the oxidant definition, the total molar flow rate, species molar fractions (consisting of O_2 and N_2 species), and inlet temperature is required. The temperature of the inlet gases can also be varied linearly along the stack height if necessary to account for heating of the gases in the manifold. Finally, the inlet system pressure of the fuel and oxidant is provided, but the model currently performs no additional calculations for pressurized operation.

To define the electrical operating target, several options are available. The user can select the total voltage for the stack, the average voltage of the cells, the average current density for the stack, or the overall fuel utilization. Based on the assigned current-voltage relationship, the program will iterate to find the voltage and current distribution that satisfies the selected target.

Supplementary spreadsheet tools are provided for the user to pre-calculate values for the conditions of interest (e.g. compute the fuel and oxidant flow rates necessary to obtained desired utilizations for a given stack current).

4.1.3 Thermal Parameters

The model accounts for thermal conduction within the solid component layers, radiation between solid component layers, convection between the solid components and fluid domains, and external heat loss to the surrounding environment. For the conduction calculation, the thermal conductivity is required for the cell, interconnect, top plate, bottom plate, and insulation layer. For the internal radiation exchange, the total emissivity values of the cell and interconnect are required. For the solid-fluid heat exchange, the film coefficients for the fuel and oxidant streams are required. Presently, only single values (i.e. no dependence on temperature, composition, flow rate, etc.) are permitted for the film coefficient parameters.

By using the external boundary conditions, the heat transfer from the stack via convection and radiation can be simulated. The user assigns values for the total emissivity of the stack, total emissivity of the insulation, convection coefficient between the stack and insulation, convection coefficient between the insulation and the ambient environment, and the temperature of the ambient environment. For example, the ambient environment can be either a high temperature furnace (representative of a typical laboratory testing condition) or room temperature (representative of the self-heating mode for an installation). These boundary conditions parameters can also be varied independently for the top, bottom, front, back, and sides of the stack. Supplementary spreadsheet tools are provided for the user to calculate these boundary condition coefficients.

4.1.4 Material Properties

The only required material properties for the thermal solution are the thermal conductivities and total emissivities of the solid components as described above. The material properties required for the electrochemical solution are described in the following section.

4.1.5 Electrochemistry

The electrochemical response of the cell was made to be flexible for the user. The simplest option is to use the default internal electrochemistry model. This model is based on the semi-empirical approach established by Chick et al. (2000) and computes the working voltage from the Nernst voltage and various cell polarizations. The open circuit Nernst voltage is provided by Eq. (1) for the O_2 partial pressure at the anode/electrolyte interface given in Eq. (2) and computed from the change in Gibbs free energy of formation for the hydrogen oxidation reaction as shown in (3). Eq. (4)-(12) provide the ohmic loss due to contact resistance, the ohmic loss due to electrolyte ionic resistance, the ohmic loss due to anode electrical resistance, the ohmic loss due to cathode electrical resistance, the ohmic loss due to interconnect electrical resistance, a Butler-Volmer activation loss for the cathode, a concentration loss for the cathode, a concentration loss for the anode, and an empirical linear over-potential, respectively. The working voltage is then obtained from these voltage losses (computed as a function of the given current density, temperature, and species concentrations) according to Eq. (13).

$$E = \frac{R_G T}{4F} \ln\left(\frac{p_{O_2}^{cathode}}{p_{O_2}^{anode}} \right) \tag{1}$$

$$p_{O_2}^{anode} = \left(\frac{p_{H_2O}}{\exp(-\Delta G_f / R_G T) p_{H_2}} \right)^2 \tag{2}$$

$$-\Delta G_f = -56930 + 6.75 * T * \log_{10}(T) - 0.64\frac{T^2}{1000} - 0.08\frac{100000}{T} - 8.74T \tag{3}$$

$$\eta_{contact} = i\left(\frac{t_{contact}}{P_e \exp(E_a / RT)} \right) \tag{4}$$

$$\eta_{ohmic}^{electrolyte} = i\left(\frac{t_{electrolyte}}{\sigma_{YSZ}} \right) \tag{5}$$

$$\eta_{ohmic}^{anode} = i\left(\frac{t_{anode}}{\sigma_{Ni:YSZ}} \right) \tag{6}$$

$$\eta_{ohmic}^{cathode} = i\left(\frac{t_{cathode}}{\sigma_{LSM}} \right) \tag{7}$$

$$\eta_{ohmic}^{int\,erconnect} = i\left(\frac{t_{int\,erconnecte}}{\sigma_{steel}} \right) \tag{8}$$

$$\eta_{activation}^{cathode} = \frac{RT}{\alpha F} a \sinh\left(\frac{i}{2i_0} \right) \tag{9}$$

$$\eta_{concentration}^{cathode} = iP_{cop} \exp(k_{cop} p_{O_2}^{cathode}) \tag{10}$$

$$\eta_{concentration}^{anode} = \max\left(\exp(B_{aop} + D_{aop}(i + C_{aop}) - A_{aop}), 0 \right) \tag{11}$$

$$\eta_{lop} = \max\left(M_{lop} i + B_{lop}, 0 \right) \tag{12}$$

$$V(i) = E - \eta_{contact} - \eta_{ohmic}^{electrolyte} - \eta_{ohmic}^{anode} - \eta_{ohmic}^{cathode} - \eta_{ohmic}^{int\,erconnect}$$
$$- \eta_{activation}^{cathode} - \eta_{concentration}^{cathode} - \eta_{concentration}^{anode} - \eta_{lop} \tag{13}$$

The most flexible approach for modeling the electrochemistry is through a user subroutine where a custom current-voltage relationship can be created. This subroutine is called frequently during solution to compute the electrochemical response at every computational point on the cells. The solution call to the subroutine provides the present current density, fuel partial pressures, oxidant partial pressures, and temperature for the EC computations. The subroutine must then return the appropriate voltage value based on the programmed electrochemistry algorithm. The subroutine uses simple structures in the programming language called Lua (2011). The user should be able to start from the provided demonstration electrochemistry routines and adapt as necessary.

4.1.6 Units

The required units for the input parameters and user subroutines are indicated. The program uses SI units for most but not all parameters. Since the code is a research tool that supports existing users while undergoing development, mixed units still exist in various places as noted.

4.1.7 Numerical Solution Controls

Several parameters for control of the numerical solution are available to the user; however, most of these will not need to be altered. The primary parameter of interest is the number of computational points along the domain. The resolution of the model may be changed as needed to obtain finer results at the cost of longer computations, but generally a minimum of 100 solution points are suggested. If high gradients occur due to reforming, then greater resolution will be beneficial for better capturing the endothermic reaction. Other advanced parameters for solution control include temperature relaxation factors, time step, temperature limits, and iteration limits.

The solution is obtained when the temperature and current are converged. The tolerances for the temperature and total current are required. The demonstration values should be sufficient for most cases, but tolerances can be loosened to speed convergence.

TimeStep is a parameter introduced to stabilize the thermal computations. For co-flow cases, the value can be set to 0.1 or even larger. For counter-flow cases, due to the more unstable nature of the numerical approach, the value should be smaller, e.g., 0.001. When TimeStep value is very small, the speed of the numerical iterations toward the real thermal solution is artificially reduced so that even when the tolerances for temperature and current are met, the thermal solution is still not valid because the energy has not been balanced. Users are advised to check the energy balance, tighten the tolerance parameters and re-run the simulation until the energy is balanced.

A flag named SmartIterations is available for the model to automatically adjust TimeStep value. If SmartIterations is not set, or set to 0, the iterations will proceed as is. If SmartIterations is set to 1, the model will adjust TimeStep value when it sees necessary. This usually brings a faster convergence to an energy-balanced solution.

4.1.8 Input File Creation

The model input is provided by a simple text file called *EC_Dimension1_InputTable.dat* with a keyword format. Values are assigned to each of the pre-defined keywords described in the following section. The user should begin by modifying an existing demonstration input file. Comment lines in the input file are indicated with the # symbol at the beginning of the line.

4.1.9 Input File Keyword Descriptions

The available keywords, keyword descriptions, and example values are described in the following tables. These parameters define the model geometry (Table 1), fuel and oxidant definitions (Table 2), electrochemical operating parameters (Table 3), numerical model options (Table 4), material properties (Table 5), thermal boundary conditions (Table 6), in-progress electrode diffusion calculations (Table 7), and the default electrochemistry model (Table 8).

Table 1 Input File Keywords for Cell Geometry Definition

Keyword	Description	Example Values (units)
CELL PARAMETERS	Flag for 2D model input	
CoFlowFlag	Flow orientation of the cell	0 = counter-flow 1 = co-flow
Ax	Cell length	0.25 (m)
Ay	Cell width	0.25 (m)
nCells	Number of cells in stack	96
BottomPlateH	Thickness of bottom plate	0.005 (m)
PEN_H	Thickness of positive electrode/electrolyte/negative electrode	0.0005 (m)
InterConnectPlateH	Thickness of interconnect	0.0005 (m)
TopPlateH	Thickness of top plate	0.005 (m)
AirFlowH	Height of oxidant channel	0.001 (m)
FuelFlowH	Height of fuel channel	0.0005 (m)
InletArea	Inlet manifold area in contact between cells	0.0001 (m^2)
InletL	Effective height of inlet manifold area in contact	0.003 (m)
OutletArea	Outlet manifold area in contact between cells	0.0001 (m^2)
OutletL	Effective height of outlet manifold area in contact	0.003 (m)

Table 2 Input File Keywords for Fuel and Oxidant Definitions

Keyword	Description	Example Values (units)
SystemPressure	Inlet pressure for fuel/oxidant	1.0 (atm)
FuelFlowRate	Total molar flow rate	0.4 (mol/s)
FuelTemperature	Fuel inlet temperature	973 (°K)
FuelTonTop	Option fuel inlet temperature at top of stack	1003 (°K)
FuelH2	Mole fraction of H_2	0.7
FuelH2O	Mole fraction of H_2O	0.2
FuelCO	Mole fraction of CO	0.005
FuelCO2	Mole fraction of CO_2	0.005
FuelCH4	Mole fraction of CH_4	0.08
FuelN2	Mole fraction of N_2	0.01

OxidantFlowRate	Total molar flow rate	0.4 (mol/s)
OxidantTemperature	Oxidant inlet temperature	973 (°K)
OxidantTonTop	Optional oxidant inlet temperature at top of stack	1003 (°K)
OxidantO2	Mole fraction of O_2	0.21
OxidantN2	Mole fraction of N_2	0.79

Table 3 Input File Keywords for Electrochemical Operation Definition

Keyword	Description	Example Values (units)
Simulation_Option	Solution mode for the desired electrical target	0 = solve for voltage 1 = solve for current density 2 = solve for fuel utilization 3 = solve for stack I-V 4 = solve for stack I-V at fixed %UF
Average_CellVoltage	Solve for mean cell voltage (option 0)	0.75 (V)
StackVoltage	Solve for total stack voltage (option 0)	72.0 (V)
Average_CurrentDensity	Solve for mean cell current density (option 1)	5000 (A/m^2)
Fuel_Utilization	Solve for fixed fuel utilization (option 2)	0.65
Average_CellVoltage_Low	Lower voltage on sweep for I-V curve (option 3)	0.4 (V)
Average_CellVoltage_High	Upper voltage on sweep for I-V curve (option 3)	1.0 (V)
Average_CellVoltage_Increment	Voltage increment on sweep for I-V curve (option 3)	0.05 (V)
EC_Model_Option	Method to compute electrochemistry	0 = internal default 1 = user subroutine
ShortCurrent	*(work in progress)*	
CH4_Option	Method to compute CH_4 reforming rate	0 = equilibrium path length 2 = Achenbach rate 3 = user subroutine
EquilibriumPathCO	Distance over which CO shift reaction reaches equilibrium	0.001 (m)
EquilibriumPathCH4	Distance over which CH_4 reforming reaction reaches equilibrium	0.01 (m)

Table 4 Input File Keywords for Numerical Model Options

Keyword	Description	Example Values (units)
Nx	Number of solution increments along flow	100

TimeStep	A stabilizing coefficient for thermal computations	0.1 for co-flow <(3/Nx) for counter-flow
SmartIterations	A flag indicating whether the model will automatically adjust TimeStep value for the purpose of speeding up the convergence	0 = do not adjust TimeStep 1 = allow model to adjust TimeStep
T_Relaxation	Relaxation factor for temperature calculation	0.9
T_TopLimit	Upper limit for temperature iterations	950 (°C)
T_BottomLimit	Lower limit for temperature iterations	650 (°C)
VoltageIncrement	Maximum increment of voltage between iterations	0.001 (V)
H2_Threshold	Lower threshold for H_2 partial pressure	0.0001 (Pa)
H2_Threshold_Current	Current generated at H_2 lower threshold	0.0001 (A/m^2)
VoltageIterationLimit	Maximum number of voltage/current iterations	100
LimitTiterations	Maximum number of temperature iterations	20
UserDefinedHeat	Use user defined thermal conductivities	0 = default 1 = user subroutine
QuasiTransient	(work in progress)	
HaveConductionOnInlet	Flag for thermal conduction between cells at inlet/outlet	0 = ignore 1 = include
PrintBalances	Flag to print species balances	0 = do not print 1 = print
NoDiffusion	Flag to activate electrode diffusion calculations	0 = include 1 = do not include
PrintDiffusionDifference	Flag to print electrode diffusion results	0 = do not print 1 = print
T_precision	Convergence criterion for maximum temperature variation between iterations	0.2 (V)
CurrentTolerance	Convergence criterion for maximum current density variation from the average	0.2 (A/m^2)

Table 5 Input File Keywords for Material Property Definitions

Keyword	Description	Example Values (units)
OxidantSolidFilmCoefficient	Film coefficient for oxidant convection with PEN and	500 (W/m^2-K)

	interconnect	
FuelSolidFilmCoefficient	Film coefficient for fuel convection with PEN and interconnect	1200 (W/m^2-K)
InterConnectEmittance	Emmissivity for radiation heat transfer from interconnect	0.9
PENEmittence	Emmissivity for radiation heat transfer from PEN	0.9
BottomPlateHC	Thermal conductivity of bottom plate	25.5 (W/m-K)
InterConnectPlateHC	Thermal conductivity of interconnect	25.5 (W/m-K)
TopPlateHC	Thermal conductivity of top plate	25.5 (W/m-K)
PEN_HC	Thermal conductivity of PEN	5.0 (W/m-K)
InletHC	Thermal conductivity of inlet manifold	25.5 (W/m-K)
OutletHC	Thermal conductivity of outlet manifold	25.5 (W/m-K)
CP_pen	Specific heat of PEN	400 (J/kg-K)
CP_plate	Specific heat of interconnect	400 (J/kg-K)

Table 6 Input File Keywords for Thermal Boundary Condition Definition

Keyword	Description	Example Values (units)
BoundaryFlag	Flag indicating type of external environment	1 = ambient temperature 2 = insulated enclosure
TopEnvironmentT	Top ambient temperature	750 (°C)
TopFilmCoefficient	Film coefficient for top insulation convection	12 (W/m^2-K)
TopEmissivity	Emmissivity for top insulation radiation	0.9
TopSIFilmCoefficient	Film coefficient for top stack-insulation convection	12 (W/m^2-K)
TopSIEmissivity	Emmissivity for top stack-insulation radiation	0.9
TopIsolationH	Thickness of top insulation	0.05 (m)
TopIsolationHC	Thermal conductivity of top insulation	1.0 (W/m-K)
TopGeometryScale	Scale factor for top area	1.2
BottomEnvironmentT	Bottom ambient temperature	750 (°C)
BottomFilmCoefficient	Film coefficient for bottom insulation convection	12 (W/m^2-K)
BottomEmissivity	Emmissivity for bottom insulation radiation	0.9

BottomSIFilmCoefficient	Film coefficient for bottom stack-insulation convection	12 (W/m^2-K)
BottomSIEmissivity	Emmissivity for bottom stack-insulation radiation	0.9
BottomIsolationH	Thickness of bottom insulation	0.05 (m)
BottomIsolationHC	Thermal conductivity of bottom insulation	1.0 (W/m-K)
BottomGeometryScale	Scale factor for bottom area	1.2
FrontEnvironmentT	Front ambient temperature	750 (°C)
FrontFilmCoefficient	Film coefficient for front insulation convection	12 (W/m^2-K)
FrontEmissivity	Emmissivity for front insulation radiation	0.9
FrontSIFilmCoefficient	Film coefficient for front stack-insulation convection	12 (W/m^2-K)
FrontSIEmissivity	Emmissivity for front stack-insulation radiation	0.9
FrontIsolationH	Thickness of front insulation	0.05 (m)
FrontIsolationHC	Thermal conductivity of front insulation	1.0 (W/m-K)
FrontGeometryScale	Scale factor for front area	1.2
BackEnvironmentT	Back ambient temperature	750 (°C)
BackFilmCoefficient	Film coefficient for back insulation convection	12 (W/m^2-K)
BackEmissivity	Emmissivity for back insulation radiation	0.9
BackSIFilmCoefficient	Film coefficient for back stack-insulation convection	12 (W/m^2-K)
BackSIEmissivity	Emmissivity for back stack-insulation radiation	0.9
BackIsolationH	Thickness of back insulation	0.05 (m)
BackIsolationHC	Thermal conductivity of back insulation	1.0 (W/m-K)
BackGeometryScale	Scale factor for back area	1.2
SideEnvironmentT	Side ambient temperature	750 (°C)
SideFilmCoefficient	Film coefficient for side insulation convection	12 (W/m^2-K)
SideEmissivity	Emmissivity for side insulation radiation	0.9
SideSIFilmCoefficient	Film coefficient for side stack-insulation convection	12 (W/m^2-K)
SideSIEmissivity	Emmissivity for side stack-insulation radiation	0.9
SideIsolationH	Thickness of side insulation	0.05 (m)

| SideIsolationHC | Thermal conductivity of side insulation | 1.0 (W/m-K) |
| SideGeometryScale | Scale factor for side area | 1.2 |

Table 7 Input File Keywords for Electrode Diffusion Computation

Keyword	Description	Example Values (units)
nLayers	Number of layers for electrode diffusion calculation *(work in progress)*	3
nSpecies	Number of species	6
Thickness	Total PEN thickness	560 (μm)
Tortuosity	Electrode tortuosity	1.1
Porosity	Electrode porosity	55 (%)
PoreRadius	Electrode pore radius	0.5 (μm)
ElectrolyteThickness	Electrolyte thickness	10 (μm)
InterconnectThickness	Interconnnect thickness	1500 (μm)
CathodeThickness	Cathode thickness	50 (μm)
CathodePorosity	Cathode porosity	55 (%)
CathodeTortuosity	Cathode tortuosity	1.1
AnodeThickness	Anode thickness	500 (μm)
AnodePorosity	Anode porosity	55 (%)
Anode Tortuosity	Anode tortuosity	1.1

Table 8 Input File Keywords for Default Electrochemistry Definition

Keyword	Description	Example Values (units)
ScaleThickness	Interconnect scale thickness	0.3 (μm)
PreExponent	Scale resistance pre-exponential constant	10
ActivationEnergy	Scale resistance activation energy	0.2
CathodePreExponent	Pre-exponential coefficient for cathode resistance	575955
CathodeActivationEnergy	Activation energy for cathode resistance	0.117
BV_AlphaCoefficient	α for Butler-Volmer activation polarization	0.55
BV_ActivationEnergy	E_a for Butler-Volmer activation polarization	1.2
BV_PreExponent_a	Pre-exponential coefficient a for Butler-Volmer activation polarization	-120
BV_PreExponent_b	Pre-exponential coefficient b for Butler-Volmer activation	2.3e5

	polarization	
CathodeDepletionCoefficinet_a	Cathode concentration overpotential coefficient	3
CathodeDepletionCoefficient_b	Cathode concentration overpotential coefficient	-35
LOP_slope	Linear overpotential coefficient	0.2027
LOP_is	Linear overpotential coefficient	-8.897e-4
LOP_ii	Linear overpotential coefficient	0.5221
AOP_ns	Anode concentration overpotential coefficient	2.439e-3
AOP_ni	Anode concentration overpotential coefficient	-2.358
AOP_qs	Anode concentration overpotential coefficient	1.747e-2
AOP_qi	Anode concentration overpotential coefficient	-17.73
AOP_ms	Anode concentration overpotential coefficient	-1.158e-2
AOP_mi	Anode concentration overpotential coefficient	11.06
AOP_ps	Anode concentration overpotential coefficient	6.560e-4
AOP_pi	Anode concentration overpotential coefficient	-1.152
VTC	(work in progress)	

4.1.10 Creation of Custom Electrochemistry Subroutine

The subroutine file *VoltageOnCurrent.dat* contains the required user subroutines for the electrochemistry calculations. The subroutine *VoltageValue* contains the coding necessary to input the current-voltage relationship for the model. The subroutine must return the voltage based on the supplied temperatures, fuel partial pressures, oxygen partial pressure, and requested current density. Using the inherent mathematical functions available in Lua (or even high level programming constructs), the user should be able to replicate their electrochemistry routine or experimental data for use in the model. The equations or data should cover the entire expected range of operation within the stack. Specifically, the iterations begin with requests for voltage at extreme currents of 1e-5 and 5e3 A/cm^2, so the routine should return a voltage value for these limits (e.g. if the requested current is above a calculated limiting current then the routine should return a voltage of 0.0).The arguments for the subroutine are shown in Table 9.

