

Solid Oxide Fuel Cell (SOFC) Thermal Management at Cell and System Scales

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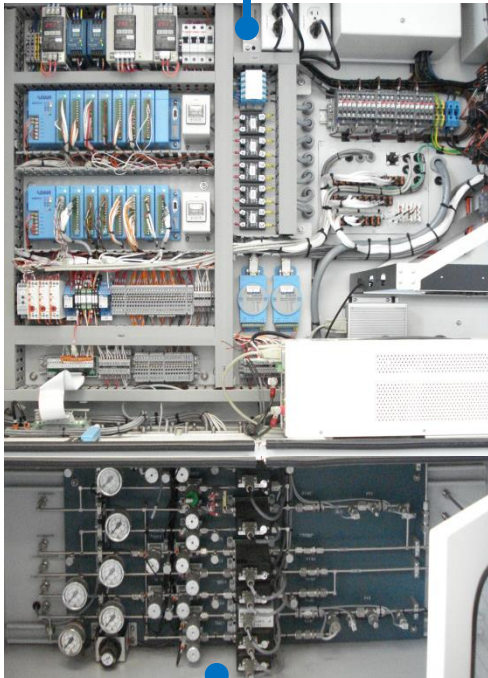
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Presentation Outline

- **A Pseudo 3D model for planar SOFC integrated with a heating furnace**
- **Temperature profiles in structural layers;**
- **System level modelling and simulation;**
- **Balance-of-Plant analysis**

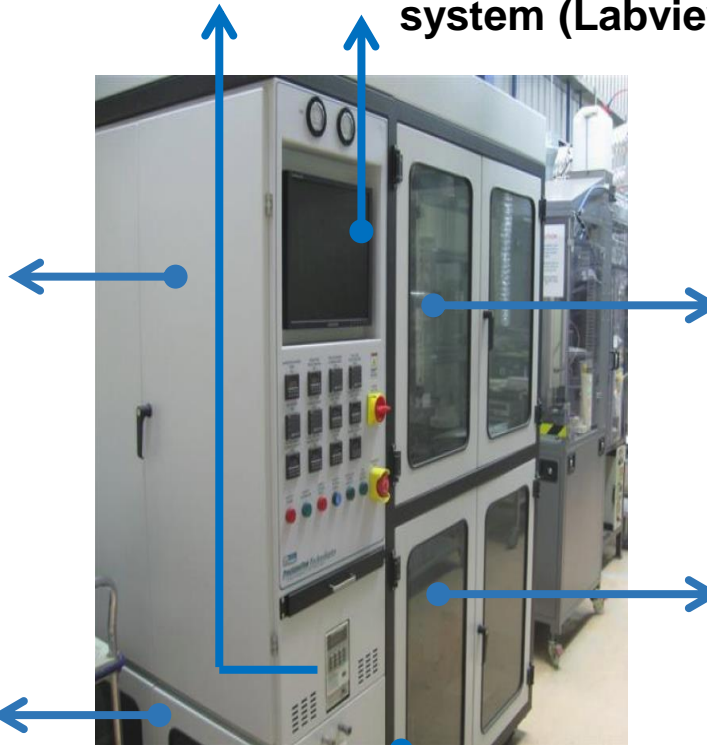
The SOFC test station at Curtin University in collaboration with Ceramic Fuel Cells Ltd.

Electronic housing & data acquisition system



Mass flow meter system

Load controller



SOFC test rig

Monitoring system (Labview)

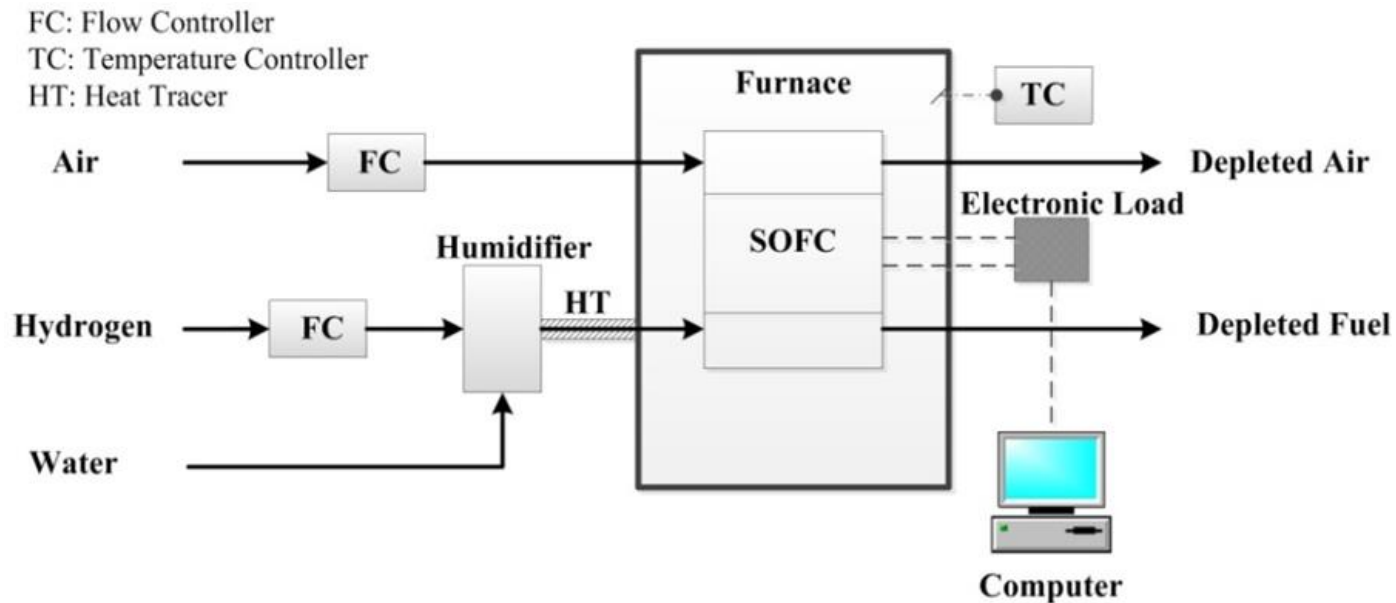
Furnace for placing cell/stack



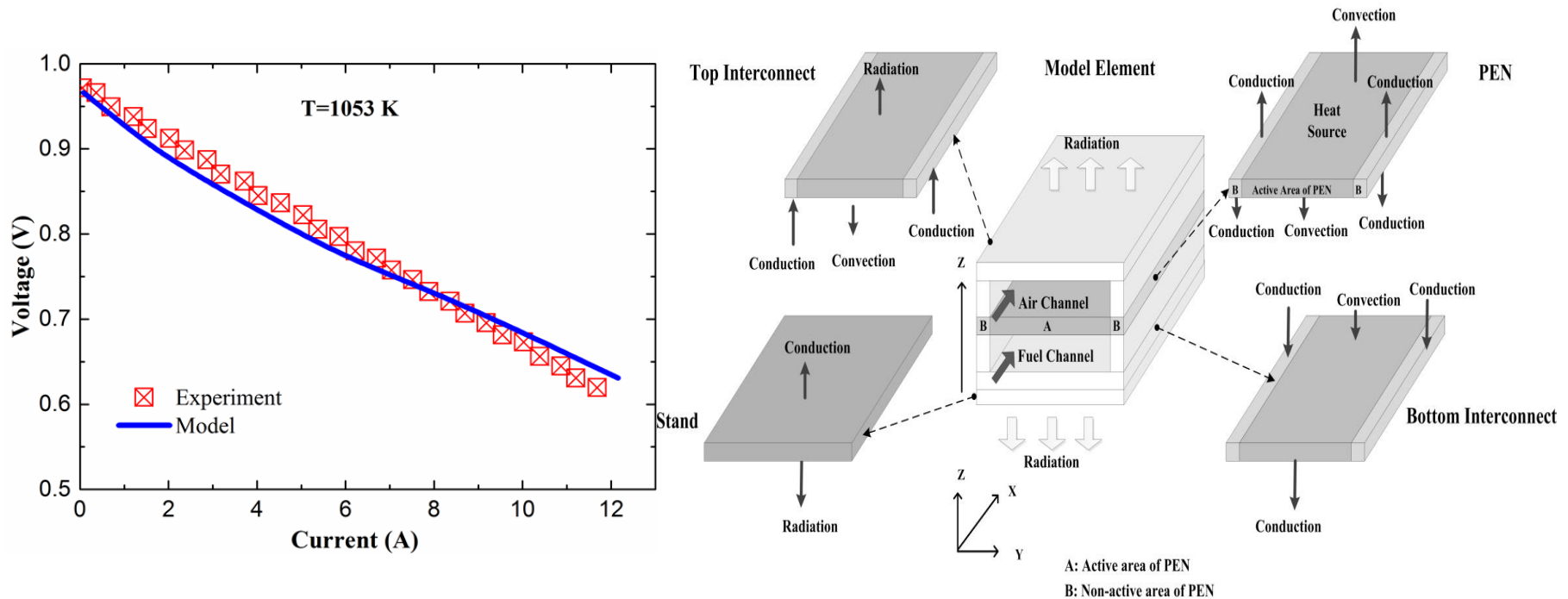
Humidifier Pre-reformer

Test Rig Modelling

A Pseudo 3D Model for Planar SOFC Integrated with a Heating Furnace



Multi-Layer modelling structure and validation

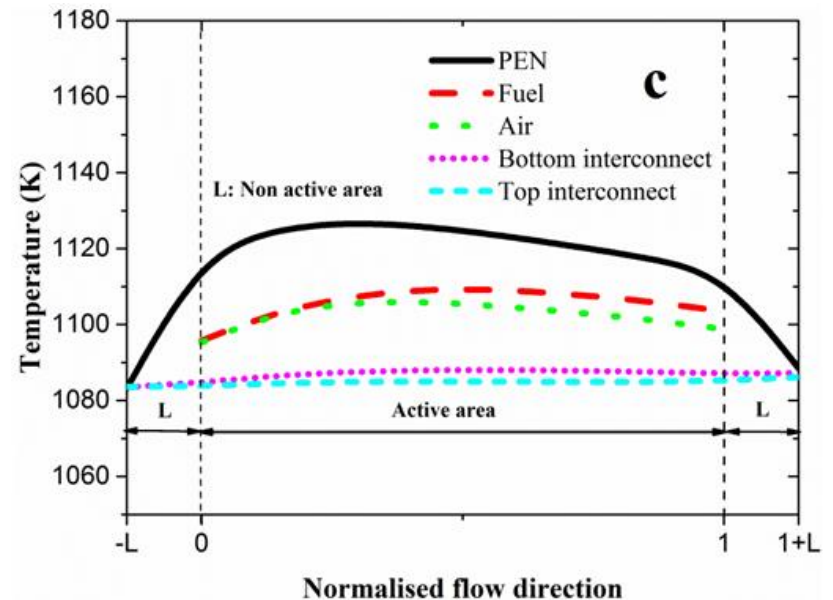
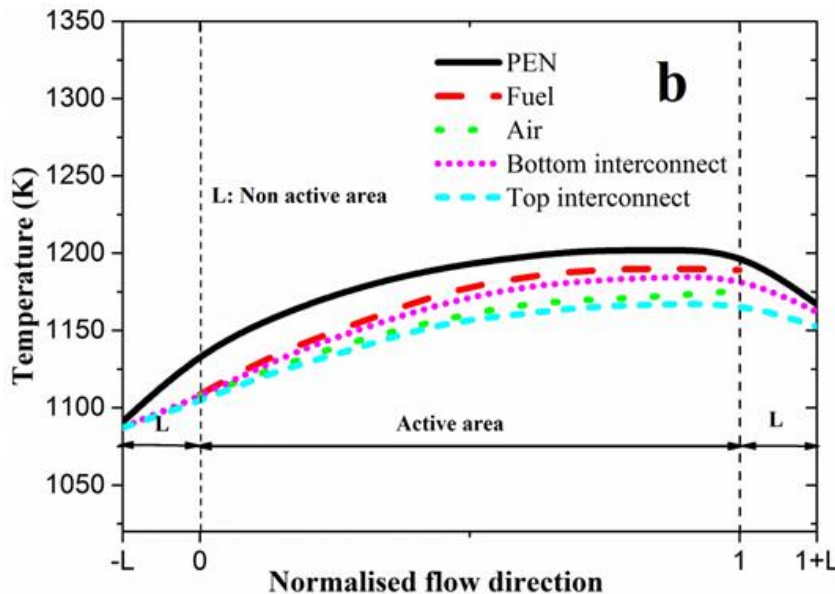


Four-layer modelling framework including stand, two interconnects, and PEN

Model Capabilities

- Detailed prediction of cell performance and thermal behaviour under both adiabatic and non-adiabatic conditions;
- Adiabatic condition is mostly consistent with cell's operation in stack (the marketable/commercial scale);
- Non-adiabatic condition is mostly consistent with cell's operation integrated with a furnace (laboratory scale);
- Detailed insights for temperature profiles in cells structure provides a design and thermal management tool;
- Model-based design of new tests is feasible

Temperature profiles in structural layers: adiabatic (left) and non-adiabatic(right)



System level modelling and simulation

Few Challenges and Opportunities:

→ A black box/lump module is numerically efficient;

BUT misses the main features of SOFC

→ A distributed module accounts for detailed transport and reaction kinetics;

BUT causes serious complexity

→ More dimensions → more analysis feasible;

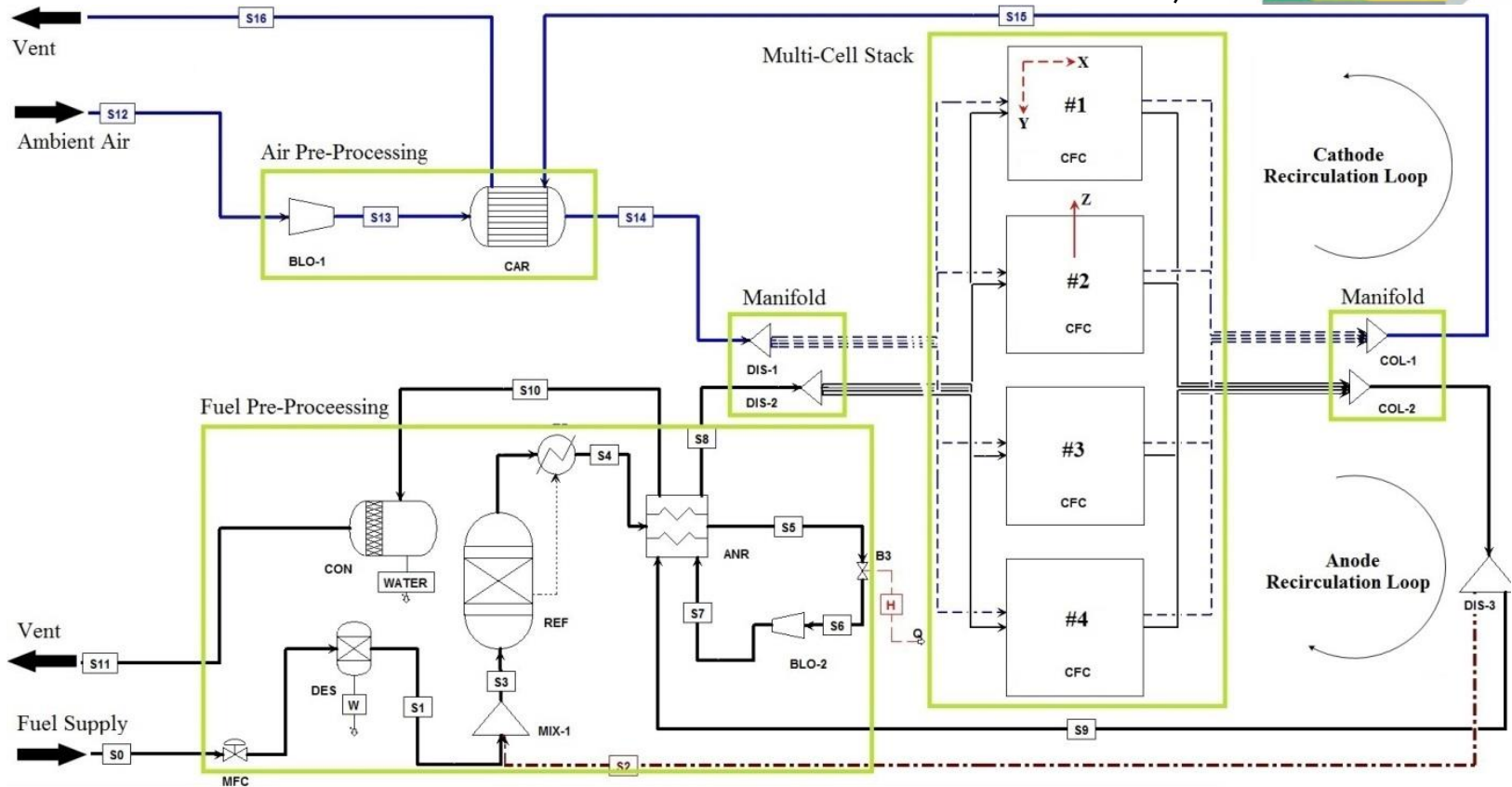
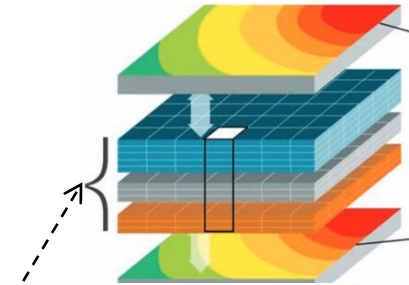
BUT more numerical facilities and proficiency needed