Table 9 Available Arguments in the I-V User Subroutine

Subroutine Arguments	Description

oT	Temperature of oxidant (°K)
cT	Temperature of cell (°K)
fT	Temperature of fuel (°K)
J	Current density (A/cm^2)
pO2air	Oxidant partial pressure O_2 (atm)
pN2air	Oxidant partial pressure N_2 (atm)
pH2	Fuel partial pressure H_2 (atm)
pH2O	Fuel partial pressure H_2O (atm)
pCO	Fuel partial pressure CO (atm)
pCO2	Fuel partial pressure CO_2 (atm)
pCH4	Fuel partial pressure CH_4 (atm)
pN2	Fuel partial pressure N_2 (atm)
nActiveCell	Cell number in the stack (1 is bottom)
DistanceFromTheEdge	Distance along the fuel flow direction (m)
DistanceFromTheEdgeRatio	Normalized distance along the fuel flow direction
Z	The voltage to be returned (V)

4.1.11 Creation of Custom Reforming Rate Subroutine

If the fuel contains methane for on-cell reforming, the reforming rate of the methane can also be customized with the subroutine *CH4ReformingRate*. The solver assumes the rate of methane reformation is kinetically controlled, so this subroutine returns the maximum rate of reforming. If used, the appropriate flag in the *EC_Dimension1_InputTable.dat* file must be set and the subroutine is placed in the same *VoltageOnCurrent.dat* file that contains the I-V user subroutine. The subroutine arguments are shown in Table 10.

Table 10 Available Arguments in the CH$_4$ Reforming User Subroutine

Subroutine Arguments	Description
fuelT	Temperature of fuel (°K)
pCH4	Fuel partial pressure CH_4 (atm)
Ch4_Usage	Rate of reformation to be returned (mol/s)

4.2 Solution

The solution is obtained by running the single executable file on the input file. This can be done using the provided execution scripts or directly from the command line. The solution procedure creates output files that provide solution status, final results, results summary, and model debugging information.

4.2.1 Submission on MS Windows Platform

To run a job on the Windows platform, it is assumed that the executable is installed correctly and in the system path so that it is accessible from any working directory. If the PATH variable was not set as indicated, then the user needs to copy the executable file and all the DLL files to the runtime directory. Then, the case can be run by the following steps:

1. To run SOFC-MP for each case, go to the appropriate directory of the selected demonstration case and double click the batch file named "^^^2D_Run_First_Time^^^.bat". It will copy all necessary files to the current directory and start the SOFC-MP 2D simulation.

2. To use an input file other than the default "EC_Dimension1_InputTable.dat", for example, "myInput.dat", type command "EC_IntegralModel.exe myInput.dat" in a DOS command prompt.

3. Check the status of the program: Depending on the size of the model, the program can last anywhere from 1 minute to up to 1 hour. Check a debugging file named "RunMonitor.dat", if the last line writes "Two Dimensional program ends at xx:xx:xx", then the program has finished. An alternative is to check the Windows Task Manager, under Processes tab, wait until "EC_IntegralModel.exe" disappears.

4.2.2 Submission on Linux Platform

Once the environment variables are set as described in Section 3.2, to run SOFC-MP 2D in the input directory simply type:

```
$ sofc [inputFile]
```

Note, without the optional parameter [inputFile], the model will assume the input file as EC_Dimension1_InputTable.dat.

4.2.3 Description of Output Files

Several output files are created upon completion of the solution. These text files may be viewed directly if needed, but usually they are simply read into the spreadsheet tool created for automated post-processing. The files are as follows:

- M odelOutput.dat – the main output file containing major result matrix such as electrical performance, temperature metrics, flow characteristics.
- CurrentInCellsLatest.dat – a result file, containing active voltage and current at each cell.
- StackTemperature.txt – a result file containing temperature at each node.
- StackFractions.txt – a result file containing fuel and air composition at each node.
- Stat.dat - data for electrochemistry heat balance.
- IterFl.dat – a debugging file detailing the convergence on temperature field matrix equation residual.
- Stack1D.txt – a result file containing temperature and fuel composition data.
- SavedState.dat – voltage and temperature data saved from last program run. If the program runs again, the data in the file will be read in and used as the initial condition. A subsequent run with SavedState.dat usually has much faster convergence.
- RunMonitor.dat – main debugging file. Useful information includes the numerical iteration and performance data.
- Solidstat.dat – a debugging file containing information on temperature matrix solver.
- WatchInitFl_00.dat – a debugging file containing information about gas species.
- FlowStat.dat – a debugging file containing fuel flow information during the numerical iteration process.

- AirStat.dat – a debugging file containing air flow information during the numerical iteration process.
- CurrentInCells.dat – a debugging file containing current distribution during the numerical iteration process.
- Cea2.out – output file from the CEA library.
- Cea_message.dat – debugging information for CEA interfacing.

4.3   Post-Processing

The model output results are contained within simple ASCII text files, so they can be viewed by the user or read into a spreadsheet if desired. However, the simplest approach is to use the provided post-processing spreadsheet tool created with Microsoft Excel 2007 for use with SOFC-MP 2D. The spreadsheet reads in the results data files from SOFC-MP 2D and automatically calculates the performance metrics of interest to the designer. The objective of this tool was to provide a mechanism for rapid evaluation and understanding of the numerical results. The file *2D_template_rev18_distribute.xlsm* is provided on the demonstration CD under the */Utilities* directory. For simulations ran on Linux, all result files can be copied to Windows file system for this post-processing purpose.

4.3.1   Open the Excel Spreadsheet Tool

Copy the spreadsheet to a convenient location and open it with Excel 2007 (the worksheet apparently works with Excel 2003, but it becomes a very large file size and all calculation features are not supported). The spreadsheet provides a method to select the working directory where the results are located, so it does not need to be re-copied to the working directory for every analysis. Upon opening the spreadsheet, a warning window may appear or the information bar at the top of the spreadsheet cells may indicate "Security Warning: Some active content has been disabled." The spreadsheet makes considerable use of Data Connections (to read in the results files) and Macros (to perform calculations and control the data input), so these advanced features must be enabled for the worksheet to function properly. Select "Enable this content" for both Macro and Data Connection.

4.3.2   Worksheets in the Excel Spreadsheet Tool

The user will primarily work with the *Summary* worksheet for their analysis as described in detail below. The preceding worksheets in the workbook are first briefly explained. The *Info* worksheet contains some basic description of the worksheet contents, and the next few worksheets hold the imported results data. The spreadsheet reads the results files and places the data into the tool's worksheets as shown in Table 11. The user generally does not need to utilize these sheets directly.

Table 11. Results Files Read Into the Post-Processing Tool

Results Filename	Worksheet	Data Contents
EC_Dimension1_InputTable.dat	Import1	All model input parameters
CurrentInCellsLatest.dat	Import2	Voltage and current for each cell
StackTemperature.txt	Import3	Temperature and current density distributions along each cell
StackFractions.txt	Import4	Species distributions along each cell

Stat.dat	Import5	Energy balance terms
IterFl.dat	Import6	Solution iteration history

The computations for data reduction and synthesis are performed on the worksheets listed in Table 12. The user generally does not need to utilize these sheets directly.

Table 12. Calculation Worksheets in the Post-Processing Tool

Worksheet Name	Calculations and Output
Calc1	Min/Max/Average temperatures for components at cell and stack level
Calc2	Min/Max/Average current, current density, and voltage
Calc3	Average outlet species compositions at cell and stack level
Calc4	Manual calculation to verify energy balance computations
Calc5	Selected distribution data for plotting

The *Summary* worksheet is the primary sheet of interest. This 'dashboard' shows all of the calculated metrics based on the latest SOFC-MP run and will be described in detail below. The remaining worksheets contain various calculators to support modeling cases or calculations used for development and verification of the model (Table 13).

Table 13. Supplementary Worksheets in the Post-Processing Tool

Worksheet Name	Description
Saved_Cases	Archival of saved results
Calculators	Supplementary calculation tools to aid the user
EnergyCheck	Simple energy balance check for the stack

4.3.3 Import Data to the Excel Spreadsheet Tool

Two large buttons on the *Summary* worksheet are used to automatically read in the results data (Figure 1). The "Change working directory and re-import all data files!" button allows the user to navigate their file system using a conventional explorer window to select the working directory where SOFC-MP 2D results are located. Upon selection, the data import process proceeds, all calculations are performed, and a window confirms successful data import. The second button entitled "Re-import all data files!" performs the same import and calculation function from the previous working directory shown above the buttons in cell **L17**. This option would be used for subsequent runs of the same model. The following discussion about the results all focus on content within this *Summary* worksheet.

Current Working Directory:	
G:\CDbenchmarks\2D\2Dcase09	
Change working directory and re-import all data files!	
Re-import all data files!	
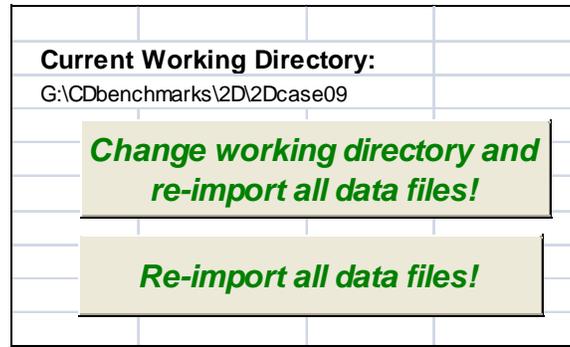
Figure 1. Worksheet buttons used for data import

4.3.4 Convergence Check

Before evaluating model results, the user should always ensure the model is fully converged. If the model did not have sufficient iterations to solve or did not converge due to other reasons, any results are likely erroneous and should be ignored. Some important indicators are shown in the lower left side of the Convergence Assessment block (Figure 2). The values for the current and temperature imbalance are shown along with the assigned tolerance limit. These are the most important values to check regarding solution convergence. If the final value is greater than the limit, then the corresponding current or temperatures are not fully converged and indicated with a warning message. The model likely needs to be run again with additional iterations. Next, the maximum and minimum model temperatures are indicated along with the assigned upper and lower limits on the solution iteration. If the solution values are near these limits, a warning message is indicated and the model may be ill defined or the limits need to be expanded. The next two values indicate the number of voltage and temperature iterations compared to the assigned limits. Usually, if the iterations reach the assigned limit, then the current and temperature is not yet converged and the model should be run with additional iterations.

Convergence Assessment				
Current converged within assigned limit				
Final value:	0.2320		Limit:	0.3
Temperature converged within assigned limit				
Final value:	0.02		Limit:	0.05
Global temperatures within user upper limit				
Maximum value:	848.6		Limit:	900
Global temperatures within user lower limit				
Minimum value:	707.9		Limit:	650.0
Voltage iterations within assigned limit				
Final value:	1		Limit:	20
Temperature iterations within assigned limit				
Final value:	0		Limit:	10

Figure 2. Convergence parameters and criteria to assess solution convergence

4.3.5 Model Data

Selected model data are summarized to verify the model under consideration. The flow orientation for the fuel and air is shown in **B3:D3** (Figure 3a). The number of cells and cell

19

geometry is shown in **C6:C11** (Figure 3b). The inlet mole fractions of the fuel are shown in **B28:E36**, and the corresponding molar flow rates are shown in **G27:J35**.

Cell Geometry		
# cells =	96	
cell length =	0.25	(m)
cell width =	0.25	(m)
cell area =	0.0625	(m^2)
cell area =	625	(cm^2)
total Area =	60000	(cm^2)
# path increments =	100	

Flow Orientation		
1	----->>>	---->>>
CO-FLOW	Fuel	Air

Figure 3. Flow orientation and cell geometry parameters

4.3.6 Performance Metrics

Many performance metrics of interest are shown on the *Summary* worksheet. The electrical performance is shown in **C15:D26** (Figure 4). Here the total current, average current density, average power density, total voltage, average voltage, and total power are reported. The fuel and air utilizations are shown **F16:J24** (Figure 5). The net output fuel mole fractions and flow rates are shown in **B28:E36** (Figure 6) and **G27:J35** (Figure 7), respectively. If CH_4 is present in the fuel, the percentage of on-cell reforming is shown in **J36**. The temperature results including average cell temperature, cell temperature difference, cathode air temperature change, and anode fuel temperature change are shown in **F2:K13** (Figure 8). The energy balance including the change of fuel enthalpy, electrical power, change in air enthalpy, and external loss to the environment is shown in **M2:P12** (Figure 9). These are expected to be the primary metrics needed by the user, although others can be easily added.

Electrical Performance		
	Current (A)	**Voltage (V)**
total =	312.425	**81.7920**
average =		**0.8520**
min =	312.193	0.8419
max =	312.447	0.8574
max delta from total =	0.2320	0.0155
%delta =	0.07%	1.82%
avg current density =	**0.4999**	(A/cm^2)
max current density =	0.6198	(A/cm^2)
avg power density =	**0.4259**	(W/cm^2)
total power =	25553.9	(W)

Figure 4. Stack electrical performance summary

Fuel/Oxidant Flow			
inlet air flow rate =	2.47E+00	mole/s
inlet air flow rate =	3319.680	slpm
O2 current =	7.77E-02	mole/s
stoichs oxidant =	6.67	
air utilization =	**14.98%**	
inlet fuel flow rate =	2.47E-01	mole/s
inlet fuel flow rate =	331.968	slpm
outlet fuel flow rate =	2.47E-01	mole/s
fuel utilization =	**64.87%**	

Figure 5. Stack air and fuel utilization

Species Mole Fractions			
Fuel	**Inlet**	**Cell edge**	**Outlet**
H2	0.9700	0.9638	0.3408
H2O	0.0300	0.0362	0.6592
CO	0.0000	0.0000	0.0000
CO2	0.0000	0.0000	0.0000
CH4	0.0000	0.0000	0.0000
N2	0.0000	0.0000	0.0000
total	1.0000	1.0000	1.0000
fuel value	0.9700	0.9638	0.3408

Figure 6. Stack inlet and outlet fuel molar fractions

Species Molar Flow Rates			
Fuel	**Inlet (mol/s)**	**Cell edge (mol/s)**	**Outlet (mol/s)**
H2	2.40E-01	2.38E-01	8.42E-02
H2O	7.41E-03	8.94E-03	1.63E-01
CO	0.00E+00	0.00E+00	0.00E+00
CO2	0.00E+00	0.00E+00	0.00E+00
CH4	0.00E+00	0.00E+00	0.00E+00
N2	0.00E+00	0.00E+00	0.00E+00
total	2.47E-01	2.47E-01	2.47E-01
fuel flow	2.40E-01	2.38E-01	8.42E-02
		OCR	**N.A.**

Figure 7. Stack inlet and outlet fuel molar flow rates

Energy Balance		
(negative = heating the stack)		
heat loss top =	271.800	(W)
heat loss bottom =	222.373	(W)
heat loss front =	-197.017	(W)
heat loss back =	590.065	(W)
heat loss sides =	1348.070	(W)
total ext heat loss =	2235.291	(W)
net chemical energy =	35650.200	(W)
electrical energy =	-25553.900	(W)
heat removed by air =	-7862.110	(W)
external heat removed =	-2235.291	(W)
imbalance =	-1.101	(W)

Figure 8. Stack energy balance

4.3.7 Distributions and Plotting

The *Summary* worksheet also permits the plotting of distributions of quantities along the cell length to aid understanding. The worksheet is created to allow the user to plot quantities for three different cells from the multi-cell stack. The green numbers in **R3:R5** can be changed to indicate the cell data to be plotted (Figure 9). The directions of fuel and air flow in the cell plots are shown in **R8:T9** where cell #1 is at the bottom of the stack by definition. The plots include:

- fuel mole fractions as a function of path length
- working voltage as a function of cell number
- current density as a function of path length
- cell temperature as a function of path length
- fuel temperature as a function of cell length
- air temperature as a function of cell length
- minimum, maximum, and average cell temperature as a function of cell number
- cell temperature difference as a function of cell number

Example plots are shown in Figure 10-Figure 13. The user may control the plotting ranges in the conventional way, but additional buttons for semiautomatic range control of the figures are included in **O45:U54** (Figure 14).