→ A flowsheeting package is not a suitable tool for discretization purposes due to meshing difficulties;

BUT offers thermodynamics data bases and process analysis and optimization tools;

Solution: Compromise

Modelling and simulation outlook



ANR: Anode Recuperator
BLO: Blower

CAR: Cathode Recuperator
COL: Collector

CON: Condenser
DES: Desulphuriser

DIS: Distributor
MFC: Mass Flow Controller

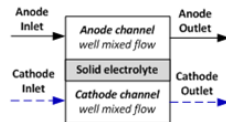
REF: Reformer
MIX: Mixer
CFC: Co-Flow Cell

Modelling Platform

Compartment Scale (1 μm – 1 cm)

Typical Issues

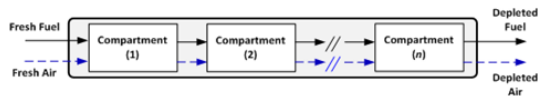
- Reaction kinetics, heat and mass transfer
- Fuel conversion, carbon deposition
- Catalyst and material improvements



Channel Scale (1 cm – 10 cm)

Typical Issues

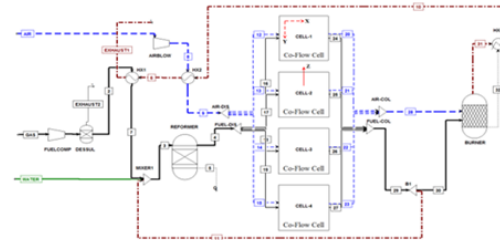
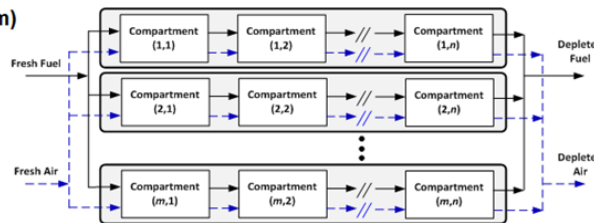
- Fuel and air flow configuration
- Fluid flow regimes
- Residence time distributions



Cell Scale (1 cm – 10 cm)

Typical Issues

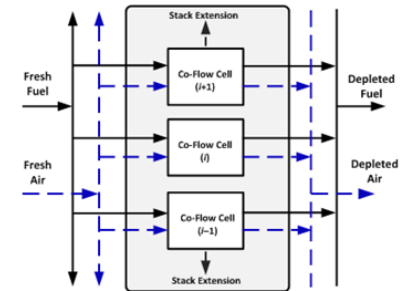
- Thermal management
- Cell life durability
- Dynamic cell behaviour



System Scale (1 m – 10 m)

Typical Issues

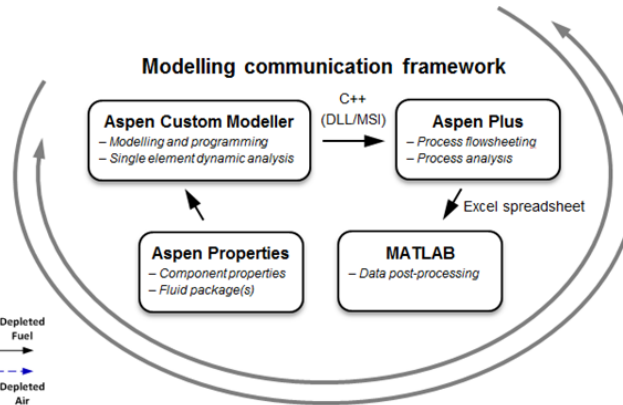
- Process optimisation
- Process dynamics and control
- Process commercialisation



Stack Scale (10 cm – 1 m)

Typical Issues

- Stack energy integration
- Process steadiness
- Start-up and shut-down dynamics



Model capabilities

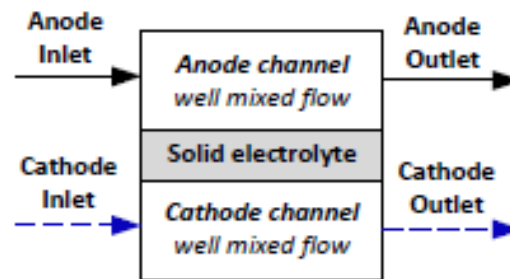
- Prediction of SOFC performance at different scales and with adjustable details(0-3D);
- System level modelling, flowsheeting, analysis, and design;
- Optimization capability through both operating variable manipulation and process flow diagram improvement;
- Potential room for dynamic and control research at system level;
- Utilization of well-established components data bases and thermodynamical packages;
- Establishment of a modular modelling library customised for electrochemical reactors such as SOFC, MCFC, ...
- Fuel processing analysis without further programming/modelling needs;

Compartment Scale Assembly capable for 0D modelling of the SOFC

Compartment Scale (1 μm – 1 cm)