Results Plotting by Cell		
Cell #	Label	
1	Cell #1	
24	Cell #24	
48	Cell #48	
Flow Directions for Path Plots		
---->>>	Fuel Flow	---->>>
---->>>	Air Flow	---->>>
Cell #1	Bottom of Stack	
Cell #96	Top of Stack	

Figure 9. Selection of different cells for results distribution plotting
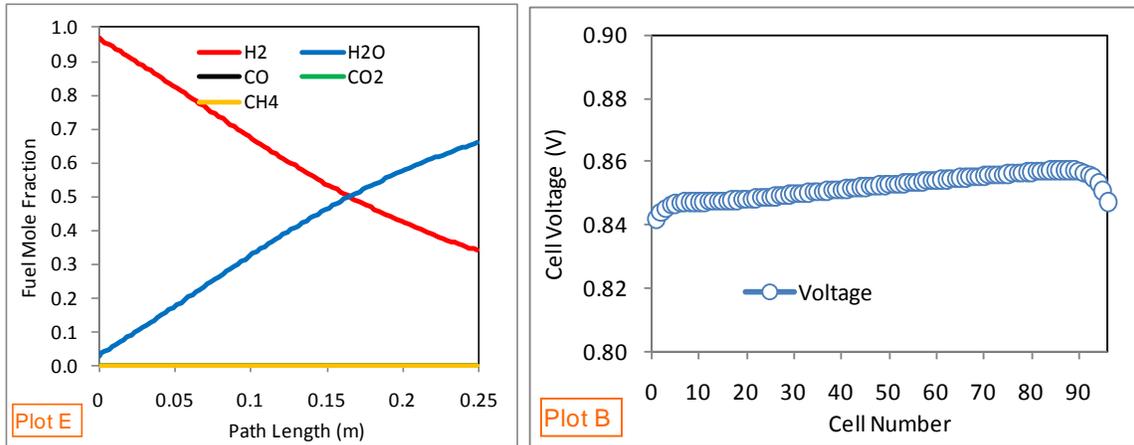
Figure 10. Contours of a) fuel mole fractions along the cell and b) distribution of the cell voltage through the stack height
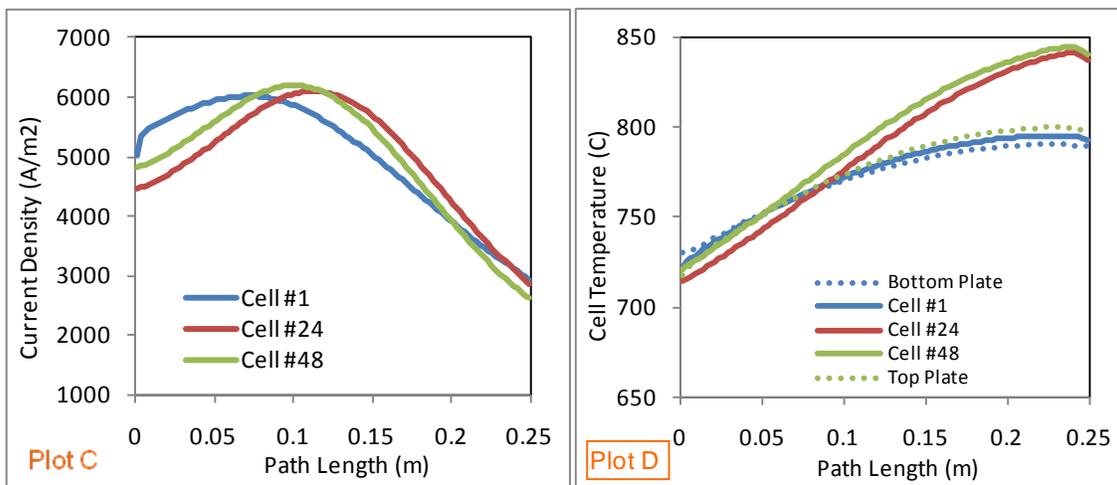
Figure 11. Contours of the a) current density and b) cell temperature along the cell
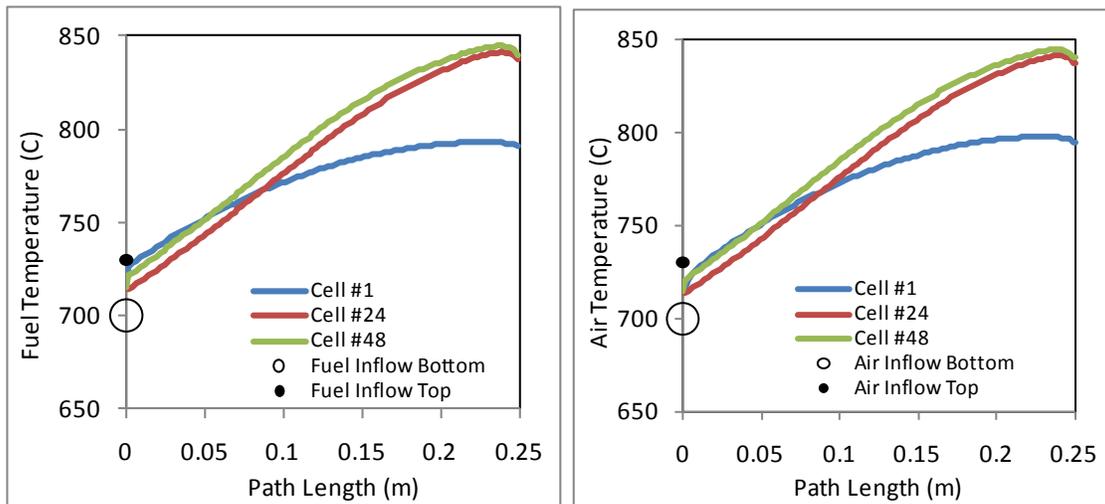
Figure 12. Contours of the a) fuel and b) air temperature along the cell
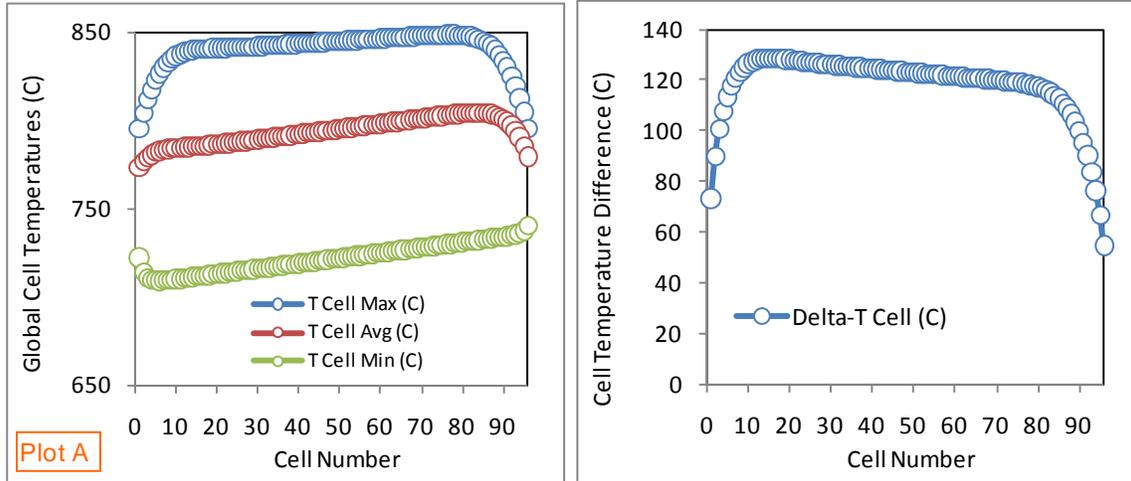
Figure 13. Distribution of the a) minimum, maximum, and average cell temperatures and b) cell temperature difference through the stack height

x_min	0	0	0	0	0	0
x_max	96	96	0.25	0.25	0.25	0.25
x_ticks	10	10	0.05	0.05	0.05	0.05
y_min	650	0.8	1000	650	0	0
y_max	850	0.9	7000	850	1	0.04
y_ticks	100	0.02	1000	50	0.1	0.02
	Format Plot A	Format Plot B	Format Plot C	Format Plot D	Format Plot E	Format Plot F
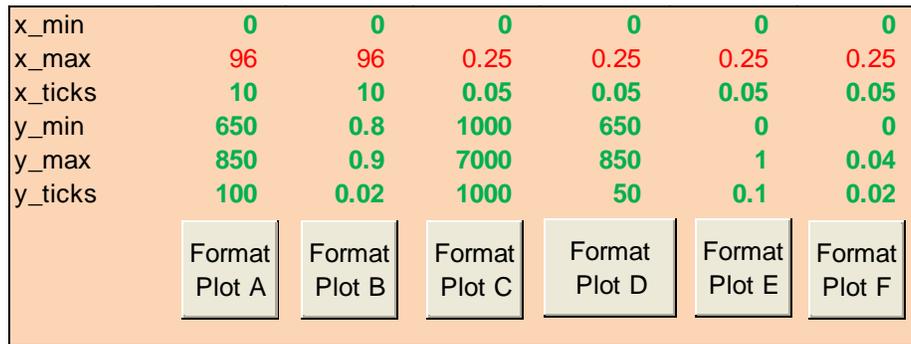
Figure 14. Buttons to control axes for results graphs.

4.3.8 Data Archival

The *Summary* worksheet also permits the user to archive results data. Buttons to archive the current results set or clear the archive are located on the *Summary* worksheet (Figure 15). This button calls a macro which most of the calculated results metrics on a single line in the *Saved_Cases* worksheet. The data can then be recalled if needed or used for plotting and comparisons between multiple cases in a sensitivity analyses.

Archive Case Results	Clear Archive
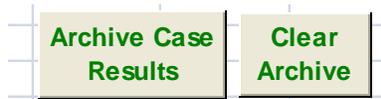
Figure 15. Buttons to archive solution data.

5.0 Demonstration Cases

Several cases are explained in further detail here to demonstrate how to use the tool to solve stack problems.

5.1 Single Co-Flow Cell with H$_2$ Fuel

The first example is a single cell co-flow model reported by the International Energy Agency (Achenbach 1996) and used subsequently as an informal benchmark in the SOFC community (Ferguson et al 1996, Braun 2002, Zhang et al 2006, Li et al 2010). This represents the simplest case that can be considered by using only a single cell, wet hydrogen fuel, adiabatic boundary conditions, and the co-flow orientation which is generally more numerically stable than counter-flow. Model development involves definition of two primary files: the input data file *EC_Dimension1_InputTable.dat* and the user subroutine *VoltageOnCurrent.dat* containing the electrochemistry routine.

5.1.1 Creation of EC_Dimension1_InputTable.dat File for Example Case 1

This file contains all of the cell geometry, thermal material properties, fuel/oxidant input conditions, thermal boundary conditions, and solution controls for the stack model. The easiest way to create this file is to modify an existing input file. Specifically, the definition of this example requires assignment of the following keywords:

Table 14 Keyword Assignments for Example Case 1

Keyword Assignment	Description
CoFlowFlag = 1	Co-flow cell
nCells=1	Use a single cell
Ax = 0.1	Cell length along flow direction is 10 cm
Ay = 0.1	Cell width is 10 cm
PEN_H = 0.00025	Cell thickness = 50 μm anode + 50 μm cathode + 150 μm electrolyte = 250 μm
InterConnectPlateH = 0.001393	Effective interconnect thickness accounting for ribs = 0.5 mm + 2.42/5.42*2 mm = 1.393 mm
BottomPlateH = 0.000946	Effective bottom plate thickness accounting for ribs = 0.5 mm + 2.42/5.42 mm = 0.946 mm
TopPlateH = 0.000946	Effective top plate thickness accounting for ribs = 0.5 mm + 2.42/5.42 mm = 0.946 mm
AirFlowH = 0.000554	Effective air flow height = 1*3/5.42 = 0.554 mm
FuelFLowH = 0.000554	Effective fuel flow height = 1*3/5.42 = 0.554 mm
CoFlowFlag = 1	Flag = 1 for co-flow, 0 for counter-flow
FuelFlowRate = 0.00020325	2.0325e-4 mol/s fuel to give 85% utilization
FuelTemperature = 1173	900°C inlet fuel temperature
FuelH2 = 0.90	90% hydrogen
FuelH2O = 0.10	10% water
OxidantFlowRate = 0.0030485	3.0485e-3 mol/s air to give 12.15% utilization
OxidantTemperature = 1173	900°C inlet air temperature
OxidantO2 = 0.21	Standard air composition
OxidantN2 = 0.79	Standard air composition
OxidantSolidFilmCoefficient = 1035	Effective film coefficient
FuelSolidFilmCoefficient = 1500	Effective film coefficient
InterConnectPlateHC = 2.0	Thermal conductivity of interconnect

PENEmittence = 0.5	Effective PEN emissivity
InterConnectEmittance = 0.5	Effective interconnect emissivity
BottomPlateHC = 2.0	Thermal conductivity of bottom plate
TopPlateHC = 2.0	Thermal conductivity of top plate
PEN_HC = 2.0	Thermal conductivity of cell
StackVoltage = 0.70875	Solve for assigned voltage to obtain a current density of 0.3 A/cm^2

The values above include effective values for the components, channel heights, and heat transfer parameters to account for the ribbed interconnect. The effective thickness for the simple plate interconnect provides the same cross-sectional area as the ribbed interconnect design for the same in-plane heat transfer by thermal conduction. The effective height for the simple flow channel provides the same cross-sectional flow area as the ribbed channel design for the same volumetric flow rate. The effective film coefficients provide the appropriate heat transfer between solid and fluid to account for both the convection through the ribbed interconnect channels and the conduction through the rib. The effective emissivities account for the different view areas between the ribbed interconnect and the simple interconnect. A pre-processing calculator to compute these effective properties based on the nominal material properties and rib geometry is included in the spreadsheet. The full details of the input file are provided in Appendix A.

5.1.2 Creation of VoltageOnCurrent.dat File for Example Case 1

The subroutine file *VoltageOnCurrent.dat* contains the required user subroutines for the electrochemistry calculations necessary to input the current-voltage relationship for the model. The subroutine returns the voltage based on the supplied temperatures, fuel partial pressures, oxygen partial pressure, and requested current density. The *VoltageOnCurrent.dat* file for the user subroutine is then created and placed in the working directory. The example subroutine *VoltageValue()* for the Achenbach benchmark case with H$_2$ fuel is shown in Figure 16. Upon being called from the main program, the code sets various parameters necessary for the computations including the ideal gas constant, Faraday's constant, a pressure conversion factor, and thickness values for the anode, electrolyte, cathode, and interconnect. Note that this model simulates an older electrolyte-supported technology which had much lower power densities than modern cell designs. Next, the reaction temperature is computed from the average of the oxidant and fuel temperatures. The partial pressures of the fuel species are then converted to units of bar to be consistent with the benchmark, and the input current density is converted from A/m^2 to A/cm^2. Next, the ohmic resistances of the cell layers are computed based on their thicknesses and resistivities, and these values are summed for the total ohmic loss. Next, the open circuit voltage is computed based on the change in Gibbs free energy of formation and adjusted for the actual partial pressures of the reactants. For this benchmark, the concentration and activation losses were not computed and it was assumed for simplicity that these polarization losses are equal to the ohmic loss. Therefore, the working voltage is then computed by subtracting the polarization losses from the Nernst voltage. The voltage is then checked, and any negative values are assigned a small positive value for improved numerical stability. Finally, the computed working voltage is returned to the solver.

```
-- EC based on Achenbach benchmark paper for H2 fuel
--
function VoltageValue()
--
-- Assign Constants/Conversions/Geometry/Material Data
R=8.3145; F=96485.3; atm2bar=1.01325
th_a=50.0e-6; th_e=150.0e-6; th_c=50.0e-6; th_ic=2500.0e-6
--
-- Compute the local cell temperature
Tk=(oT+fT)/2.0
--
-- Compute the total pressure & convert to bar
pO2airc=pO2air*atm2bar; pN2airc=pN2air*atm2bar
pH2c=pH2*atm2bar;       pH2Oc=pH2O*atm2bar;    pCOc=pCO*atm2bar
pCO2c=pCO2*atm2bar;     pCH4c=pCH4*atm2bar;    pN2c=pN2*atm2bar
Ptotal=pH2c+pH2Oc+pCOc+pCO2c+pCH4c+pN2c
--
-- Convert the passed current density
Jcalc=J*10000.
--
-- Calculate ohmic resistance
siga=95.0e6/Tk*math.exp(-1150.0/Tk)
sigc=42.0e6/Tk*math.exp(-1200.0/Tk)
sige=3.34e4*math.exp(-10300.0/Tk)
sigic=9.3e6/Tk*math.exp(-1100.0/Tk)
RohmIC=0.0025/sigic
Rohm=th_a/siga+th_c/sigc+th_e/sige+RohmIC
--
-- Calculate the open cell voltage
U00H2O=(241.106-3.804e-2*Tk-1.402e-5*Tk^2+3.551e-9*Tk^3)*1000.0/2.0/F
U0H2=U00H2O-R*Tk/2.0/F*math.log(pH2Oc/pH2c/pO2airc^0.5)
--
-- Calculate the working voltage
UH2=U0H2-(Rohm*Jcalc+Rohm*Jcalc+Rohm*Jcalc)
Z=UH2
--
-- Return the voltage value (not less than zero)
if Z<0.0 then
  Z=0.001
end
return Z
end
```

Figure 16. I-V user subroutine for example Case 1.

5.1.3 Results for Example Case 1

Selected results for this case are shown in Figure 17. These species distribution indicates consumption of the H_2 fuel along the cell (Figure 17a) resulting in a current density distribution that is highest at the fuel rich inlet (Figure 17c) and a temperature distribution that is hottest at the outlet due to the heat removal from the oxidant and fuel gases (Figure 17d). The results predictions were also compared to the metrics in the literature (Figure 18, Figure 19) and found that the model results fall well within the range of the reported values. More details on the model validation and comparisons are found in Lai et al (2010).
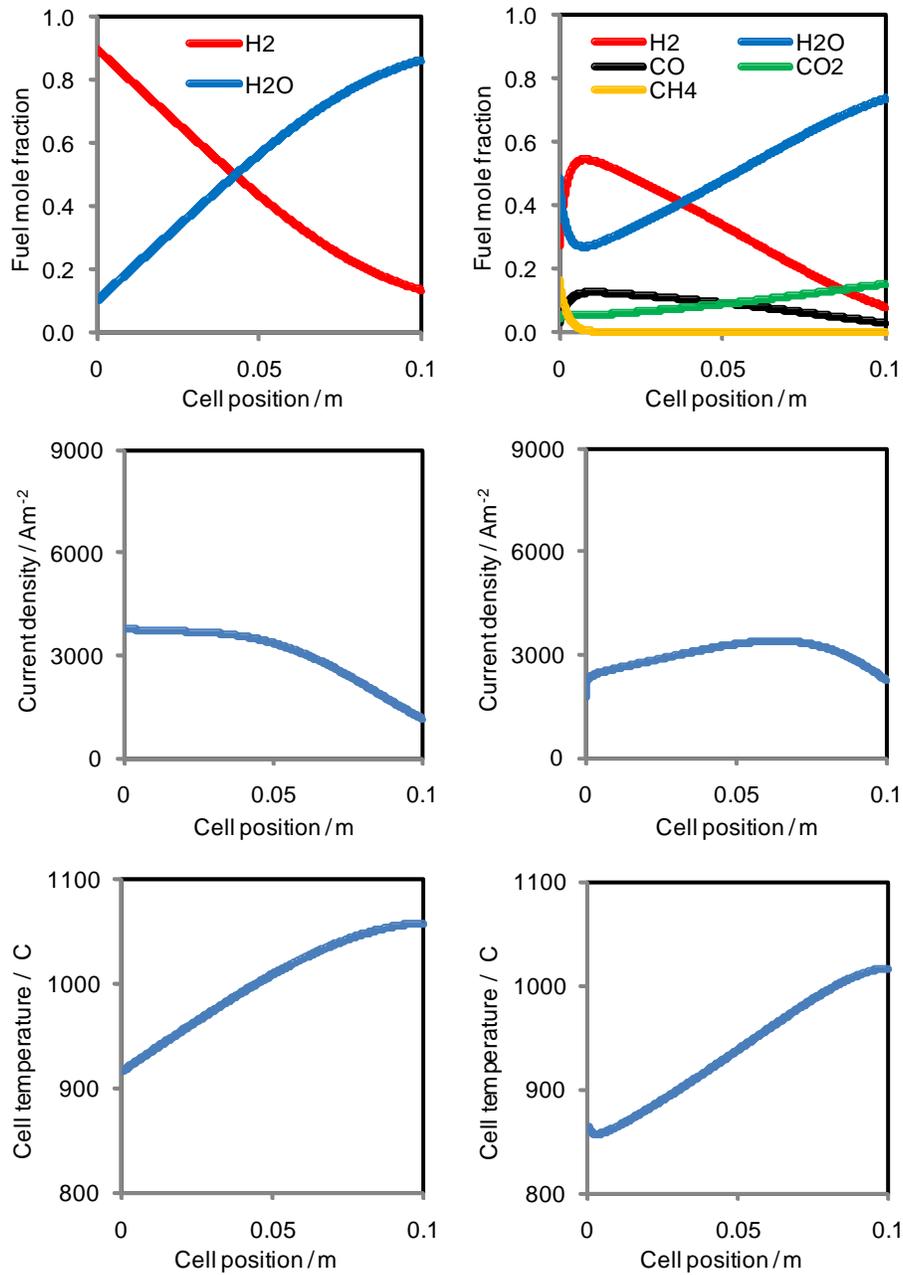
Figure 17. Contours of the species distribution for a) H$_2$ and b) CH$_4$ fuels, the current density distribution for c) H$_2$ and d) CH$_4$ fuels, and the cell temperature for the e) H$_2$ and f) CH$_4$ fuels.
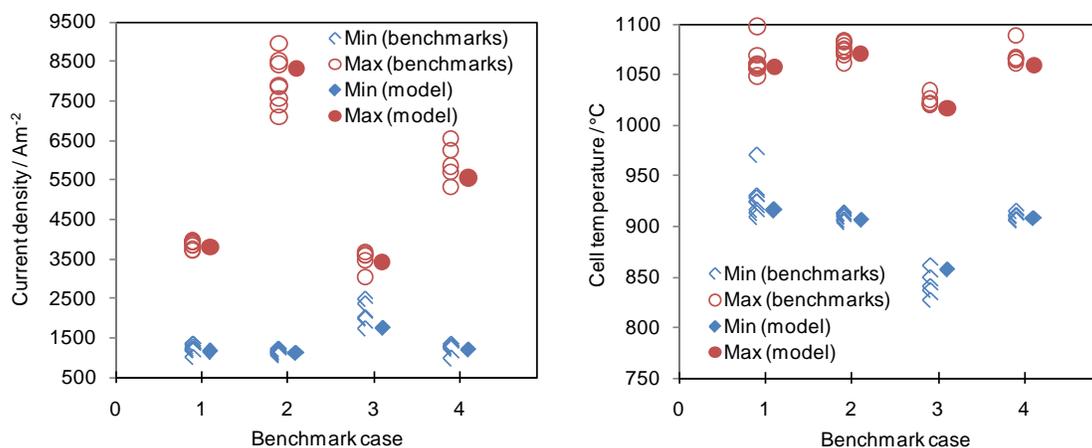
Figure 18. Comparison of minimum and maximum a) current densities and b) cell temperatures between the model and the benchmark cases.
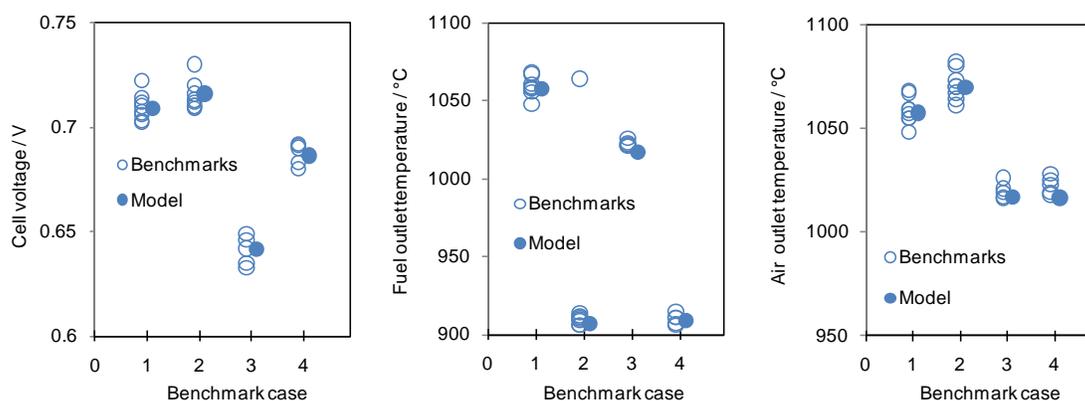
Figure 19. Comparison of a) cell voltage, b) fuel outlet temperature, and c) oxidant outlet temperature between the model and the benchmark cases.

5.2 Single Co-Flow Cell with CH$_4$ Fuel

The next example is identical to the previous case except that a fuel with methane is used. Carbon-based fuels are widely available from natural gas, gasification processes, generation processes for biological materials, etc. and of interest for the SOFC. The nickel in the anode acts as a catalyst for steam reformation of the methane on the cell. The reformation reaction of methane along with the water-gas shift reaction of carbon monoxide produces four models of hydrogen from each mole of methane. Also favorably, the reformation reaction is endothermic which can be utilized to beneficially remove heat from the stack. Therefore, the modeling tool must handle carbon-based fuels also.

5.2.1 Creation of EC_Dimension1_InputTable.dat File for Example Case 2

The input file is very similar to the H$_2$ case. The additional changes to the file are shown in Figure 16 and the full input file is provided in Appendix B. The fuel flow rate is smaller because the H$_2$ content of the methane fuel is greater and will result in the same utilization after on-cell

reforming. Next, the fuel composition is appropriately updated. Finally, the stack voltage for the required current density is slightly lower because of a lower Nernst voltage with the methane.

Table 15 Keyword Assignments for Example Case 2

Keyword Assignment	Description
FuelFlowRate = 0.00018741	1.8741e-4 mol/s fuel to give 85% utilization
FuelH2 = 0.2626	26.26% hydrogen
FuelH2O = 0.4934	49.34% water
FuelCO = 0.0294	2.94% carbon monoxide
FuelCO2 = 0.0436	4.36% carbon dioxide
FuelCH4 = 0.1710	17.1% methane
StackVoltage = 0.6374	Solve for assigned voltage to obtain a current density of 0.3 A/cm^2

5.2.2 Creation of VoltageOnCurrent.dat File for Example Case 2

The I-V calculation for the carbon-based fuel is the same as the H_2 case. In general, this may not be true because the possibility for oxidation of H_2, CO, and CH_4 exists in the cell, where each of these reactions proceed such that the total anode current consists of contributions from each oxidation reaction. However, in this model it is assumed that the methane is not oxidized and converted to H_2 via on-cell steam reformation. It is also assumed that the relatively fast water-gas shift equation is always in equilibrium everywhere on the cell. With these assumptions, the working voltage for the H_2 and CO oxidation has been shown to be identical, so the predicted open circuit voltage considering only H_2 oxidation is acceptable. The steam reformation reaction is kinetically controlled though, so a rate expression is required. The Achenbach rate (1994) is implemented in the *CH4ReformingRate()* subroutine and placed in the *VoltageOnCurrent.dat* file as shown in Figure 20.

```
function CH4ReformingRate()
GasConstant=8.3144
Ch4_Usage=4274.0*pCH4*math.exp(-82000.0/fuelT/GasConstant)
return Ch4_Usage
end
```

Figure 20. CH$_4$ reforming rate subroutine for the example Case 2.

5.2.3 Results for Example Case 2

The results for the Achenbach case 3 are also shown in Figure 17-Figure 19. The species distribution indicates the production of H_2 at the inlet from reformed CH_4 (Figure 17b). This reduces the temperature at the inlet region (Figure 17f) which reduces the current density (Figure 17d). The current density increases further downstream as the cell becomes hotter but then reduces again due to low fuel concentration. Overall, the cell temperature is lower due to the on-cell reformation. Comparison of the total output power indicates about a 10% loss from the H_2 case.

5.3 Multi-Cell Co-Flow Cell with H₂ Fuel

While many models for single SOFC cells exist in the literature and have been used for studies, very few have been demonstrated for tall stack analyses. The SOFC-MP 2D model is well suited for evaluating distributions and performance of tall stacks. A tall stack consisting of 96 625 cm² cells was created by increasing the number of cells and flow rates in the model definition. This stack assumes an anode-supported cell with much higher performance (Figure 21). The input files for this case are shown in Appendix C.
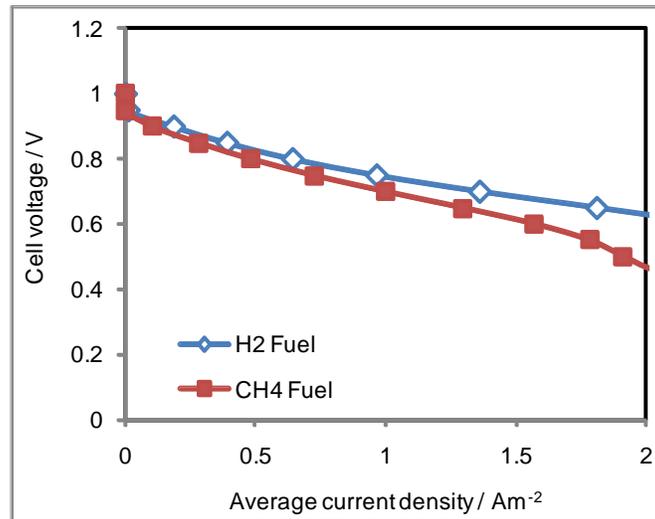
Figure 21. I-V curve for the modeled H₂ and CH₄ fuels.

Various results are shown in Figure 22 and Figure 23. Several observations can be made about the stack performance:

- The voltage varies ~2% along the stack height with the highest value near the top of the stack (which is hotter and reduces the electrolyte ionic conductivity).
- The current density profile varies along the stack height. Due to hotter inlet gases at the top of the stack, the peak current density shifts toward the inlet compared to the bottom of the stack. The center cells in the stack are hotter because they see less influence from the top and bottom boundary conditions, so the peak current density for the these cells occurs at the middle of the cell.
- The temperature difference is greatest for cell #15 (130°C) compared to the end cells (50-70), which is important for structural reliability.

Clearly the effect of the boundary conditions and stack size will affect the response in different cells, indicating that single cell models do not provide all the necessary information for design and operation of realistic tall stacks.
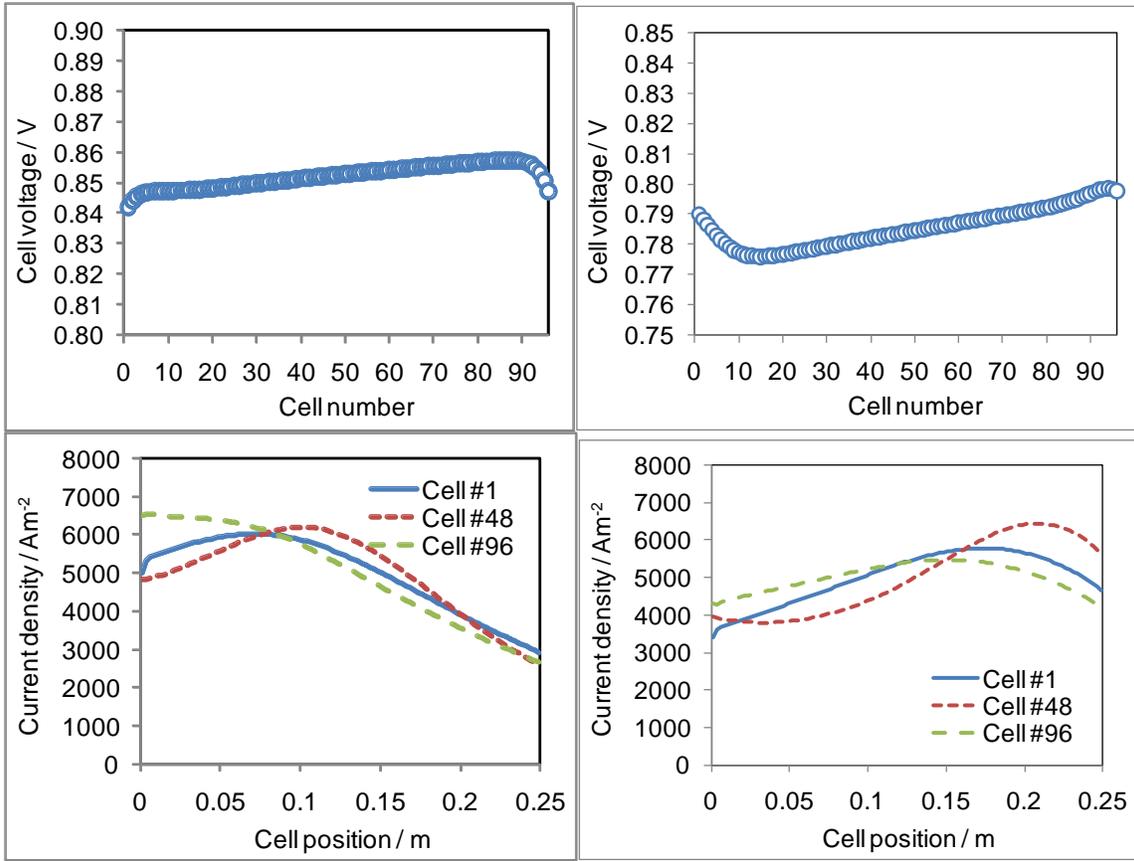
Figure 22. Comparison of the predicted results between the a) cell voltage and c) current density distribution for the H₂ fuel case and the b) cell voltage and d) current density distribution for the CH₄ fuel case.
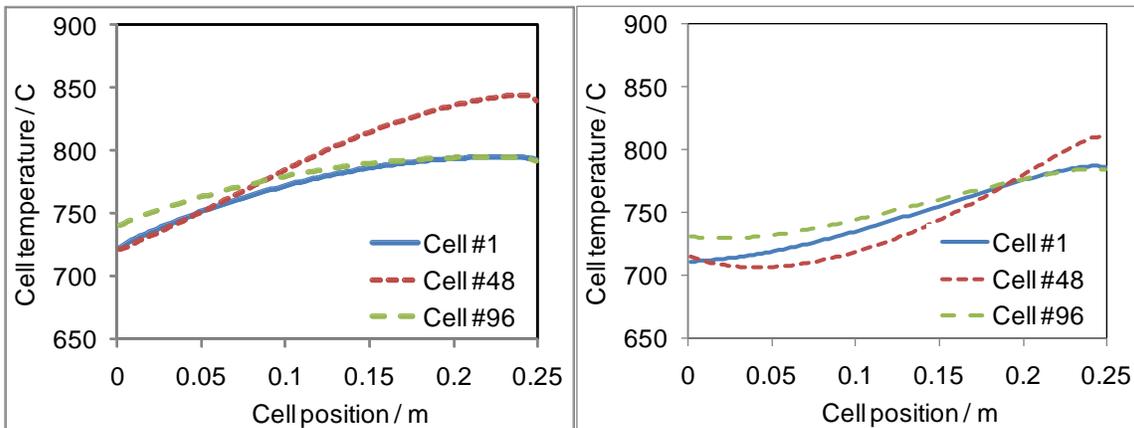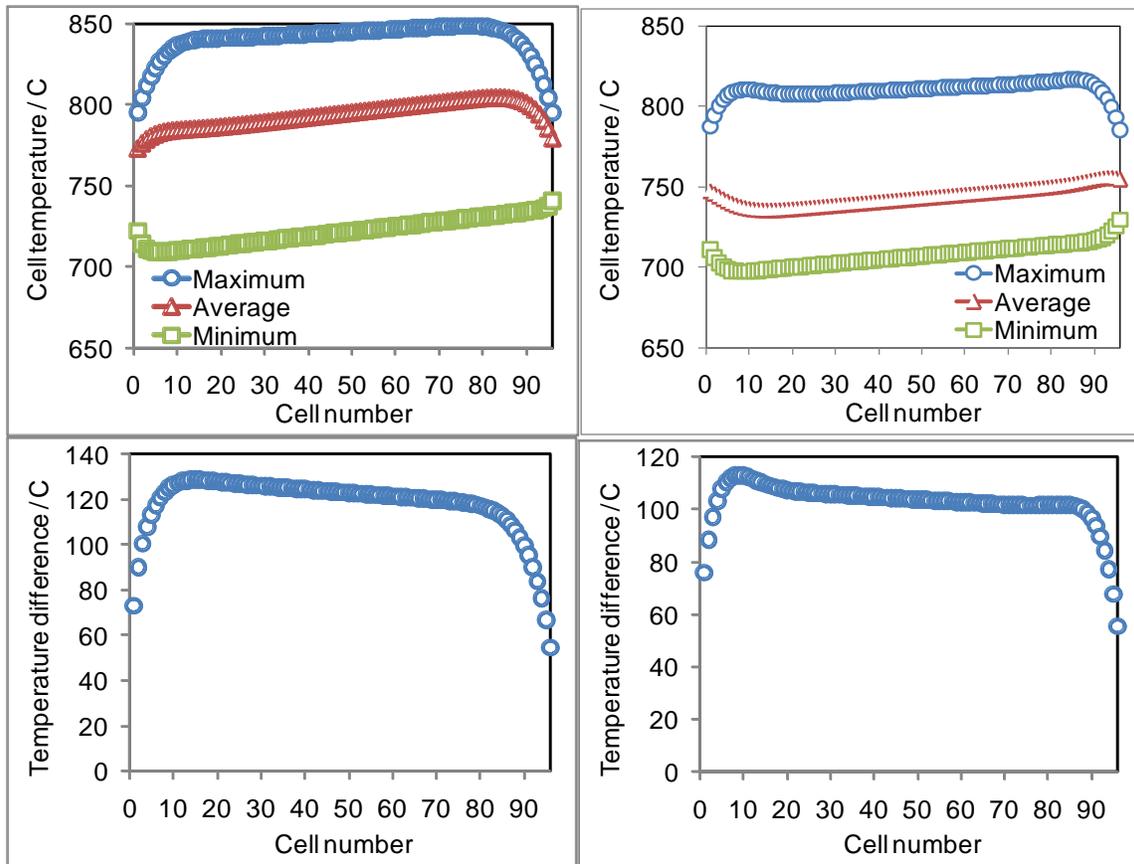
Figure 23. Comparison of the predicted results between the a) cell temperature, c) temperature extremes, and e) temperature difference for the H₂ fuel case and the b) cell temperature, d) temperature extremes, and f) temperature difference for the CH₄ fuel case

5.4 Multi-Cell Co-Flow Cell with CH₄ Fuel

The tall stack example was also repeated with a carbon-based fuel composition which gave the performance shown in Figure 21. The input files for this case are provided in Appendix D. The results are shown in Figure 22 and Figure 23. Several observations can be made about these stack results:

- The voltage varies ~2% along the stack height with the highest value near the top of the stack (which is hotter and reduces the electrolyte ionic conductivity).
- The current density profile varies along the stack height. Due to hotter inlet gases at the top of the stack, the peak current density shifts toward the inlet compared to the bottom of the stack. The center cells in the stack are hotter because they see less influence from the top and bottom boundary conditions, so the peak current density for the these cells occurs at the middle of the cell.
- The temperature difference is greatest for cell #15 (130°C) compared to the end cells (50-70), which is important for structural reliability.

5.5 Effect of Cell Aspect Ratio

The primary driver for thermal-mechanical stresses in the SOFC is the temperature profile of the cells and associated mismatches in component thermal expansion

coefficients. The SOFC-MP software was used to evaluate the effect of cell aspect ratio on the stack thermal profile. The influence of cell aspect ratio (AR) values of 0.2-5.0 on the thermal temperature difference (ΔT) was evaluated, where the AR is defined as the ratio of the cell length along the flow direction to the cell width. The temperature field was more uniform with high aspect ratios due to stronger thermal influence of either the inlet flow gas temperature (AR=0.2) or heat transfer with the furnace (AR=5.0). The maximum cell ΔT and global ΔT were 128°C and 139°C respectively for AR=1.0. For AR=0.2, the cell ΔT decreased by 12°C and the global ΔT decreased by 10°C. For AR=5.0, the cell ΔT decreased by 7°C and the global ΔT decreased by 11°C. This type of analyses could aid the stack engineers with potential changes to the cell design to minimize thermal stresses.
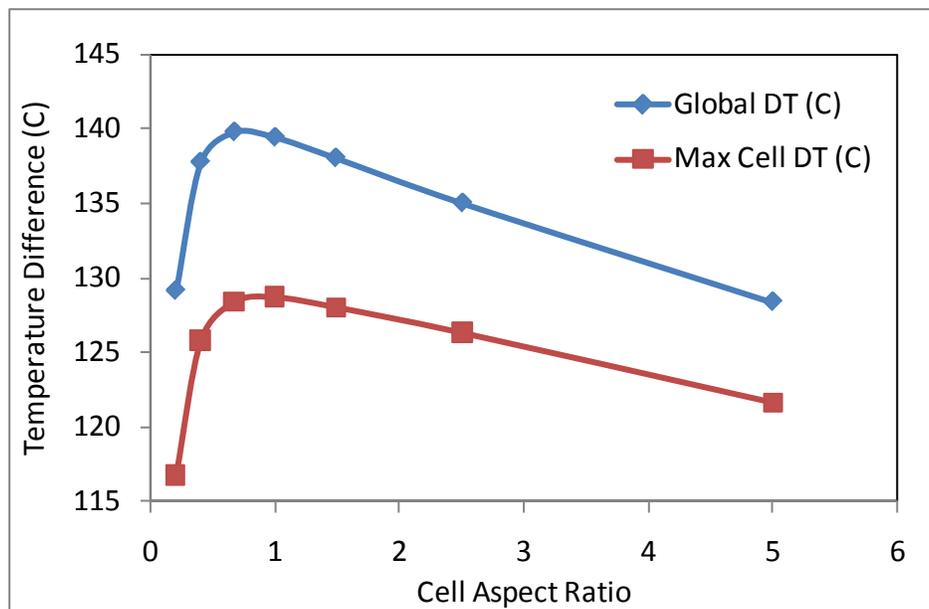
Figure 24. Effect of cell aspect ratio on stack temperature difference.