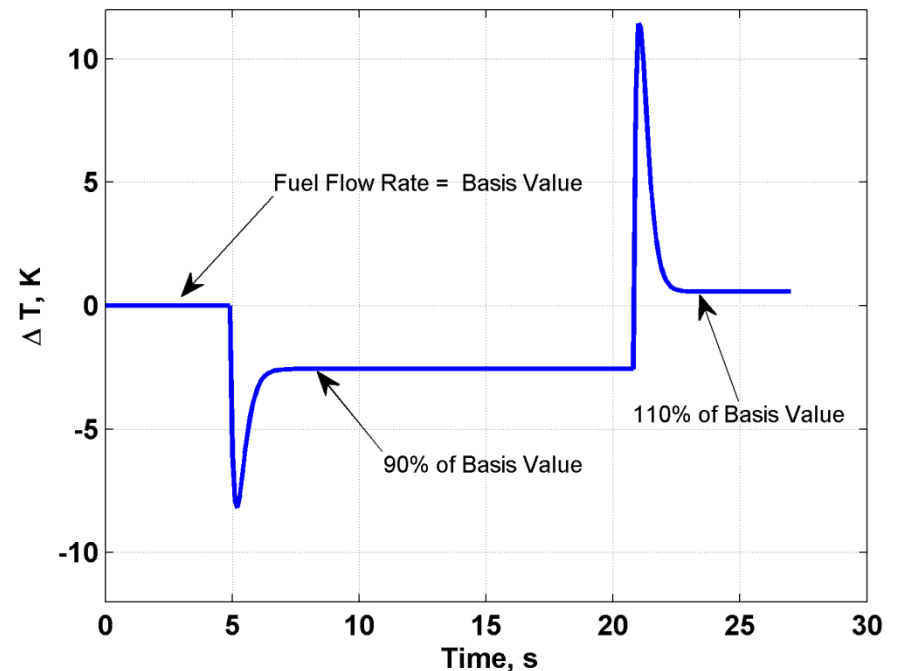
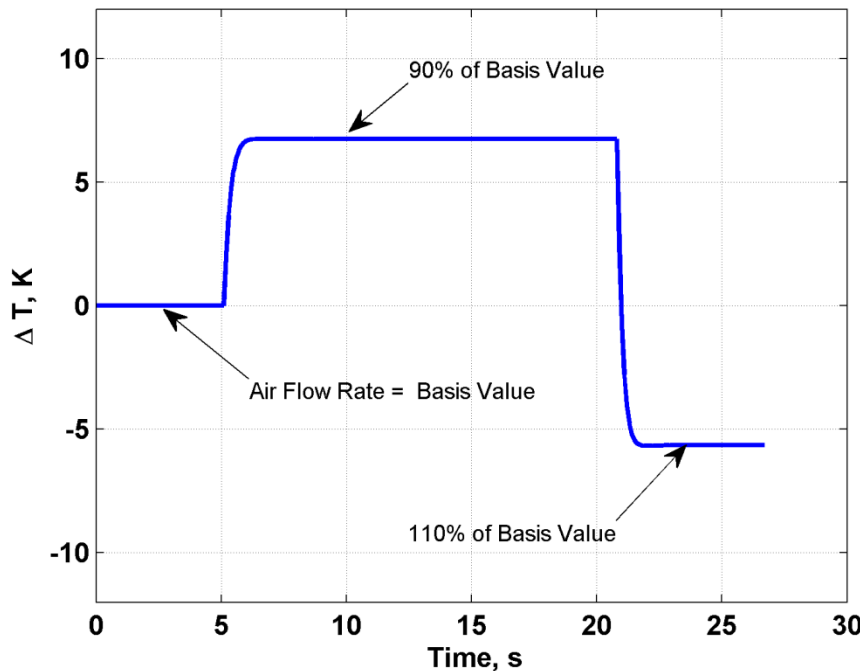
Typical Issues

- Reaction kinetics, heat and mass transfer
- Fuel conversion, carbon deposition
- Catalyst and material improvements



Recommended for flowsheeting purposes and dynamic studies

Dynamic sensitivity analysis at compartment scale: temperature response to the air and fuel perturbation

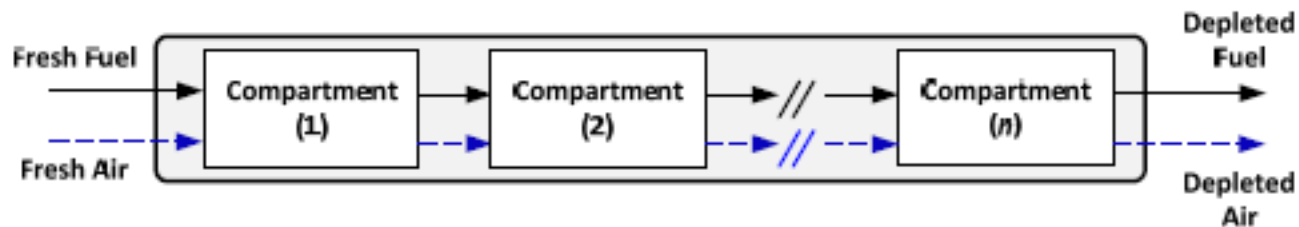


Channel Scale Assembly capable for 1D modelling of the SOFC

Channel Scale (1 cm – 10 cm)

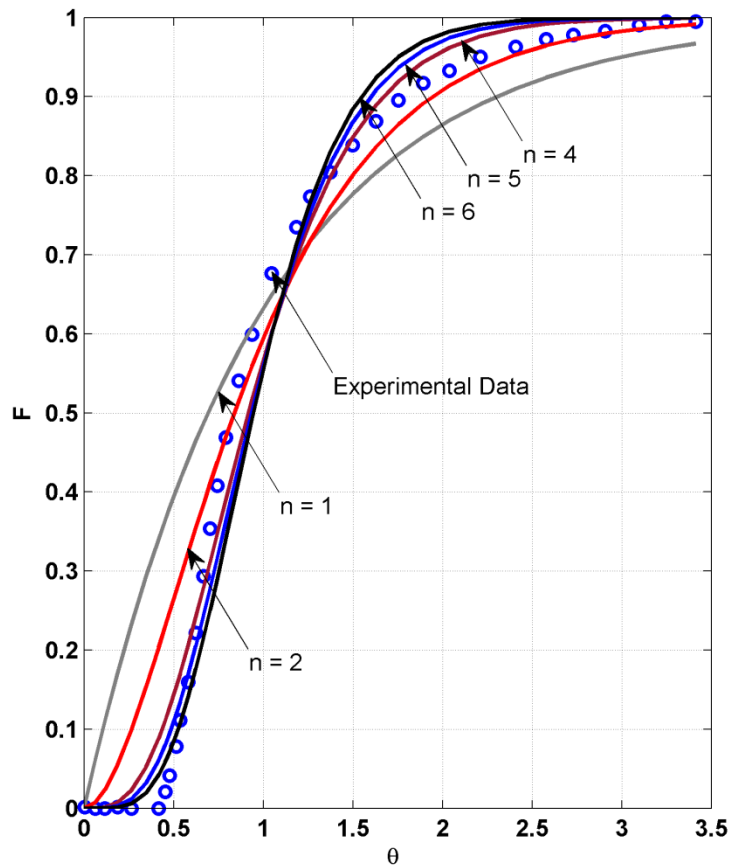
Typical Issues

- Fuel and air flow configuration
- Fluid flow regimes
- Residence time distributions



Recommended for Co-flow and Counter flow SOFC modelling as well as flowsheeting purposes

Estimation of number of compartments in series based on reactor's Residence Time Distribution



Circles:

Experimental RTD data (Krewer et al. (2004))

Solid lines:

Prediction based on n compartments

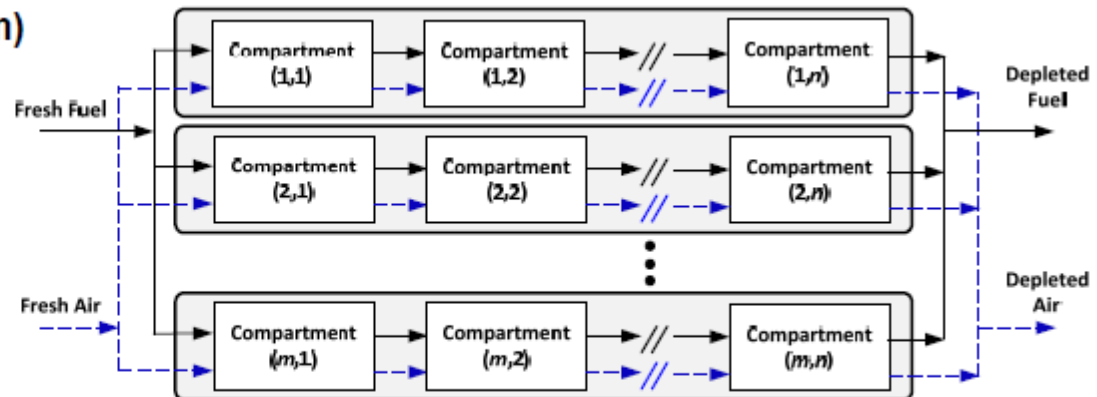
$$F = 1 - e^{-n\theta} \sum_{i=1}^n \frac{(n\theta)^{i-1}}{(i-1)!}$$