5.6 Effect of Interconnect Thickness

The effect of interconnect thickness (IC) on the stack thermal profile was also evaluated. Thinner ICs may provide cost reduction; however, thermal management will be impacted because the IC also conducts the electrochemical heat from the stack interior. Thinner IC's with the same thermal conductivity have less ability to conduct heat laterally. IC thickness reduction from 1.5 mm to 0.5 mm resulted in an undesirable increase of peak temperature by 11°C, global stack ΔT by 17°C, and maximum cell ΔT by 16°C. This type of analyses could help the stack engineers identify potential impacts on the stress state due to cost reduction strategies.
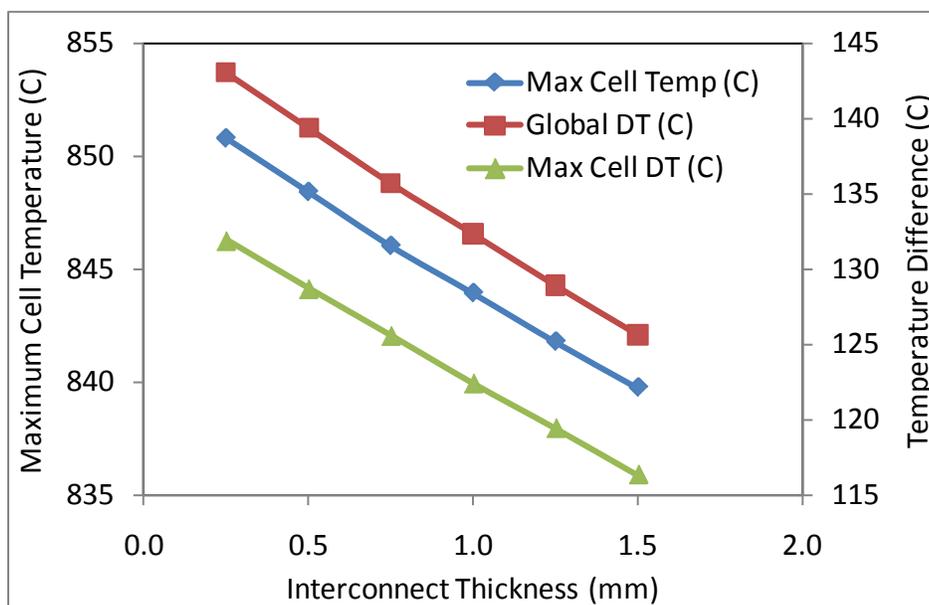
Figure 25. Effect of interconnect thickness on stack temperatures.

6.0   Summary

An efficient numerical tool was developed to evaluate the effects of cell design, geometric parameters, material properties, electrochemical properties, thermal boundary conditions, and operating conditions on stack performance. Detailed instructions for installation, model development, usage, and post-processing were provided. Various example cases using the software were demonstrated. This manual should provide the user with enough knowledge to construct their own model and perform independent analyses.

7.0   References

Achenbach E and E Riensche. 1994. Methane/Steam Reforming Kinetics for Solid Oxide Fuel Cells, Journal of Power Sources 52:283-288.

Achenbach E. 1996. IEA Programme on R&D on Advanced Fuel Cells – Annex II: Modeling and Evaluation of Advanced Solid Oxide Fuel Cells, Forschungszentrum Jülich.

Braun RJ. 2002. Optimal Design and Operation of Solid Oxide Fuel Cell Systems for Small-Scale Stationary Applications, PhD thesis, University of Wisconsin-Madison.

Chick LA, JW Stevenson, KD Meinhardt, SP Simner, JE Jaffe, and RE Williford. 2000. Modeling and Performance of Anode-Supported SOFC, 2000 Fuel Cell Seminar-Abstracts 619-622.

Ferguson JR, JM Fiard, and R Herbin. 1995. Three-Dimensional Numerical Simulation for Various Geometries of Solid Oxide Fuel Cells, Journal of Power Sources 58:109-122.

Khaleel MA, Z Lin, P Singh, W Surdoval, and D Collins. 2004. "A Finite Element Analysis Modeling Tool for Solid Oxide Fuel Cell Development: Coupled Electrochemistry, Thermal and Flow Analysis in MARC, Journal of Power Sources 130:136-148.

Lai K, BJ Koeppel, KS Choi, KP Recknagle, X Sun, LA Chick, V Korolev, and MA Khaleel. 2010. "A Quasi-Two Dimensional Electrochemistry Modeling Tool for Planar Solid Oxide Fuel Cell Stacks," Journal of Power Sources 196(6):3204-3222.

Li M, JD Powers, J Brouwer. 2010. A Finite Volume SOFC Model for Coal-Based Integrated Gasification Fuel Cell Systems Analysis, Journal of Fuel Cell Science and Technology 7(4): 041017-1-12.

Lua 5.1 Reference Manual, http://www.lua.org/manual/5.1/.

Zhang X, J Li, G Li, and Z Feng. 2006. Development of a Control-Oriented Model for the Solid Oxide Fuel Cell, Journal of Power Sources 160:258-267.

Appendix A

EC_Dimension1_InputTable.dat for Example Case 1

Description: Achenbach single cell co-flow benchmark with H_2 fuel

```
CELL PARAMETERS
nLayers = 10
nSpecies = 6
Thickness = 250.0
Tortuosity = 2.5
Porosity  = 30.0
PoreRadius  = 0.5
ElectrolyteThickness = 150.0
InterconnectThickness = 1500.0
CathodeThickness = 50.0
CathodePorosity = 30.0
CathodeTortuosity = 2.5
AnodeThickness = 50.0
AnodePorosity = 30.0

CONTACT RESISTANCE PARAMETERS
ScaleThickness  = 30.0
PreExponent = 10.0
ActivationEnergy = 0.20

CATHODE RESISTANCE PARAMETERS
CathodePreExponent = 575955.0
CathodeActivationEnergy = 0.117

CATHODE BUTLER-VOLMER PARAMETERS
BV_AlphaCoefficient = 0.55
BV_ActivationEnergy = 1.2
BV_PreExponent_a = -120
BV_PreExponent_b = 2.3e5

CATHODE O2 DEPLETION PARAMETERS
CathodeDepletionCoefficient_a = 3
CathodeDepletionCoefficient_b = -35

ANODE DEPLETION POLARIZATION PARAMETERS
LOP_slope = 0.2027
LOP_is = -8.897e-4
LOP_ii = 0.5221
AOP_ns = 2.439e-3
AOP_ni = -2.358
AOP_qs = 1.747e-2
AOP_qi = -17.73
AOP_ms = -1.158e-2
AOP_mi = 11.06
AOP_ps = 6.560e-4
AOP_pi = -1.152

SystemPressure = 1.0

FUEL PARAMETERS (FLOW RATE IS MOLE/SEC; TEMP IS K)
FuelFlowRate = 0.00020325
FuelTemperature = 1173
FuelTonTop = 1173
FuelH2 = 0.90
FuelH2O = 0.10
FuelCO = 0.00
FuelCO2 = 0.00
```

```
FuelCH4 = 0.00
FuelN2 = 0.00


OXIDANT PARAMETERS (FLOW RATE IS MOLE/SEC; TEMP IS K)
OxidantFlowRate = 0.0030485
OxidantTemperature  = 1173
OxidantTonTop = 1173
OxidantO2 = 0.21
OxidantN2 = 0.79


DIMENSION IN DIRECTION OF GAS FLOW (M)
Ax = 0.1

DIMENSION PERPENDICULAR TO GAS FLOW (M)
Ay = 0.1

NUMBER OF INCREMENTS PER CELL
Nx = 1000

NUMBER OF CELLS IN STACK
nCells=1

--Average_CurrentDensity=3000
StackVoltage=0.7082
--Average_CellVoltage=0.7098
ShortCurrent=0.0
DISTANCE REQUIRED TO REACH GAS EQUILIBRIUM
EquilibriumPathCO = 0.001
EquilibriumPathCH4 = 0.01


EMISSIVITY OF INTERCONNECT AND CELL
InterConnectEmittance = 0.5
PENEmittence = 0.5


THICKNESSES OF BOTTOM, INTERCONNECT, TOP PLATE AND PEN
BottomPlateH = 0.000946
InterConnectPlateH = 0.001393
TopPlateH = 0.000946
PEN_H = 0.00025


THERMAL COND. OF BOTTOM, INTERCONNECT, TOP PLATE AND PEN
BottomPlateHC = 2.0
InterConnectPlateHC = 2.0
TopPlateHC = 2.0
PEN_HC = 2.0


HEIGHT OF GAS FLOW PASSAGES
AirFlowH = 0.000554
FuelFLowH = 0.000554


OxidantSolidFilmCoefficient = 134.0
FuelSolidFilmCoefficient = 510.0


SWITCH:COFLOW IS 1, COUNTERFLOW IS 0
CoFlowFlag = 1


relaxation parameter between old T distribution and new T distribution
T_Relaxation = 0.5
T_precision = 0.05
maximum temperature admissible in iterations (C)
T_TopLimit = 1420.0


minimum temperature admissible in iterations (C)
T_BottomLimit = 580.0


maximum admissible total current difference in the cells in stack
CurrentTolerance = 0.001


voltage increment for the cell during multicell stack solution
VoltageIncrement = 0.001
VoltageIterationLimit = 5
```

```
TopEnvironmentT = 950
TopFilmCoefficient = .00010
TopEmissivity = 0.00003
TopSIFilmCoefficient = .010000
TopSIEmissivity = 0.009
TopIsolationH = 0.2
TopIsolationHC = 0.006
TopGeometryScale = 10e-8


BottomEnvironmentT = 950
BottomFilmCoefficient = .00010
BottomEmissivity = 0.00003
BottomSIFilmCoefficient = .010000
BottomSIEmissivity = 0.009
BottomIsolationH = 0.2
BottomIsolationHC = 0.006
BottomGeometryScale = 10e-8

FrontEnvironmentT = 950
FrontFilmCoefficient = .00010
FrontEmissivity = 0.00003
FrontSIFilmCoefficient = .010000
FrontSIEmissivity = 0.009
FrontIsolationH = 0.2
FrontIsolationHC = 0.006
FrontGeometryScale = 10e-8

BackEnvironmentT = 950
BackFilmCoefficient = .00010
BackEmissivity = 0.00003
BackSIFilmCoefficient = .010000
BackSIEmissivity = 0.009
BackIsolationH = 0.2
BackIsolationHC = 0.006
BackGeometryScale = 10e-8

SideEnvironmentT = 950
SideFilmCoefficient = 0.000010
SideEmissivity = 0.000003
SideSIFilmCoefficient = 0.000010
SideSIEmissivity = 0.000003
SideIsolationH = 0.20000111
SideIsolationHC = 0.0006
SideGeometryScale = 10e-8

InletArea = 0.0001
InletHC = 20.0
InletL = 0.003
OutletArea = 0.0001
OutletHC = 20.0
OutletL = 0.003
BoundaryFlag = 2

CP_pen = 400.0
CP_plate = 400.0

EC_Model_Option = 4
VTC = -0.017
UserDefinedHeat = 1
QuasiTransient = 0
TimeStep=0.01
LimitTiterations = 40
PrintBalances = 1
HaveConductionOnInlet = 0

H2_Threshold=0.01
H2_Threshold_Current=0.01
```

VoltageOnCurrent.dat for Example Case 1

```
-- EC based on Achenbach benchmark paper for H2 fuel
--
function VoltageValue()
--
-- Assign Constants/Conversions/Geometry/Material Data
R=8.3145; F=96485.3; atm2bar=1.01325
th_a=50.0e-6; th_e=150.0e-6; th_c=50.0e-6; th_ic=2500.0e-6
--
-- Compute the local cell temperature
Tk=(oT+fT)/2.0
--
-- Compute the total pressure & convert to bar
pO2airc=pO2air*atm2bar; pN2airc=pN2air*atm2bar
pH2c=pH2*atm2bar;        pH2Oc=pH2O*atm2bar;    pCOc=pCO*atm2bar
pCO2c=pCO2*atm2bar;      pCH4c=pCH4*atm2bar;    pN2c=pN2*atm2bar
Ptotal=pH2c+pH2Oc+pCOc+pCO2c+pCH4c+pN2c
--
-- Convert the passed current density
Jcalc=J*10000.
--
-- Calculate ohmic resistance
siga=95.0e6/Tk*math.exp(-1150.0/Tk)
sigc=42.0e6/Tk*math.exp(-1200.0/Tk)
sige=3.34e4*math.exp(-10300.0/Tk)
sigic=9.3e6/Tk*math.exp(-1100.0/Tk)
RohmIC=0.0025/sigic
Rohm=th_a/siga+th_c/sigc+th_e/sige+RohmIC
--
-- Calculate the open cell voltage
U00H2O=(241.106-3.804e-2*Tk-1.402e-5*Tk^2+3.551e-9*Tk^3)*1000.0/2.0/F
U0H2=U00H2O-R*Tk/2.0/F*math.log(pH2Oc/pH2c/pO2airc^0.5)
--
-- Calculate the working voltage
UH2=U0H2-(Rohm*Jcalc+Rohm*Jcalc+Rohm*Jcalc)
Z=UH2
--
-- Return the voltage value (not less than zero)
if Z<0.0 then
  Z=0.001
end
return Z
end
```

Appendix B

EC_Dimension1_InputTable.dat for Example Case 2

Description: Achenbach single cell co-flow benchmark with CH_4 fuel

```
CELL PARAMETERS
nLayers = 10
nSpecies = 6
Thickness = 250.0
Tortuosity = 2.5
Porosity  = 30.0
PoreRadius  = 0.5
ElectrolyteThickness = 150.0
InterconnectThickness = 1500.0
CathodeThickness = 50.0
CathodePorosity = 30.0
CathodeTortuosity = 2.5
AnodeThickness = 50.0
AnodePorosity = 30.0

CONTACT RESISTANCE PARAMETERS
ScaleThickness  = 30.0
PreExponent = 10.0
ActivationEnergy = 0.20

CATHODE RESISTANCE PARAMETERS
CathodePreExponent = 575955.0
CathodeActivationEnergy = 0.117

CATHODE BUTLER-VOLMER PARAMETERS
BV_AlphaCoefficient = 0.55
BV_ActivationEnergy = 1.2
BV_PreExponent_a = -120
BV_PreExponent_b = 2.3e5

CATHODE O2 DEPLETION PARAMETERS
CathodeDepletionCoefficient_a = 3
CathodeDepletionCoefficient_b = -35

ANODE DEPLETION POLARIZATION PARAMETERS
LOP_slope = 0.2027
LOP_is = -8.897e-4
LOP_ii = 0.5221
AOP_ns = 2.439e-3
AOP_ni = -2.358
AOP_qs = 1.747e-2
AOP_qi = -17.73
AOP_ms = -1.158e-2
AOP_mi = 11.06
AOP_ps = 6.560e-4
AOP_pi = -1.152

SystemPressure = 1.0

FUEL PARAMETERS (FLOW RATE IS MOLE/SEC; TEMP IS K)
FuelFlowRate = 0.0001873849
FuelTemperature = 1173
FuelTonTop = 1173
FuelH2 = 0.2626
FuelH2O = 0.4934
FuelCO = 0.0294
FuelCO2 = 0.0436
FuelCH4 = 0.1710
FuelN2 = 0.00
```

```
OXIDANT PARAMETERS (FLOW RATE IS MOLE/SEC; TEMP IS K)
OxidantFlowRate = 0.0030485
OxidantTemperature  = 1173
OxidantTonTop = 1173
OxidantO2 = 0.21
OxidantN2 = 0.79


DIMENSION IN DIRECTION OF GAS FLOW (M)
Ax = 0.1

DIMENSION PERPENDICULAR TO GAS FLOW (M)
Ay = 0.1

NUMBER OF INCREMENTS PER CELL
Nx = 1000

NUMBER OF CELLS IN STACK
nCells=1

--Average_CurrentDensity=3000
StackVoltage=0.64645
--Average_CellVoltage=0.7098
ShortCurrent=0.0
DISTANCE REQUIRED TO REACH GAS EQUILIBRIUM
EquilibriumPathCO = 0.001
EquilibriumPathCH4 = 0.01

EMISSIVITY OF INTERCONNECT AND CELL
InterConnectEmittance = 0.5
PENEmittence = 0.5

THICKNESSES OF BOTTOM, INTERCONNECT, TOP PLATE AND PEN
BottomPlateH = 0.000946
InterConnectPlateH = 0.001393
TopPlateH = 0.000946
PEN_H = 0.00025

THERMAL COND. OF BOTTOM, INTERCONNECT, TOP PLATE AND PEN
BottomPlateHC = 2.0
InterConnectPlateHC = 2.0
TopPlateHC = 2.0
PEN_HC = 2.0

HEIGHT OF GAS FLOW PASSAGES
AirFlowH = 0.000554
FuelFLowH = 0.000554

OxidantSolidFilmCoefficient = 132.0
FuelSolidFilmCoefficient = 321.0

SWITCH:COFLOW IS 1, COUNTERFLOW IS 0
CoFlowFlag = 1

relaxation parameter between old T distribution and new T distribution
T_Relaxation = 0.5
T_precision = 0.05
maximum temperature admissible in iterations (C)
T_TopLimit = 1420.0

minimum temperature admissible in iterations (C)
T_BottomLimit = 580.0

maximum admissible total current difference in the cells in stack
CurrentTolerance = 0.001

voltage increment for the cell during multicell stack solution
VoltageIncrement = 0.001
VoltageIterationLimit = 5

TopEnvironmentT = 950
```

```
TopFilmCoefficient = .00010
TopEmissivity = 0.00003
TopSIFilmCoefficient = .010000
TopSIEmissivity = 0.009
TopIsolationH = 0.2
TopIsolationHC = 0.006
TopGeometryScale = 10e-8


BottomEnvironmentT = 950
BottomFilmCoefficient = .00010
BottomEmissivity = 0.00003
BottomSIFilmCoefficient = .010000
BottomSIEmissivity = 0.009
BottomIsolationH = 0.2
BottomIsolationHC = 0.006
BottomGeometryScale = 10e-8

FrontEnvironmentT = 950
FrontFilmCoefficient = .00010
FrontEmissivity = 0.00003
FrontSIFilmCoefficient = .010000
FrontSIEmissivity = 0.009
FrontIsolationH = 0.2
FrontIsolationHC = 0.006
FrontGeometryScale = 10e-8

BackEnvironmentT = 950
BackFilmCoefficient = .00010
BackEmissivity = 0.00003
BackSIFilmCoefficient = .010000
BackSIEmissivity = 0.009
BackIsolationH = 0.2
BackIsolationHC = 0.006
BackGeometryScale = 10e-8

SideEnvironmentT = 950
SideFilmCoefficient = 0.000010
SideEmissivity = 0.000003
SideSIFilmCoefficient = 0.000010
SideSIEmissivity = 0.000003
SideIsolationH = 0.20000111
SideIsolationHC = 0.0006
SideGeometryScale = 10e-8

InletArea = 0.0001
InletHC = 20.0
InletL = 0.003
OutletArea = 0.0001
OutletHC = 20.0
OutletL = 0.003
BoundaryFlag = 2

CP_pen = 400.0
CP_plate = 400.0

EC_Model_Option = 4
VTC = -0.017
UserDefinedHeat = 1
QuasiTransient = 0
TimeStep=0.01
LimitTiterations = 40
PrintBalances = 1
HaveConductionOnInlet = 0

H2_Threshold=0.01
H2_Threshold_Current=0.01

CH4_Option=2
```

VoltageOnCurrent.dat for Example Case 2

```
-- EC based on Achenbach benchmark paper for CH4 fuel
--   assume no CH4 oxidation, just steam reforming
--   assume not CO oxidation, just water-gas shift
--
function VoltageValue()
--
-- Assign Constants/Conversions/Geometry/Material Data
R=8.3145; F=96485.3; atm2bar=1.01325
th_a=50.0e-6; th_e=150.0e-6; th_c=50.0e-6; th_ic=2500.0e-6
--
-- Compute the local cell temperature
Tk=(oT+fT)/2.0
--
-- Compute the total pressure & convert to bar
pO2airc=pO2air*atm2bar; pN2airc=pN2air*atm2bar
pH2c=pH2*atm2bar;        pH2Oc=pH2O*atm2bar;     pCOc=pCO*atm2bar
pCO2c=pCO2*atm2bar;      pCH4c=pCH4*atm2bar;     pN2c=pN2*atm2bar
Ptotal=pH2c+pH2Oc+pCOc+pCO2c+pCH4c+pN2c
--
-- Convert the passed current density
Jcalc=J*10000.
--
-- Calculate ohmic resistance
siga=95.0e6/Tk*math.exp(-1150.0/Tk)
sigc=42.0e6/Tk*math.exp(-1200.0/Tk)
sige=3.34e4*math.exp(-10300.0/Tk)
sigic=9.3e6/Tk*math.exp(-1100.0/Tk)
RohmIC=0.0025/sigic
Rohm=th_a/siga+th_c/sigc+th_e/sige+RohmIC
--
-- Calculate the open cell voltage
U00H2O=(241.106-3.804e-2*Tk-1.402e-5*Tk^2+3.551e-9*Tk^3)*1000.0/2.0/F
U0H2=U00H2O-R*Tk/2.0/F*math.log(pH2Oc/pH2c/pO2airc^0.5)
--
-- Calculate the working voltage
UH2=U0H2-(Rohm*Jcalc+Rohm*Jcalc+Rohm*Jcalc)
Z=UH2
--
-- Return the voltage value (not less than zero)
if Z<0.0 then
  Z=0.001
end
return Z
end


------------------------------------------------------------------
--        CH4 conversion rate for on-cell reformation          --
------------------------------------------------------------------
function CH4ReformingRate()
GasConstant=8.3144
Ch4_Usage=4274.0*pCH4*math.exp(-82000.0/fuelT/GasConstant)
return Ch4_Usage
end
```

Appendix C

EC_Dimension1_InputTable.dat for Example Case 3

Description: Tall stack co-flow example with H_2 fuel

```
#CELL PARAMETERS

                                 #--------------------------------------#
                                 #          FLOW GEOMETRY SWITCH         #
                                 # (co-flow is 1, counter-flow is 0)     #
                                 #--------------------------------------#
CoFlowFlag = 1


                                 #--------------------------------------#
                                 #        STACK GEOMETRY PARAMETERS      #
                                 #--------------------------------------#
                                 # dimension along flow (m)              #
Ax = 0.25
                                 # dimension perpendicular to flow (m)   #
Ay = 0.25
                                 # number of cells                       #
nCells=96
                                 # solid layer thickness (m)             #
BottomPlateH = 0.005
PEN_H = 0.0005
InterConnectPlateH = 0.0005
TopPlateH = 0.005
                                 # flow channel height (m)               #
AirFlowH = 0.001
FuelFLowH = 0.0005
                                 # inlet/outlet manifold area (m^2) and  #
                                 # length (m)                            #
InletArea = 0.0001
InletL = 0.003
OutletArea = 0.0001
OutletL = 0.003
                                 # set to 1 for cell-to-cell variations  #
Cell_Variation = 0


                                 #--------------------------------------#
                                 #        AIR-FUEL FLOW PARAMETERS       #
                                 # pressure (atm), flow rate (mol/s),    #
                                 # temp (K)                              #
                                 #--------------------------------------#
SystemPressure = 1.0
                                 # fuel inlet state                      #
FuelTemperature = 973
FuelTonTop = 1003
#FuelFlowRate = 0.0147
#FuelH2 = 0.485
#FuelH2O = 0.03
#FuelCO = 0.0
#FuelCO2 = 0.0
#FuelCH4 = 0.0
#FuelN2 = 0.485
FuelFlowRate = 0.247
FuelH2 = 0.97
FuelH2O = 0.03
FuelCO = 0.0
FuelCO2 = 0.0
FuelCH4 = 0.0
FuelN2 = 0.0
```

```
#FuelFlowRate = 0.0147
#FuelH2 = 0.538
#FuelH2O = 0.181
#FuelCO = 0.127
#FuelCO2 = 0.052
#FuelCH4 = 0.101
#FuelN2 = 0.0


                                    # oxidant inlet state              #
OxidantFlowRate = 2.47
OxidantTemperature  = 973
OxidantTonTop = 1003
OxidantO2 = 0.21
OxidantN2 = 0.79



                                    #---------------------------------------#
                                    #          STACK SOLUTION MODE          #
                                    # Comment out all modes except one!     #
                                    #---------------------------------------#
                                    # Mode 1: cell average voltage (V)      #
Average_CellVoltage=0.852
                                    # Mode 2: total stack voltage (V)       #
#StackVoltage=0.64175
                                    # Mode 3: current density (A/m^2)       #
#Average_CurrentDensity=3000
                                    # Mode 4: fixed fuel utilization        #
#Fuel_Utilization=0.65
                                    # Mode 5: solve the stack V-I curve     #
#Average_CellVoltage_Low=0.4
#Average_CellVoltage_High=1.0
#Average_CellVoltage_Increment=0.05



                                    #---------------------------------------#
                                    #       ELECTROCHEMISTRY OPTIONS        #
                                    #---------------------------------------#
                                    # I-V relation: internal is 0,          #
                                    # subroutine is 4                       #
EC_Model_Option = 4
                                    # short current switch?                 #
ShortCurrent=0.0
                                    # CH4 consumption option                #
                                    # 0 is path length, 2 is Achenbach rate #
                                    # expression, 3 is user subroutine      #
CH4_Option=3
                                    # species equilibrium distance (m)      #
EquilibriumPathCO = 0.001
EquilibriumPathCH4 = 0.01



                                    #---------------------------------------#
                                    #      SOLUTION CONTROL PARAMETERS      #
                                    #---------------------------------------#
                                    # number of increments                  #
Nx = 100
                                    # timestep for counter-flow             #
TimeStep=0.5
                                    # temp iteration relaxation factor      #
T_Relaxation = 1.0
                                    # temperature iteration limits (C)      #
T_TopLimit = 900.0
T_BottomLimit = 650.0
                                    # multicell voltage increment           #
VoltageIncrement = 0.001
                                    # minimum threshold on H2               #
H2_Threshold=0.0001
H2_Threshold_Current=0.0001
                                    # maximum voltage/temperature iterations #
VoltageIterationLimit = 30
```

```
LimitTiterations = 10
                                # gas heat capacity                 #
                                # (user defined is 1, CEA is 0)     #
UserDefinedHeat = 1
                                # quasi-transient switch            #
                                # (not used is 0, hold temperature is 1) #
QuasiTransient = 0
                                # manifold conduction?              #
HaveConductionOnInlet = 0
                                # print species balance info        #
PrintBalances = 1
                                # Electrode diffusion calculations  #
                                # 0 is perform as before, 1 is do not #
                                # perform                           #
NoDiffusion = 1
                                # print diffusion results (1 is yes) #
PrintDiffusionDifference = 1


                                #---------------------------------------#
                                #         CONVERGENCE PARAMETERS     #
                                #---------------------------------------#
                                # max temp variation between iterations #
T_precision = 0.05
                                # max cell current density variation #
                                # from stack nominal value          #
CurrentTolerance = 0.3



                                #---------------------------------------#
                                #          MATERIAL PROPERTIES       #
                                #---------------------------------------#
                                # film coefficient (W/m^2-K)        #
OxidantSolidFilmCoefficient = 2700.0
FuelSolidFilmCoefficient = 2700.0
                                # emissivity                        #
InterConnectEmittance = 0.5
PENEmittence = 0.5
                                # thermal conductivity (W/m-K)      #
BottomPlateHC = 25.0
InterConnectPlateHC = 25.0
TopPlateHC = 25.0
PEN_HC = 4.0
InletHC = 25.0
OutletHC = 25.0
                                # specific heat capacity (J/kg-K)   #
CP_pen = 400.0
CP_plate = 400.0



                                #---------------------------------------#
                                #          BOUNDARY CONDITIONS       #
                                # temp (C), film (W/m^2-K), H (m),  #
                                # HC (W/m-K)                        #
                                #---------------------------------------#
                                # BC flag 1 is ambient temperature  #
                                # BC flag 2 is insulation layer     #
BoundaryFlag = 2
                                # top                               #
TopEnvironmentT = 750
TopFilmCoefficient = 1.5
TopEmissivity = 0.7
TopSIFilmCoefficient = 1000.0
TopSIEmissivity = 0.9
TopIsolationH = 0.25
TopIsolationHC = 25.0
TopGeometryScale = 2.5
                                # bottom                            #
BottomEnvironmentT = 750
BottomFilmCoefficient = 0.3
BottomEmissivity = 0.7
BottomSIFilmCoefficient = 1000.0
```

```
BottomSIEmissivity = 0.9
BottomIsolationH = 0.25
BottomIsolationHC = 25.0
BottomGeometryScale = 2.5
                                        # front                         #
FrontEnvironmentT = 750
FrontFilmCoefficient = 0.3
FrontEmissivity = 0.7
FrontSIFilmCoefficient = 1000.0
FrontSIEmissivity = 0.9
FrontIsolationH = 0.12
FrontIsolationHC = 25.0
FrontGeometryScale = 1.3
                                        # back                          #
BackEnvironmentT = 750
BackFilmCoefficient = 0.3
BackEmissivity = 0.7
BackSIFilmCoefficient = 1000.0
BackSIEmissivity = 0.9
BackIsolationH = 0.12
BackIsolationHC = 25.0
BackGeometryScale = 1.3
                                        # sides                         #
SideEnvironmentT = 750
SideFilmCoefficient = 0.3
SideEmissivity = 0.7
SideSIFilmCoefficient = 1000.0
SideSIEmissivity = 0.9
SideIsolationH = 0.03
SideIsolationHC = 25.0
SideGeometryScale = 2.0


                                        #---------------------------------------#
                                        #           ELECTRODE DIFFUSION          #
                                        # thickness and radius in (micron)       #
                                        # porosity in (%)                        #
                                        #---------------------------------------#
nLayers = 3
nSpecies = 6
Thickness = 250.0
Tortuosity = 1.1
Porosity  = 55.0
PoreRadius  = 0.5
ElectrolyteThickness = 150.0
InterconnectThickness = 1500.0
CathodeThickness = 50.0
CathodePorosity = 55.0
CathodeTortuosity = 1.1
AnodeThickness = 50.0
AnodePorosity = 55.0



                                        #---------------------------------------#
                                        #    INTERNAL I-V CURVE PARAMETERS       #
                                        #---------------------------------------#
                                        # contact resistance                     #
ScaleThickness  = 30.0
PreExponent = 10.0
ActivationEnergy = 0.20
                                        # cathode resistance                     #
CathodePreExponent = 575955.0
CathodeActivationEnergy = 0.117
                                        # cathode BV activation                  #
BV_AlphaCoefficient = 0.55
BV_ActivationEnergy = 1.2
BV_PreExponent_a = -120
BV_PreExponent_b = 2.3e5
                                        # cathode O2 depletion                   #
CathodeDepletionCoefficient_a = 3
CathodeDepletionCoefficient_b = -35
```

```
                                        # anode depletion                    #
LOP_slope = 0.2027
LOP_is = -8.897e-4
LOP_ii = 0.5221
AOP_ns = 2.439e-3
AOP_ni = -2.358
AOP_qs = 1.747e-2
AOP_qi = -17.73
AOP_ms = -1.158e-2
AOP_mi = 11.06
AOP_ps = 6.560e-4
AOP_pi = -1.152
                                        # miscellaneous                      #
VTC = -0.017
```

VoltageOnCurrent.dat for Example Case 3

```
-- B Koeppel
-- 4-1-11
--
------------------------------------------------------------------
--                                                              --
--      VoltageValue()                                          --
--                                                              --
--      V-I performance based on spreadsheet EC model           --
--                                                              --
------------------------------------------------------------------
--
-- Available Local Inputs From SOFC-MP
--   oT                 Temperature oxidant (K)
--   fT                 Temperature fuel (K)
--   J                  Current density (A/cm2)
--   pO2air             Air side partial pressure O2 (atm)
--   pN2air             Air side partial pressure N2 (atm)
--   pH2               Fuel side partial pressure H2 (atm)
--   pH2O              Fuel side partial pressure H2O (atm)
--   pCO               Fuel side partial pressure CO (atm)
--   pCO2              Fuel side partial pressure CO2 (atm)
--   pCH4              Fuel side partial pressure CH4 (atm)
--   pN2               Fuel side partial pressure N2 (atm)
--   nActiveCell        Cell number
--   DistanceFromTheEdge      Distance along path (m)
--   DistanceFromTheEdgeRatio Relative distance along the path
--
-- Required Subroutine Outputs
--   Z                  Voltage (V)
--
------------------------------------------------------------------
--
-- User-Assigned Geometry/Material Inputs
--   th_a      Thickness anode (microns)
--   th_e      Thickness electrolyte (microns)
--   th_c      Thickness cathode (microns)
--   th_ic     Thickness interconnect (microns)
--   por_a     Porosity anode (%)
--   por_c     Porosity cathode (%)
--   tort_a    Tortuosity anode
--   tort_c    Tortuosity cathode
--   BV_alpha  Butler-Volmer 'alpha' constant
--   BV_prexp  Butler-Volmer pre-exponential constant
--   BV_Eact   Butler-Volmer activation energy
--   R_cont    Contact resistance
--
-- User-Assigned Constants/Conversions
--   R         Ideal gas constant
--   F         Faraday's constant
--   atm2Pa    Conversion for pressure atm -> Pa
```

```
--   mic2m     Conversion for length micron -> m
----------------------------------------------------------------------
--
function VoltageValue()
--
-- Assign Constants/Conversions
R=8.3145
F=96485.0
atm2Pa=101325.0
mic2m=1.0e-6
--
-- Assign Flags
BVflag=1        -- 0=old method, 1=pressurized method
--
-- Assign Geometry/Material Data
th_a=   450.0
th_e=   10.0
th_c=   40.0
th_ic=         500.0
por_a=         40.0
por_c=         40.0
tort_a=        2.5
tort_c=        2.5
BV_alpha=      0.3
BV_prexp=      105000.0
BV_Eact=       107489.0
R_cont=        0.0
BV_alpha2a=    2.0
BV_prexp2a=    465000.0
BV_Eact2a=     125000.0
BV_gamma2a=    0.5
BV_alpha2f=    1.0
BV_prexp2f=    75000000.0
BV_Eact2f=     110000.0
BV_gamma2f=    0.133
V_loss=        0.0
--
-- Compute the local cell temperature
----------------------------------------------------------------------
Tk=(oT+fT)/2.0
Tc=Tk-273.0
--
-- Compute the Nernst open circuit voltage
----------------------------------------------------------------------
Keq_dHo=-56930.0
Keq_A=6.75
Keq_B=-0.64
Keq_C=-0.08
Keq_L=-8.74
Keq_dG=Keq_dHo+Keq_A*Tk*math.log10(Tk)+Keq_B*Tk*Tk/1000+Keq_C*100000/Tk+Keq_L*Tk
Kequib=math.exp(-Keq_dG*4.184/R/Tk)
pO2anode=(pH2O/Kequib/pH2)^2
Voc=(R*Tk/4.0/F)*math.log(pO2air/pO2anode)
--
-- Compute the ohmic polarization
----------------------------------------------------------------------
-- Compute the electrolyte conductivity
s_eA=8.588e-10
s_eB=-1.101e-6
s_eC=4.679e-4
s_eD=-0.0654
s_e=s_eA*Tc^3+s_eB*Tc^2+s_eC*Tc+s_eD
-- Compute the interconnect conductivity
s_icA=0.069
s_icB=70.9
s_ic=1000000.0/(s_icA*Tc+s_icB)
-- Compute the cathode conductivity
s_cA=575955.0
s_cEa=0.117
s_c=(s_cA/Tk)*math.exp(-s_cEa/0.00008617/Tk)*(1.0-(0.018*por_c))
-- Compute the anode conductivity
```