Cell scale assembly capable for 2D modelling of the SOFC

Cell Scale (1 cm – 10 cm)

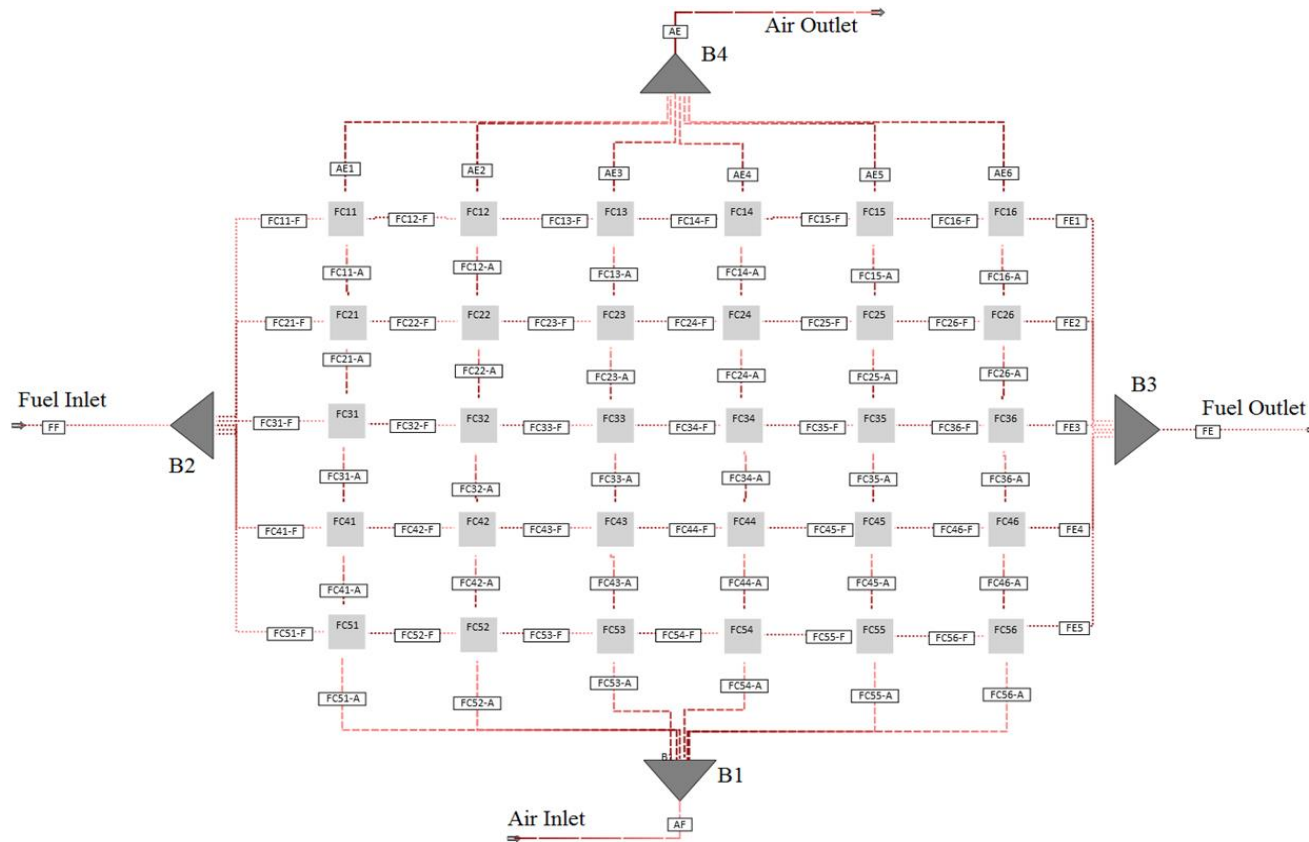
Typical Issues

- Thermal management
- Cell life durability
- Dynamic cell behaviour



Recommended for SOFC modelling at lab scale and flowsheeting purposes

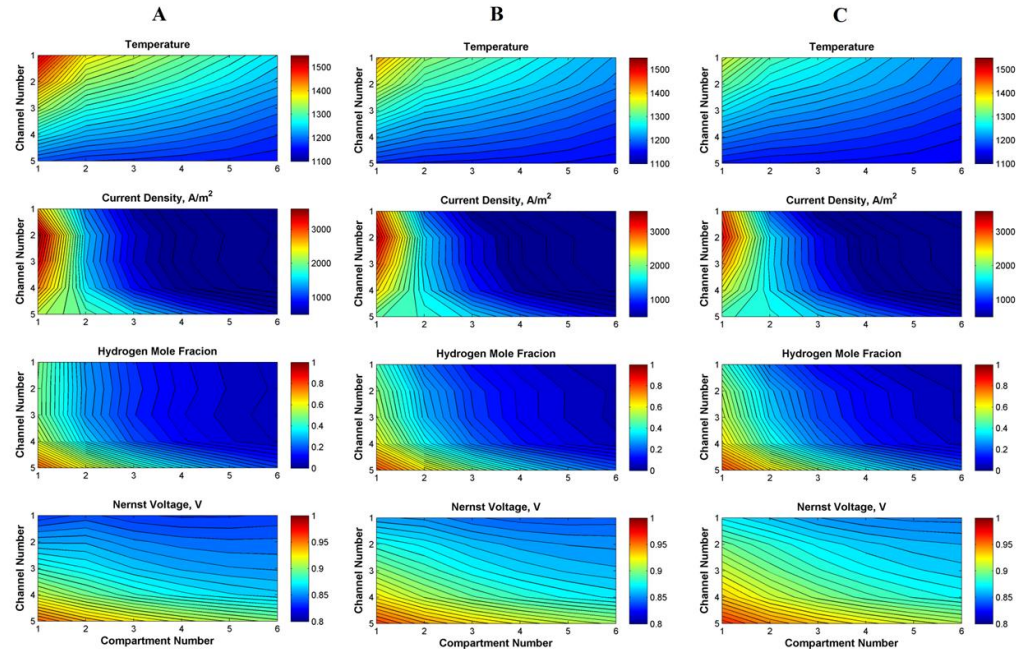
Distributed Cell embedded in a Balance of Plant (Aspen Plus implementation)



Sensitivity Analysis at Cell Scale: Air Flow Rate Impact

Higher air flow rate results in

- more homogeneity in cell's distributed variables
- Lower average temperature and suppressing the electrochemical reaction/current generation;
- Higher pressure drop/costs