C-6

```
s_aA=1000
s_a=s_aA*(1.0-(0.018*por_a))
-- Compute the effective cell resistivity
Ri=R_cont+(th_e/s_e+th_a/s_a+th_ic/s_ic+th_c/s_c)*0.0001
-- Compute the total ohmic loss
Ohmic=Ri*J
--
-- Compute the activation polarization (old method or new pressurized method)
----------------------------------------------------------------
if BVflag==0 then
  -- Old method
  i0=BV_prexp*math.exp(-BV_Eact/R/Tk)
  BV=(R*Tk/BV_alpha/F)*math.log((J/2.0/i0)+math.sqrt((J/2.0/i0)^2+1))
else
  -- New method
  ioeff_f=BV_prexp2f*math.exp(-BV_Eact2f/R/Tk)*pO2anode^BV_gamma2f
  ioeff_a=BV_prexp2a*math.exp(-BV_Eact2a/R/Tk)*pO2air^BV_gamma2a
  eta_f=R*Tk/BV_alpha2f/F*math.log((J/2.0/ioeff_f)+math.sqrt((J/2.0/ioeff_f)^2+1))
  eta_a=R*Tk/BV_alpha2a/F*math.log((J/2.0/ioeff_a)+math.sqrt((J/2.0/ioeff_a)^2+1))
  BV=eta_f+eta_a
end
--
-- Compute the diffusion coefficients
----------------------------------------------------------------
-- Make 0.0 species non-zero to make equations defined
if pCO<=0 then
  pCOc=1e-16
else
  pCOc=pCO
end
if pCO2<=0 then
  pCO2c=1e-16
else
  pCO2c=pCO2
end
Ptotal=pH2+pH2O+pCOc+pCO2c+pN2+pCH4
H2_mf=pH2/Ptotal
H2O_mf=pH2O/Ptotal
CO_mf=pCOc/Ptotal
CO2_mf=pCO2c/Ptotal
N2_mf=pN2/Ptotal
CH4_mf=pCH4/Ptotal
-- Diffusion constants (empirical radii and molecular weights)
H2i=1.92
H2Oi=2.33
COi=2.66
CO2i=3.0
N2i=2.62
O2i=2.55
CH4i=2.9
H2ii=2.0
H2Oii=18.0
COii=28.0
CO2ii=44.0
N2ii=28.0
O2ii=32.0
CH4ii=16.0
-- Compute anode binary diffusion constants
H2H2O=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2ii+1/H2Oii)/((H2i+H2Oi)^2)
H2CO=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2ii+1/COii)/((H2i+COi)^2)
H2CO2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2ii+1/CO2ii)/((H2i+CO2i)^2)
H2N2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2ii+1/N2ii)/((H2i+N2i)^2)
H2CH4=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2ii+1/CH4ii)/((H2i+CH4i)^2)
O2N2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/O2ii+1/N2ii)/((O2i+N2i)^2)
H2OCO=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2Oii+1/COii)/((H2Oi+COi)^2)
H2OCO2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2Oii+1/CO2ii)/((H2Oi+CO2i)^2)
H2ON2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2Oii+1/N2ii)/((H2Oi+N2i)^2)
H2OCH4=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2Oii+1/CH4ii)/((H2Oi+CH4i)^2)
N2CH4=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/N2ii+1/CH4ii)/((N2i+CH4i)^2)
COCO2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/COii+1/CO2ii)/((COi+CO2i)^2)
CON2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/COii+1/N2ii)/((COi+N2i)^2)
```

```
COCH4=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/COii+1/CH4ii)/((COi+CH4i)^2)
CO2N2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/CO2ii+1/N2ii)/((CO2i+N2i)^2)
CO2CH4=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/CO2ii+1/CH4ii)/((CO2i+CH4i)^2)
-- Compute anode unitary diffusion constants
H2_UD=(1-H2_mf)/(H2O_mf/H2H2O+CO_mf/H2CO+CO2_mf/H2CO2+N2_mf/H2N2+CH4_mf/H2CH4)
H2O_UD=(1-H2O_mf)/(H2_mf/H2H2O+CO_mf/H2OCO+CO2_mf/H2OCO2+N2_mf/H2ON2+CH4_mf/H2OCH4)
CO_UD=(1-CO_mf)/(H2_mf/H2CO+H2O_mf/H2OCO+CO2_mf/COCO2+N2_mf/CON2+CH4_mf/COCH4)
CO2_UD=(1-CO2_mf)/(H2_mf/H2CO2+H2O_mf/H2OCO2+CO_mf/COCO2+N2_mf/CO2N2+CH4_mf/CO2CH4)
N2_UD=(1-N2_mf)/(H2_mf/H2N2+H2O_mf/H2ON2+CO_mf/CON2+CO2_mf/CO2N2+CH4_mf/N2CH4)
CH4_UD=(1-CH4_mf)/(H2_mf/H2CH4+H2O_mf/H2OCH4+CO_mf/COCH4+CO2_mf/CO2CH4+N2_mf/N2CH4)
-- Compute anode adsorption and surface diffusion modifications
area_H2=math.pi*(H2i*10^-10)^2
area_H2O=math.pi*(H2Oi*10^-10)^2
area_CO=math.pi*(COi*10^-10)^2
area_CO2=math.pi*(CO2i*10^-10)^2
area_N2=math.pi*(N2i*10^-10)^2
area_O2=math.pi*(O2i*10^-10)^2
area_CH4=math.pi*(CH4i*10^-10)^2
pres_H2=math.max(0,pH2-J*82.058*Tk*(th_a/10000)/(2*F)*(tort_a/(H2_UD*por_a/100)))
pres_H2O=math.max(0,pH2O+J*82.058*Tk*(th_a/10000)/(2*F)*(tort_a/(H2O_UD*por_a/100)))
pres_CO=math.max(0,pCOc-J*82.058*Tk*(th_a/10000)/(2*F)*(tort_a/(CO_UD*por_a/100)))
pres_CO2=math.max(0,pCO2c+J*82.058*Tk*(th_a/10000)/(2*F)*(tort_a/(CO2_UD*por_a/100)))
pres_N2=math.max(0,pN2)
pres_O2=math.max(0,pO2anode)
pres_CH4=math.max(0,pCH4)
Qev_H2=0.425
Qev_H2O=0.549
Qev_CO=0.5
Qev_CO2=0.5
Qev_N2=0.5
Qev_O2=0.5
Qev_CH4=0.5
bP_H2=6.023*10^23*area_H2*10^-
    13/math.sqrt(2*math.pi*R*Tk*H2ii)*math.exp(Qev_H2/(0.026*Tk/298))*pres_H2
bP_H2O=6.023*10^23*area_H2O*10^-
    13/math.sqrt(2*math.pi*R*Tk*H2Oii)*math.exp(Qev_H2O/(0.026*Tk/298))*pres_H2O
bP_CO=6.023*10^23*area_CO*10^-
    13/math.sqrt(2*math.pi*R*Tk*COii)*math.exp(Qev_CO/(0.026*Tk/298))*pres_CO
bP_CO2=6.023*10^23*area_CO2*10^-
    13/math.sqrt(2*math.pi*R*Tk*CO2ii)*math.exp(Qev_CO2/(0.026*Tk/298))*pres_CO2
bP_N2=6.023*10^23*area_N2*10^-
    13/math.sqrt(2*math.pi*R*Tk*N2ii)*math.exp(Qev_N2/(0.026*Tk/298))*pres_N2
bP_O2=6.023*10^23*area_O2*10^-
    13/math.sqrt(2*math.pi*R*Tk*O2ii)*math.exp(Qev_O2/(0.026*Tk/298))*pres_O2
bP_CH4=6.023*10^23*area_CH4*10^-
    13/math.sqrt(2*math.pi*R*Tk*CH4ii)*math.exp(Qev_CH4/(0.026*Tk/298))*pres_CH4
bP_sum=bP_H2+bP_H2O+bP_CO+bP_CO2+bP_N2+bP_O2+bP_CH4
cov_H2=bP_H2/(1+bP_sum)
cov_H2O=bP_H2O/(1+bP_sum)
cov_CO=bP_CO/(1+bP_sum)
cov_CO2=bP_CO2/(1+bP_sum)
cov_N2=bP_N2/(1+bP_sum)
cov_O2=bP_O2/(1+bP_sum)
cov_CH4=bP_CH4/(1+bP_sum)
cov_sum=cov_H2+cov_H2O+cov_CO+cov_CO2+cov_N2+cov_O2+cov_CH4
fij_H2=cov_H2/cov_sum
fij_H2O=cov_H2O/cov_sum
fij_CO=cov_CO/cov_sum
fij_CO2=cov_CO2/cov_sum
fij_N2=cov_N2/cov_sum
fij_O2=cov_O2/cov_sum
fij_CH4=cov_CH4/cov_sum
DsurfH2th1=0.1
DsurfH2th2=4.51e-5
D_H2=H2_UD^fij_H2*((DsurfH2th1^(1-fij_H2)*DsurfH2th2^fij_H2)/(1-fij_H2))^(1-fij_H2)
D_H2O=H2O_UD^fij_H2O*(10^-4)^(1-fij_H2O)
D_CO=CO_UD^fij_CO*(10^-4)^(1-fij_CO)
D_CO2=CO2_UD^fij_CO2*(10^-4)^(1-fij_CO2)
D_N2=N2_UD^fij_N2*(10^-4)^(1-fij_N2)
D_O2=O2N2^fij_O2*(10^-4)^(1-fij_O2)
D_CH4=CH4_UD^fij_CH4*(10^-4)^(1-fij_CH4)
```

```
--
-- Compute the cathode concentration polarization
----------------------------------------------------------------
Deffc=0.01*por_c*O2N2/tort_c
ics=1.0e-8*(4.0*F*Ptotal*atm2Pa*Deffc)/(R*Tk*th_c*mic2m)*math.log(1.0/(1.0-pO2air))
Cath=(R*Tk/4.0/F)*math.log(1.0-(J/ics))
--
-- Compute the anode concentration polarization
----------------------------------------------------------------
DeffH2=D_H2
DeffH2O=0.01*H2O_UD*por_a/tort_a
DeffCO=0.01*CO_UD*por_a/tort_a
DeffCO2=0.01*CO2_UD*por_a/tort_a
alim=2*F*pH2*atm2Pa*DeffH2/(831.45*Tk*th_a)
blim=2*F*pH2O*atm2Pa*DeffH2O/(831.45*Tk*th_a)
clim=2*F*pCOc*atm2Pa*DeffCO/(831.45*Tk*th_a)
dlim=2*F*pCO2c*atm2Pa*DeffCO2/(831.45*Tk*th_a)
-- Adjust calculation for iteration case of too high current requested
if J>(alim+clim) then
  Jcalc=(alim+clim)*0.99
else
  Jcalc=J
end
OPa_A=(Jcalc+blim+dlim)/blim/dlim
OPa_B=(Jcalc*(alim*dlim+blim*clim)+blim*clim*dlim+alim*blim*dlim-alim*clim*dlim-
    alim*blim*clim)/alim/blim/clim/dlim
OPa_C=(Jcalc-alim-clim)/alim/clim
holdA1=OPa_A
holdB1=OPa_B
holdC1=OPa_C
stabcheck=OPa_B^2-4.0*OPa_A*OPa_C
stabcheck2=(-OPa_B+math.sqrt(OPa_B^2-4.0*OPa_A*OPa_C))/2.0/OPa_A
if stabcheck>0 then
  if stabcheck2>0 then
    Anod=(R*Tk/2.0/F)*math.log((-OPa_B+math.sqrt(OPa_B^2-4.0*OPa_A*OPa_C))/2.0/OPa_A)
    holdA2=0
    holdB2=0
    holdC2=0
  else
    DeffH2=0.01*H2_UD*por_a/tort_a
    DeffH2O=0.01*H2O_UD*por_a/tort_a
    DeffCO=0.01*CO_UD*por_a/tort_a
    DeffCO2=0.01*CO2_UD*por_a/tort_a
    alim=2*F*pH2*atm2Pa*DeffH2/(831.45*Tk*th_a)
    blim=2*F*pH2O*atm2Pa*DeffH2O/(831.45*Tk*th_a)
    clim=2*F*pCOc*atm2Pa*DeffCO/(831.45*Tk*th_a)
    dlim=2*F*pCO2c*atm2Pa*DeffCO2/(831.45*Tk*th_a)
    OPa_A=(Jcalc+blim+dlim)/blim/dlim
    OPa_B=(Jcalc*(alim*dlim+blim*clim)+blim*clim*dlim+alim*blim*dlim-alim*clim*dlim-
    alim*blim*clim)/alim/blim/clim/dlim
    OPa_C=(Jcalc-alim-clim)/alim/clim
    holdA2=OPa_A
    holdB2=OPa_B
    holdC2=OPa_C
    Anod=(R*Tk/2.0/F)*math.log((-OPa_B+math.sqrt(OPa_B^2-4.0*OPa_A*OPa_C))/2.0/OPa_A)
  end
end
--
-- Compute the final voltage result
----------------------------------------------------------------
V=(Voc-Ohmic-BV+Cath+Anod)+V_loss
Z=V
--
-- return the voltage value
return Z
end
```

Appendix D

EC_Dimension1_InputTable.dat for Example Case 4

Description: Tall stack co-flow example with CH_4 fuel

```
#CELL PARAMETERS
#CELL PARAMETERS

                                  #--------------------------------------#
                                  #          FLOW GEOMETRY SWITCH        #
                                  # (co-flow is 1, counter-flow is 0)    #
                                  #--------------------------------------#
CoFlowFlag = 1


                                  #--------------------------------------#
                                  #        STACK GEOMETRY PARAMETERS     #
                                  #--------------------------------------#
                                  # dimension along flow (m)             #
Ax = 0.25
                                  # dimension perpendicular to flow (m)  #
Ay = 0.25
                                  # number of cells                      #
nCells=96
                                  # solid layer thickness (m)            #
BottomPlateH = 0.005
PEN_H = 0.0005
InterConnectPlateH = 0.0005
TopPlateH = 0.005
                                  # flow channel height (m)              #
AirFlowH = 0.001
FuelFLowH = 0.0005
                                  # inlet/outlet manifold area (m^2) and #
                                  # length (m)                           #
InletArea = 0.0001
InletL = 0.003
OutletArea = 0.0001
OutletL = 0.003
                                  # set to 1 for cell-to-cell variations #
Cell_Variation = 0


                                  #--------------------------------------#
                                  #        AIR-FUEL FLOW PARAMETERS      #
                                  # pressure (atm), flow rate (mol/s),   #
                                  # temp (K)                             #
                                  #--------------------------------------#
SystemPressure = 1.0
                                  # fuel inlet state                     #
FuelTemperature = 973
FuelTonTop = 1003
#FuelFlowRate = 0.0147
#FuelH2 = 0.485
#FuelH2O = 0.03
#FuelCO = 0.0
#FuelCO2 = 0.0
#FuelCH4 = 0.0
#FuelN2 = 0.485
FuelFlowRate = 0.294
FuelH2 = 0.324
FuelH2O = 0.333
FuelCO = 0.049
```

```
FuelCO2 = 0.061
FuelCH4 = 0.110
FuelN2 = 0.124
#FuelFlowRate = 0.0147
#FuelH2 = 0.538
#FuelH2O = 0.181
#FuelCO = 0.127
#FuelCO2 = 0.052
#FuelCH4 = 0.101
#FuelN2 = 0.0


                                      # oxidant inlet state               #
OxidantFlowRate = 2.47
OxidantTemperature  = 973
OxidantTonTop = 1003
OxidantO2 = 0.21
OxidantN2 = 0.79


                                      #---------------------------------------#
                                      #          STACK SOLUTION MODE          #
                                      # Comment out all modes except one!     #
                                      #---------------------------------------#
                                      # Mode 1: cell average voltage (V)      #
Average_CellVoltage=0.7841
                                      # Mode 2: total stack voltage (V)       #
#StackVoltage=0.64175
                                      # Mode 3: current density (A/m^2)       #
#Average_CurrentDensity=3000
                                      # Mode 4: fixed fuel utilization        #
#Fuel_Utilization=0.65
                                      # Mode 5: solve the stack V-I curve     #
#Average_CellVoltage_Low=0.4
#Average_CellVoltage_High=1.0
#Average_CellVoltage_Increment=0.05


                                      #---------------------------------------#
                                      #       ELECTROCHEMISTRY OPTIONS        #
                                      #---------------------------------------#
                                      # I-V relation: internal is 0,          #
                                      # subroutine is 4                       #
EC_Model_Option = 4
                                      # short current switch?                 #
ShortCurrent=0.0
                                      # CH4 consumption option                #
                                      # 0 is path length, 2 is Achenbach rate #
                                      # expression, 3 is user subroutine      #
CH4_Option=3
                                      # species equilibrium distance (m)      #
EquilibriumPathCO = 0.001
EquilibriumPathCH4 = 0.01


                                      #---------------------------------------#
                                      #     SOLUTION CONTROL PARAMETERS       #
                                      #---------------------------------------#
                                      # number of increments                  #
Nx = 100
                                      # timestep for counter-flow             #
TimeStep=0.5
                                      # temp iteration relaxation factor      #
T_Relaxation = 1.0
                                      # temperature iteration limits (C)      #
T_TopLimit = 900.0
T_BottomLimit = 650.0
                                      # multicell voltage increment           #
VoltageIncrement = 0.001
                                      # minimum threshold on H2               #
H2_Threshold=0.0001
```

```
H2_Threshold_Current=0.0001
                                  # maximum voltage/temperature iterations #
VoltageIterationLimit = 30
LimitTiterations = 10
                                  # gas heat capacity                      #
                                  # (user defined is 1, CEA is 0)          #
UserDefinedHeat = 1
                                  # quasi-transient switch                 #
                                  # (not used is 0, hold temperature is 1) #
QuasiTransient = 0
                                  # manifold conduction?                   #
HaveConductionOnInlet = 0
                                  # print species balance info             #
PrintBalances = 1
                                  # Electrode diffusion calculations       #
                                  # 0 is perform as before, 1 is do not    #
                                  # peform                                 #
NoDiffusion = 1
                                  # print diffusion results (1 is yes)     #
PrintDiffusionDifference = 1


                                  #---------------------------------------#
                                  #        CONVERGENCE PARAMETERS         #
                                  #---------------------------------------#
                                  # max temp variation between iterations  #
T_precision = 0.05
                                  # max cell current density variation     #
                                  # from stack nominal value               #
CurrentTolerance = 0.1


                                  #---------------------------------------#
                                  #         MATERIAL PROPERTIES           #
                                  #---------------------------------------#
                                  # film coefficient (W/m^2-K)             #
OxidantSolidFilmCoefficient = 2700.0
FuelSolidFilmCoefficient = 2700.0
                                  # emissivity                             #
InterConnectEmittance = 0.5
PENEmittence = 0.5
                                  # thermal conductivity (W/m-K)           #
BottomPlateHC = 25.0
InterConnectPlateHC = 25.0
TopPlateHC = 25.0
PEN_HC = 4.0
InletHC = 25.0
OutletHC = 25.0
                                  # specific heat capacity (J/kg-K)        #
CP_pen = 400.0
CP_plate = 400.0


                                  #---------------------------------------#
                                  #         BOUNDARY CONDITIONS           #
                                  # temp (C), film (W/m^2-K), H (m),       #
                                  # HC (W/m-K)                             #
                                  #---------------------------------------#
                                  # BC flag 1 is ambient temperature       #
                                  # BC flag 2 is insulation layer          #
BoundaryFlag = 2
                                  # top                                    #
TopEnvironmentT = 750
TopFilmCoefficient = 1.5
TopEmissivity = 0.7
TopSIFilmCoefficient = 1000.0
TopSIEmissivity = 0.9
TopIsolationH = 0.25
TopIsolationHC = 25.0
TopGeometryScale = 2.5
                                  # bottom                                 #
BottomEnvironmentT = 750
```

```
BottomFilmCoefficient = 0.3
BottomEmissivity = 0.7
BottomSIFilmCoefficient = 1000.0
BottomSIEmissivity = 0.9
BottomIsolationH = 0.25
BottomIsolationHC = 25.0
BottomGeometryScale = 2.5
                                        # front                               #
FrontEnvironmentT = 750
FrontFilmCoefficient = 0.3
FrontEmissivity = 0.7
FrontSIFilmCoefficient = 1000.0
FrontSIEmissivity = 0.9
FrontIsolationH = 0.12
FrontIsolationHC = 25.0
FrontGeometryScale = 1.3
                                        # back                                #
BackEnvironmentT = 750
BackFilmCoefficient = 0.3
BackEmissivity = 0.7
BackSIFilmCoefficient = 1000.0
BackSIEmissivity = 0.9
BackIsolationH = 0.12
BackIsolationHC = 25.0
BackGeometryScale = 1.3
                                        # sides                               #
SideEnvironmentT = 750
SideFilmCoefficient = 0.3
SideEmissivity = 0.7
SideSIFilmCoefficient = 1000.0
SideSIEmissivity = 0.9
SideIsolationH = 0.03
SideIsolationHC = 25.0
SideGeometryScale = 2.0


                                        #-------------------------------------#
                                        #           ELECTRODE DIFFUSION       #
                                        # thickness and radius in (micron)    #
                                        # porosity in (%)                     #
                                        #-------------------------------------#
nLayers = 3
nSpecies = 6
Thickness = 250.0
Tortuosity = 1.1
Porosity  = 55.0
PoreRadius  = 0.5
ElectrolyteThickness = 150.0
InterconnectThickness = 1500.0
CathodeThickness = 50.0
CathodePorosity = 55.0
CathodeTortuosity = 1.1
AnodeThickness = 50.0
AnodePorosity = 55.0


                                        #-------------------------------------#
                                        #    INTERNAL I-V CURVE PARAMETERS    #
                                        #-------------------------------------#
                                        # contact resistance                  #
ScaleThickness  = 30.0
PreExponent = 10.0
ActivationEnergy = 0.20
                                        # cathode resistance                  #
CathodePreExponent = 575955.0
CathodeActivationEnergy = 0.117
                                        # cathode BV activation               #
BV_AlphaCoefficient = 0.55
BV_ActivationEnergy = 1.2
BV_PreExponent_a = -120
BV_PreExponent_b = 2.3e5
```

```
                                         # cathode O2 depletion                    #
CathodeDepletionCoefficient_a = 3
CathodeDepletionCoefficient_b = -35
                                         # anode depletion                         #
LOP_slope = 0.2027
LOP_is = -8.897e-4
LOP_ii = 0.5221
AOP_ns = 2.439e-3
AOP_ni = -2.358
AOP_qs = 1.747e-2
AOP_qi = -17.73
AOP_ms = -1.158e-2
AOP_mi = 11.06
AOP_ps = 6.560e-4
AOP_pi = -1.152
                                         # miscellaneous                           #
VTC = -0.17
```