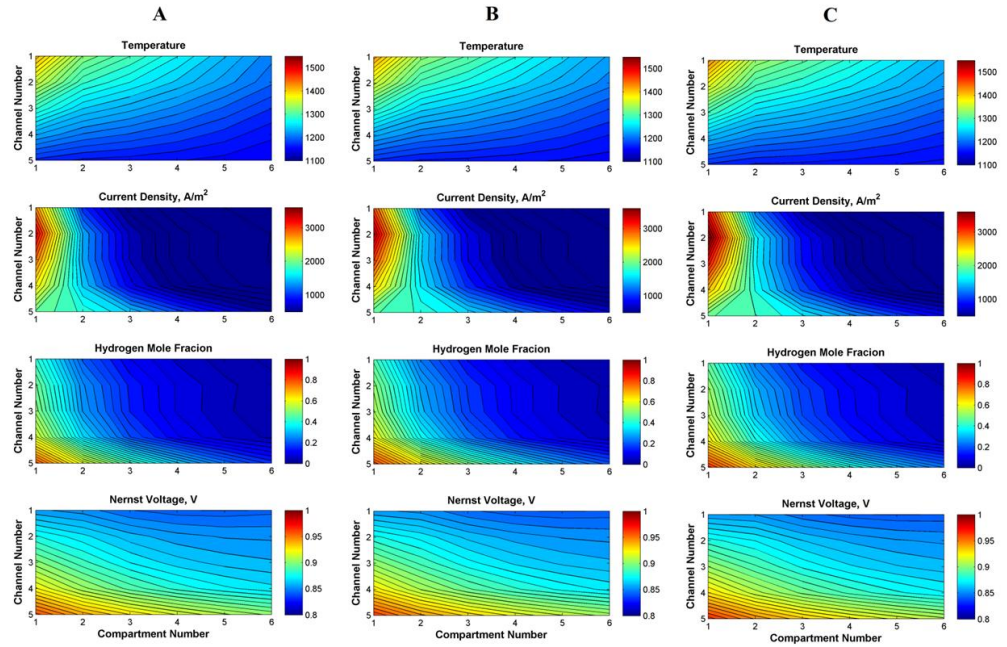
Variable	A (Air flow rate 20% lower than base case)	B (Base case air flow rate)	C (Air flow rate 20% higher than base case)
Average Temperature, K	1265	1235	1215
Temperature Coefficient of Variation	0.0663	0.0522	0.0432
Average Current Density, A/m ²	1113	1108	1099
Current Density Coefficient of Variation	0.8854	0.8482	0.8119
Average Nernst Voltage, V	0.873	0.883	0.891
Average Hydrogen Mole Fraction	0.25	0.26	0.27
Fuel Utilization	0.91	0.90	0.89

Sensitivity Analysis at Cell Scale: Fuel Flow Rate Impact

Higher fuel flow rate results in

- less homogeneity in cell's distributed temperature
- Higher average temperature and improved electrochemical reaction/current generation;
- Less fuel utilization

All due to more reactant availability in all parts of the cell



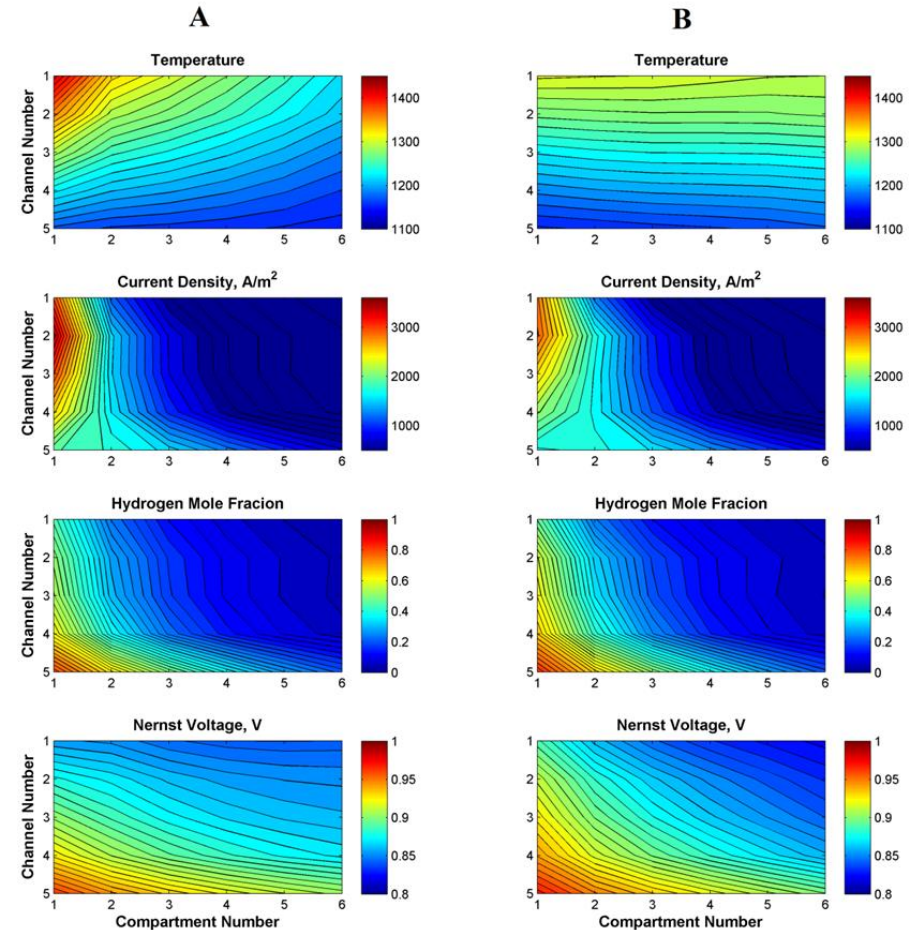
Variable	A (Fuel flow rate 10% lower than base case)	B (Base case fuel flow rate)	C (Fuel flow rate 10% higher than base case)
Average Temperature, K	1229	1235	1239
Temperature Coefficient of Variation	0.0517	0.0522	0.0532
Average Current Density, A/m ²	1012	1108	1195
Current Density Coefficient of Variation	0.9056	0.8482	0.8199
Average Nernst Voltage, V	0.881	0.883	0.885
Average Hydrogen Mole Fraction	0.24	0.26	0.28
Fuel Utilization	0.92	0.90	0.88

Optimization at Cell Scale: Air Distribution

Optimized Air distribution (B) shows:

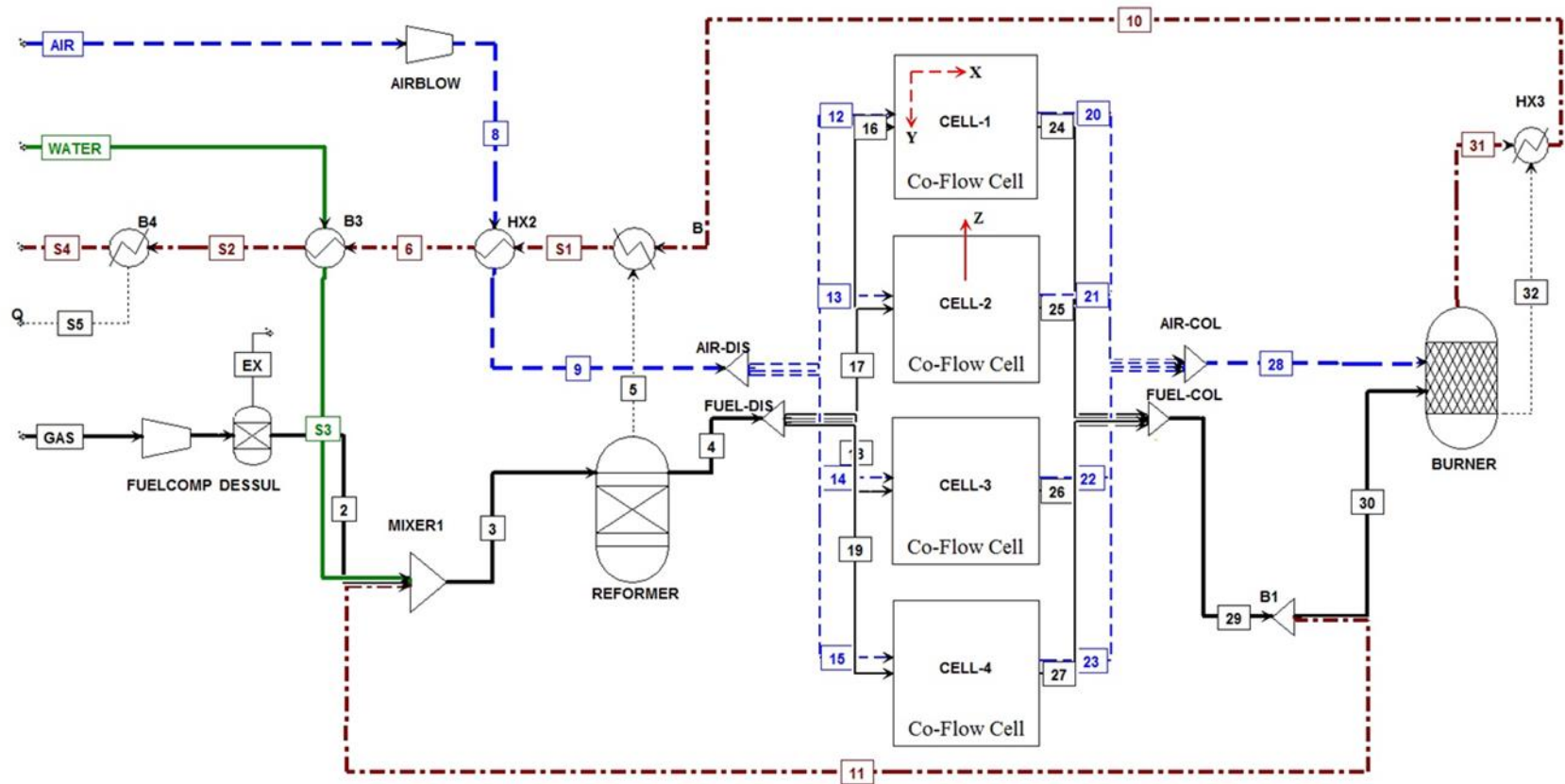
- more homogeneity in cell's distributed variables for both temperature and current (desired) ;
- Hot spot is removed (desired). ;
- Not significant change in generated current and fuel utilization (desired).

Variable	Non-Optimised	Optimised
Average Temperature, K	1235	1238
Temperature Coefficient of Variation	0.0522	0.0407
Average Current Density, A/m ²	1108	1098
Current Density Coefficient of Variation	0.8482	0.7554
Average Nernst Voltage, V	0.883	0.884
Average Hydrogen Mole Fraction	0.26	0.28
Fuel Utilization	0.90	0.89



System scale assembly

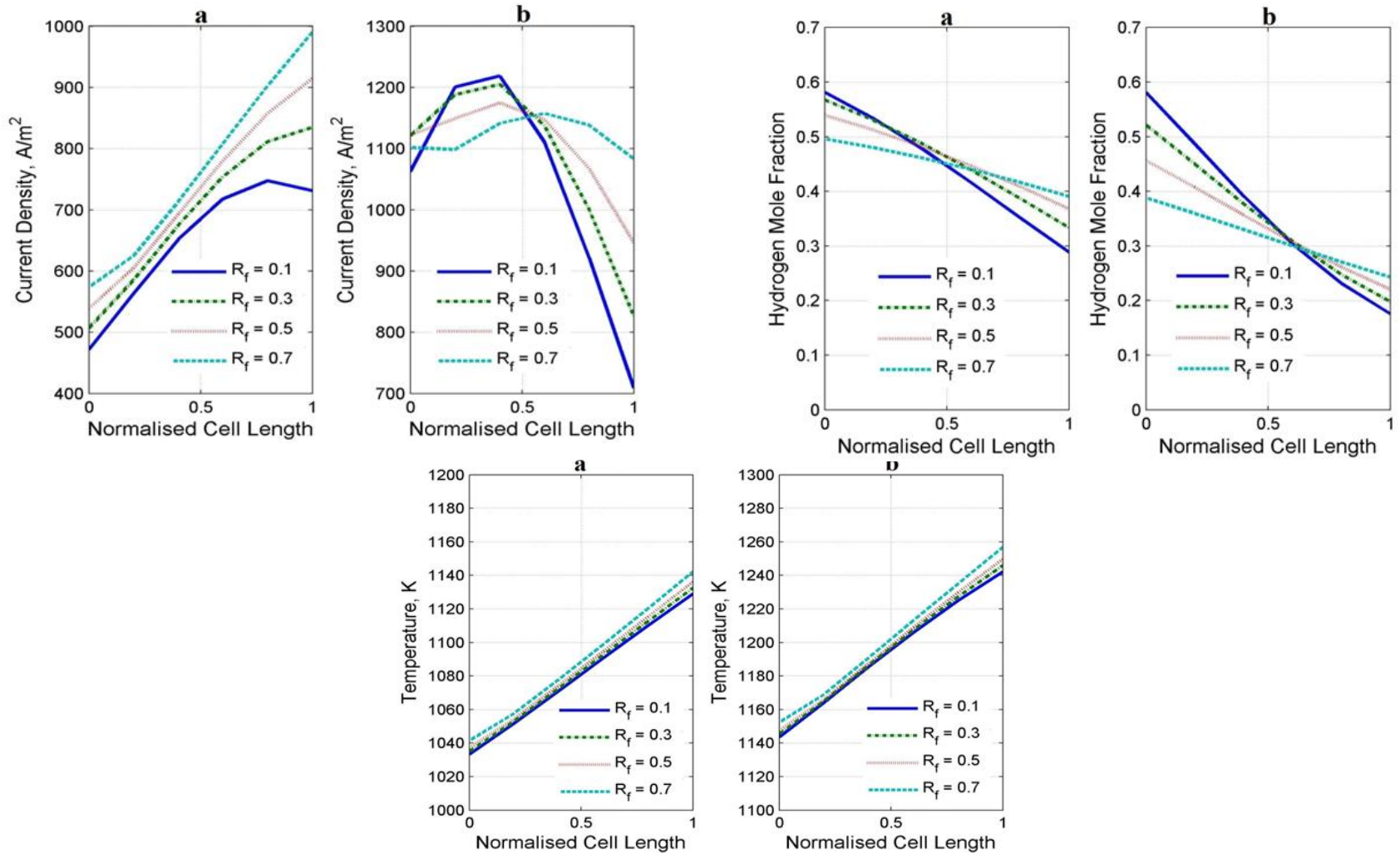
Simulated plant with external Methane reforming process