VoltageOnCurrent.dat for Example Case 4

```
-- B Koeppel
-- 4-1-11
--
-------------------------------------------------------------------
--                                                               --
--      VoltageValue()                                           --
--                                                               --
--      V-I performance based on spreadsheet EC model            --
--                                                               --
-------------------------------------------------------------------
--
-- Available Local Inputs From SOFC-MP
--   oT                    Temperature oxidant (K)
--   fT                    Temperature fuel (K)
--   J                     Current density (A/cm2)
--   pO2air                Air side partial pressure O2 (atm)
--   pN2air                Air side partial pressure N2 (atm)
--   pH2                   Fuel side partial pressure H2 (atm)
--   pH2O                  Fuel side partial pressure H2O (atm)
--   pCO                   Fuel side partial pressure CO (atm)
--   pCO2                  Fuel side partial pressure CO2 (atm)
--   pCH4                  Fuel side partial pressure CH4 (atm)
--   pN2                   Fuel side partial pressure N2 (atm)
--   nActiveCell           Cell number
--   DistanceFromTheEdge      Distance along path (m)
--   DistanceFromTheEdgeRatio Relative distance along the path
--
-- Required Subroutine Outputs
--   Z                     Voltage (V)
--
----------------------------------------------------------------
--
-- User-Assigned Geometry/Material Inputs
--   th_a     Thickness anode (microns)
--   th_e     Thickness electrolyte (microns)
--   th_c     Thickness cathode (microns)
--   th_ic    Thickness interconnect (microns)
--   por_a    Porosity anode (%)
--   por_c    Porosity cathode (%)
--   tort_a   Tortuosity anode
--   tort_c   Tortuosity cathode
--   BV_alpha Butler-Volmer 'alpha' constant
--   BV_prexp Butler-Volmer pre-exponential constant
--   BV_Eact  Butler-Volmer activation energy
--   R_cont   Contact resistance
--
```

```
-- User-Assigned Constants/Conversions
--   R         Ideal gas constant
--   F         Faraday's constant
--   atm2Pa    Conversion for pressure atm -> Pa
--   mic2m     Conversion for length micron -> m
------------------------------------------------------------------
--
function VoltageValue()
--
-- Assign Constants/Conversions
R=8.3145
F=96485.0
atm2Pa=101325.0
mic2m=1.0e-6
--
-- Assign Flags
BVflag=1        -- 0=old method, 1=pressurized method
--
-- Assign Geometry/Material Data
th_a=   450.0
th_e=   10.0
th_c=   40.0
th_ic=          500.0
por_a=          40.0
por_c=          40.0
tort_a=         2.5
tort_c=         2.5
BV_alpha=       0.3
BV_prexp=       105000.0
BV_Eact=        107489.0
R_cont=         0.0
BV_alpha2a=     2.0
BV_prexp2a=     465000.0
BV_Eact2a=      125000.0
BV_gamma2a=     0.5
BV_alpha2f=     1.0
BV_prexp2f=     75000000.0
BV_Eact2f=      110000.0
BV_gamma2f=     0.133
V_loss=         0.0
--
-- Compute the local cell temperature
------------------------------------------------------------------
Tk=(oT+fT)/2.0
Tc=Tk-273.0
--
-- Compute the Nernst open circuit voltage
------------------------------------------------------------------
Keq_dHo=-56930.0
Keq_A=6.75
Keq_B=-0.64
Keq_C=-0.08
Keq_L=-8.74
Keq_dG=Keq_dHo+Keq_A*Tk*math.log10(Tk)+Keq_B*Tk*Tk/1000+Keq_C*100000/Tk+Keq_L*Tk
Kequib=math.exp(-Keq_dG*4.184/R/Tk)
pO2anode=(pH2O/Kequib/pH2)^2
Voc=(R*Tk/4.0/F)*math.log(pO2air/pO2anode)
--
-- Compute the ohmic polarization
------------------------------------------------------------------
-- Compute the electrolyte conductivity
s_eA=8.588e-10
s_eB=-1.101e-6
s_eC=4.679e-4
s_eD=-0.0654
s_e=s_eA*Tc^3+s_eB*Tc^2+s_eC*Tc+s_eD
-- Compute the interconnect conductivity
s_icA=0.069
s_icB=70.9
s_ic=1000000.0/(s_icA*Tc+s_icB)
-- Compute the cathode conductivity
```

```
s_cA=575955.0
s_cEa=0.117
s_c=(s_cA/Tk)*math.exp(-s_cEa/0.00008617/Tk)*(1.0-(0.018*por_c))
-- Compute the anode conductivity
s_aA=1000
s_a=s_aA*(1.0-(0.018*por_a))
-- Compute the effective cell resistivity
Ri=R_cont+(th_e/s_e+th_a/s_a+th_ic/s_ic+th_c/s_c)*0.0001
-- Compute the total ohmic loss
Ohmic=Ri*J
--
-- Compute the activation polarization (old method or new pressurized method)
----------------------------------------------------------------
if BVflag==0 then
  -- Old method
  i0=BV_prexp*math.exp(-BV_Eact/R/Tk)
  BV=(R*Tk/BV_alpha/F)*math.log((J/2.0/i0)+math.sqrt((J/2.0/i0)^2+1))
else
  -- New method
  ioeff_f=BV_prexp2f*math.exp(-BV_Eact2f/R/Tk)*pO2anode^BV_gamma2f
  ioeff_a=BV_prexp2a*math.exp(-BV_Eact2a/R/Tk)*pO2air^BV_gamma2a
  eta_f=R*Tk/BV_alpha2f/F*math.log((J/2.0/ioeff_f)+math.sqrt((J/2.0/ioeff_f)^2+1))
  eta_a=R*Tk/BV_alpha2a/F*math.log((J/2.0/ioeff_a)+math.sqrt((J/2.0/ioeff_a)^2+1))
  BV=eta_f+eta_a
end
--
-- Compute the diffusion coefficients
----------------------------------------------------------------
-- Make 0.0 species non-zero to make equations defined
if pCO<=0 then
  pCOc=1e-16
else
  pCOc=pCO
end
if pCO2<=0 then
  pCO2c=1e-16
else
  pCO2c=pCO2
end
Ptotal=pH2+pH2O+pCOc+pCO2c+pN2+pCH4
H2_mf=pH2/Ptotal
H2O_mf=pH2O/Ptotal
CO_mf=pCOc/Ptotal
CO2_mf=pCO2c/Ptotal
N2_mf=pN2/Ptotal
CH4_mf=pCH4/Ptotal
-- Diffusion constants (empirical radii and molecular weights)
H2i=1.92
H2Oi=2.33
COi=2.66
CO2i=3.0
N2i=2.62
O2i=2.55
CH4i=2.9
H2ii=2.0
H2Oii=18.0
COii=28.0
CO2ii=44.0
N2ii=28.0
O2ii=32.0
CH4ii=16.0
-- Compute anode binary diffusion constants
H2H2O=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2ii+1/H2Oii)/((H2i+H2Oi)^2)
H2CO=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2ii+1/COii)/((H2i+COi)^2)
H2CO2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2ii+1/CO2ii)/((H2i+CO2i)^2)
H2N2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2ii+1/N2ii)/((H2i+N2i)^2)
H2CH4=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2ii+1/CH4ii)/((H2i+CH4i)^2)
O2N2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/O2ii+1/N2ii)/((O2i+N2i)^2)
H2OCO=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2Oii+1/COii)/((H2Oi+COi)^2)
H2OCO2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2Oii+1/CO2ii)/((H2Oi+CO2i)^2)
H2ON2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2Oii+1/N2ii)/((H2Oi+N2i)^2)
```

```
H2OCH4=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/H2Oii+1/CH4ii)/((H2Oi+CH4i)^2)
N2CH4=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/N2ii+1/CH4ii)/((N2i+CH4i)^2)
COCO2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/COii+1/CO2ii)/((COi+CO2i)^2)
CON2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/COii+1/N2ii)/((COi+N2i)^2)
COCH4=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/COii+1/CH4ii)/((COi+CH4i)^2)
CO2N2=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/CO2ii+1/N2ii)/((CO2i+N2i)^2)
CO2CH4=(1e-3/Ptotal)*(Tk^1.75)*math.sqrt(1/CO2ii+1/CH4ii)/((CO2i+CH4i)^2)
-- Compute anode unitary diffusion constants
H2_UD=(1-H2_mf)/(H2O_mf/H2H2O+CO_mf/H2CO+CO2_mf/H2CO2+N2_mf/H2N2+CH4_mf/H2CH4)
H2O_UD=(1-H2O_mf)/(H2_mf/H2H2O+CO_mf/H2OCO+CO2_mf/H2OCO2+N2_mf/H2ON2+CH4_mf/H2OCH4)
CO_UD=(1-CO_mf)/(H2_mf/H2CO+H2O_mf/H2OCO+CO2_mf/COCO2+N2_mf/CON2+CH4_mf/COCH4)
CO2_UD=(1-CO2_mf)/(H2_mf/H2CO2+H2O_mf/H2OCO2+CO_mf/COCO2+N2_mf/CO2N2+CH4_mf/CO2CH4)
N2_UD=(1-N2_mf)/(H2_mf/H2N2+H2O_mf/H2ON2+CO_mf/CON2+CO2_mf/CO2N2+CH4_mf/N2CH4)
CH4_UD=(1-CH4_mf)/(H2_mf/H2CH4+H2O_mf/H2OCH4+CO_mf/COCH4+CO2_mf/CO2CH4+N2_mf/N2CH4)
-- Compute anode adsorption and surface diffusion modifications
area_H2=math.pi*(H2i*10^-10)^2
area_H2O=math.pi*(H2Oi*10^-10)^2
area_CO=math.pi*(COi*10^-10)^2
area_CO2=math.pi*(CO2i*10^-10)^2
area_N2=math.pi*(N2i*10^-10)^2
area_O2=math.pi*(O2i*10^-10)^2
area_CH4=math.pi*(CH4i*10^-10)^2
pres_H2=math.max(0,pH2-J*82.058*Tk*(th_a/10000)/(2*F)*(tort_a/(H2_UD*por_a/100)))
pres_H2O=math.max(0,pH2O+J*82.058*Tk*(th_a/10000)/(2*F)*(tort_a/(H2O_UD*por_a/100)))
pres_CO=math.max(0,pCOc-J*82.058*Tk*(th_a/10000)/(2*F)*(tort_a/(CO_UD*por_a/100)))
pres_CO2=math.max(0,pCO2c+J*82.058*Tk*(th_a/10000)/(2*F)*(tort_a/(CO2_UD*por_a/100)))
pres_N2=math.max(0,pN2)
pres_O2=math.max(0,pO2anode)
pres_CH4=math.max(0,pCH4)
Qev_H2=0.425
Qev_H2O=0.549
Qev_CO=0.5
Qev_CO2=0.5
Qev_N2=0.5
Qev_O2=0.5
Qev_CH4=0.5
bP_H2=6.023*10^23*area_H2*10^-
    13/math.sqrt(2*math.pi*R*Tk*H2ii)*math.exp(Qev_H2/(0.026*Tk/298))*pres_H2
bP_H2O=6.023*10^23*area_H2O*10^-
    13/math.sqrt(2*math.pi*R*Tk*H2Oii)*math.exp(Qev_H2O/(0.026*Tk/298))*pres_H2O
bP_CO=6.023*10^23*area_CO*10^-
    13/math.sqrt(2*math.pi*R*Tk*COii)*math.exp(Qev_CO/(0.026*Tk/298))*pres_CO
bP_CO2=6.023*10^23*area_CO2*10^-
    13/math.sqrt(2*math.pi*R*Tk*CO2ii)*math.exp(Qev_CO2/(0.026*Tk/298))*pres_CO2
bP_N2=6.023*10^23*area_N2*10^-
    13/math.sqrt(2*math.pi*R*Tk*N2ii)*math.exp(Qev_N2/(0.026*Tk/298))*pres_N2
bP_O2=6.023*10^23*area_O2*10^-
    13/math.sqrt(2*math.pi*R*Tk*O2ii)*math.exp(Qev_O2/(0.026*Tk/298))*pres_O2
bP_CH4=6.023*10^23*area_CH4*10^-
    13/math.sqrt(2*math.pi*R*Tk*CH4ii)*math.exp(Qev_CH4/(0.026*Tk/298))*pres_CH4
bP_sum=bP_H2+bP_H2O+bP_CO+bP_CO2+bP_N2+bP_O2+bP_CH4
cov_H2=bP_H2/(1+bP_sum)
cov_H2O=bP_H2O/(1+bP_sum)
cov_CO=bP_CO/(1+bP_sum)
cov_CO2=bP_CO2/(1+bP_sum)
cov_N2=bP_N2/(1+bP_sum)
cov_O2=bP_O2/(1+bP_sum)
cov_CH4=bP_CH4/(1+bP_sum)
cov_sum=cov_H2+cov_H2O+cov_CO+cov_CO2+cov_N2+cov_O2+cov_CH4
fij_H2=cov_H2/cov_sum
fij_H2O=cov_H2O/cov_sum
fij_CO=cov_CO/cov_sum
fij_CO2=cov_CO2/cov_sum
fij_N2=cov_N2/cov_sum
fij_O2=cov_O2/cov_sum
fij_CH4=cov_CH4/cov_sum
DsurfH2th1=0.1
DsurfH2th2=4.51e-5
D_H2=H2_UD^fij_H2*((DsurfH2th1^(1-fij_H2)*DsurfH2th2^fij_H2)/(1-fij_H2))^(1-fij_H2)
D_H2O=H2O_UD^fij_H2O*(10^-4)^(1-fij_H2O)
D_CO=CO_UD^fij_CO*(10^-4)^(1-fij_CO)
```

```
D_CO2=CO2_UD^fij_CO2*(10^-4)^(1-fij_CO2)
D_N2=N2_UD^fij_N2*(10^-4)^(1-fij_N2)
D_O2=O2N2^fij_O2*(10^-4)^(1-fij_O2)
D_CH4=CH4_UD^fij_CH4*(10^-4)^(1-fij_CH4)
--
-- Compute the cathode concentration polarization
----------------------------------------------------------------
Deffc=0.01*por_c*O2N2/tort_c
ics=1.0e-8*(4.0*F*Ptotal*atm2Pa*Deffc)/(R*Tk*th_c*mic2m)*math.log(1.0/(1.0-pO2air))
Cath=(R*Tk/4.0/F)*math.log(1.0-(J/ics))
--
-- Compute the anode concentration polarization
----------------------------------------------------------------
DeffH2=D_H2
DeffH2O=0.01*H2O_UD*por_a/tort_a
DeffCO=0.01*CO_UD*por_a/tort_a
DeffCO2=0.01*CO2_UD*por_a/tort_a
alim=2*F*pH2*atm2Pa*DeffH2/(831.45*Tk*th_a)
blim=2*F*pH2O*atm2Pa*DeffH2O/(831.45*Tk*th_a)
clim=2*F*pCOc*atm2Pa*DeffCO/(831.45*Tk*th_a)
dlim=2*F*pCO2c*atm2Pa*DeffCO2/(831.45*Tk*th_a)
-- Adjust calculation for iteration case of too high current requested
if J>(alim+clim) then
  Jcalc=(alim+clim)*0.99
else
  Jcalc=J
end
OPa_A=(Jcalc+blim+dlim)/blim/dlim
OPa_B=(Jcalc*(alim*dlim+blim*clim)+blim*clim*dlim+alim*blim*dlim-alim*clim*dlim-
    alim*blim*clim)/alim/blim/clim/dlim
OPa_C=(Jcalc-alim-clim)/alim/clim
holdA1=OPa_A
holdB1=OPa_B
holdC1=OPa_C
stabcheck=OPa_B^2-4.0*OPa_A*OPa_C
stabcheck2=(-OPa_B+math.sqrt(OPa_B^2-4.0*OPa_A*OPa_C))/2.0/OPa_A
if stabcheck>0 then
  if stabcheck2>0 then
    Anod=(R*Tk/2.0/F)*math.log((-OPa_B+math.sqrt(OPa_B^2-4.0*OPa_A*OPa_C))/2.0/OPa_A)
    holdA2=0
    holdB2=0
    holdC2=0
  else
    DeffH2=0.01*H2_UD*por_a/tort_a
    DeffH2O=0.01*H2O_UD*por_a/tort_a
    DeffCO=0.01*CO_UD*por_a/tort_a
    DeffCO2=0.01*CO2_UD*por_a/tort_a
    alim=2*F*pH2*atm2Pa*DeffH2/(831.45*Tk*th_a)
    blim=2*F*pH2O*atm2Pa*DeffH2O/(831.45*Tk*th_a)
    clim=2*F*pCOc*atm2Pa*DeffCO/(831.45*Tk*th_a)
    dlim=2*F*pCO2c*atm2Pa*DeffCO2/(831.45*Tk*th_a)
    OPa_A=(Jcalc+blim+dlim)/blim/dlim
    OPa_B=(Jcalc*(alim*dlim+blim*clim)+blim*clim*dlim+alim*blim*dlim-alim*clim*dlim-
    alim*blim*clim)/alim/blim/clim/dlim
    OPa_C=(Jcalc-alim-clim)/alim/clim
    holdA2=OPa_A
    holdB2=OPa_B
    holdC2=OPa_C
    Anod=(R*Tk/2.0/F)*math.log((-OPa_B+math.sqrt(OPa_B^2-4.0*OPa_A*OPa_C))/2.0/OPa_A)
  end
end
--
-- Compute the final voltage result
----------------------------------------------------------------
V=(Voc-Ohmic-BV+Cath+Anod)+V_loss
Z=V
--
-- return the voltage value
return Z
end
```

```
------------------------------------------------------------------
--                                                              --
--      CH4ReformingRate()                                      --
--                                                              --
--      CH4 conversion rate for on-cell reformation             --
--                                                              --
------------------------------------------------------------------
function CH4ReformingRate()
GasConstant=8.3144
Ch4_Usage=4274.0*pCH4*math.exp(-82000.0/fuelT/GasConstant)
return Ch4_Usage
end
```

Distribution

No. of
Copies

No. of
Copies

3 U.S. Department of Energy
    National Energy Technology Laboratory
    3610 Collins Ferry Road
    P.O. Box 880
    Morgantown, WV 26507-0880
      T Shultz
      B White
      S Vora

3 **Local Distribution**
3 Pacific Northwest National Laboratory
      K Lai   (PDF)
      MA Khaleel   (PDF)
      BJ Koeppel   (PDF)