Recommended for Balance of Plant modelling and flowsheeting purposes

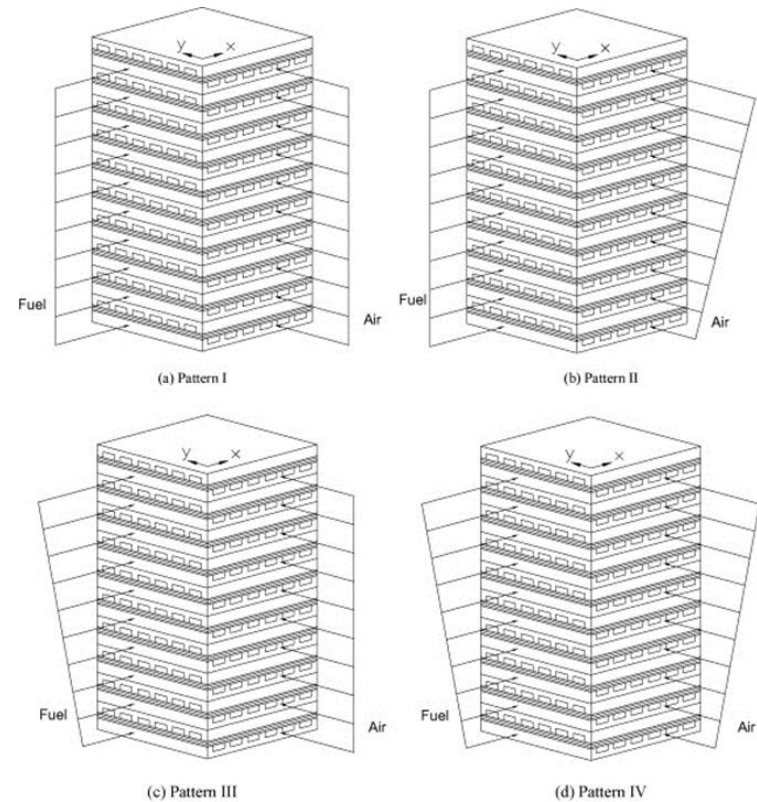
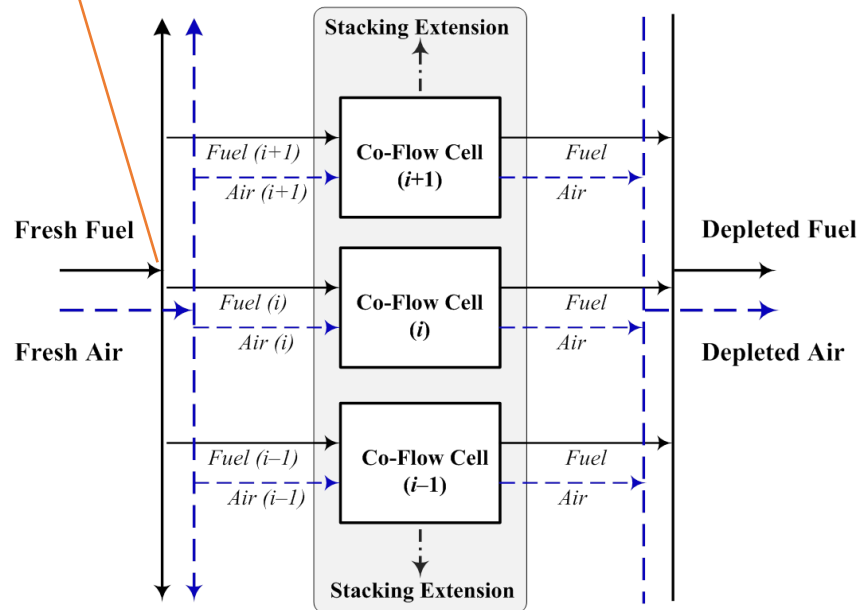
Balance of Plant Analysis

Distributed variables affected by reformer temperature: (a) Reformer T = 973 K; (b) Reformer T = 1073 K.



A stack analysis: effect of manifold maldistribution

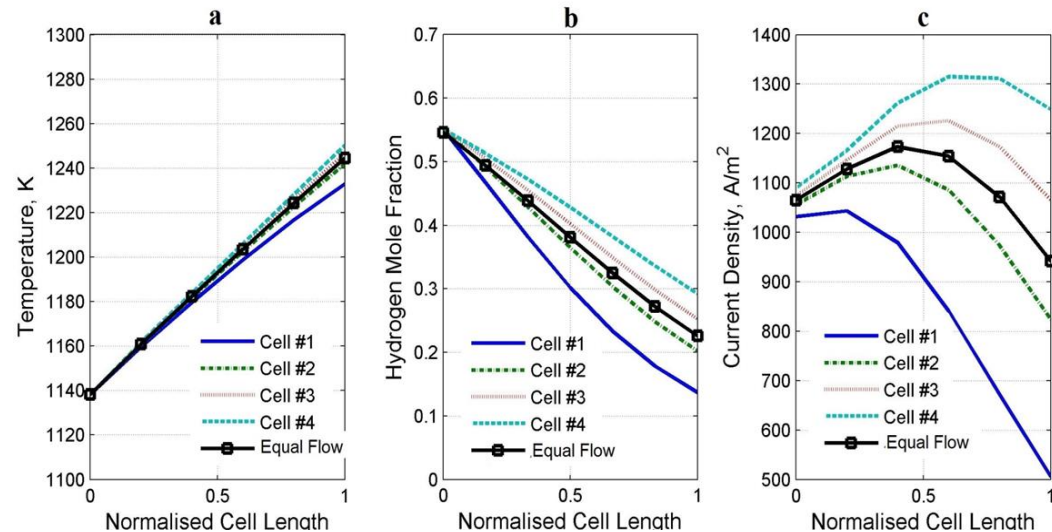
$$f^n = \bar{f} \left(\frac{2d_{stack}}{(n_{stack}-1)}(n-1) + (1-d_{stack}) \right)$$



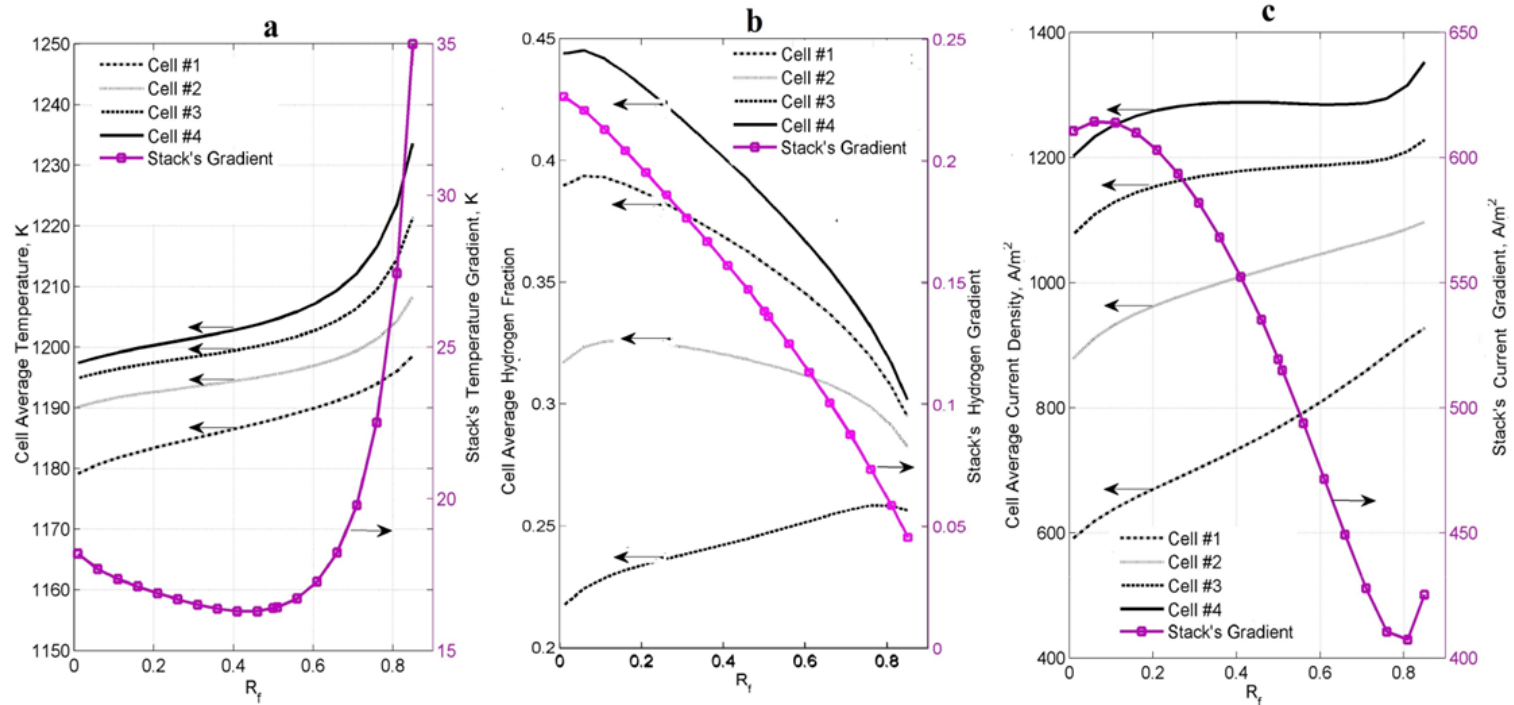
Cell-to-Cell variation of distributed variables caused by the fuel manifold malfunction

Significant deviation from even distribution

- The temperature of the cell with less fuel share is minimum but more smoother ;
- The generated current and average reactant availability are minimum in cell with min fuel share but not necessary result in smoother profile
- Current peaks in each cell are significantly shifted by fuel shares

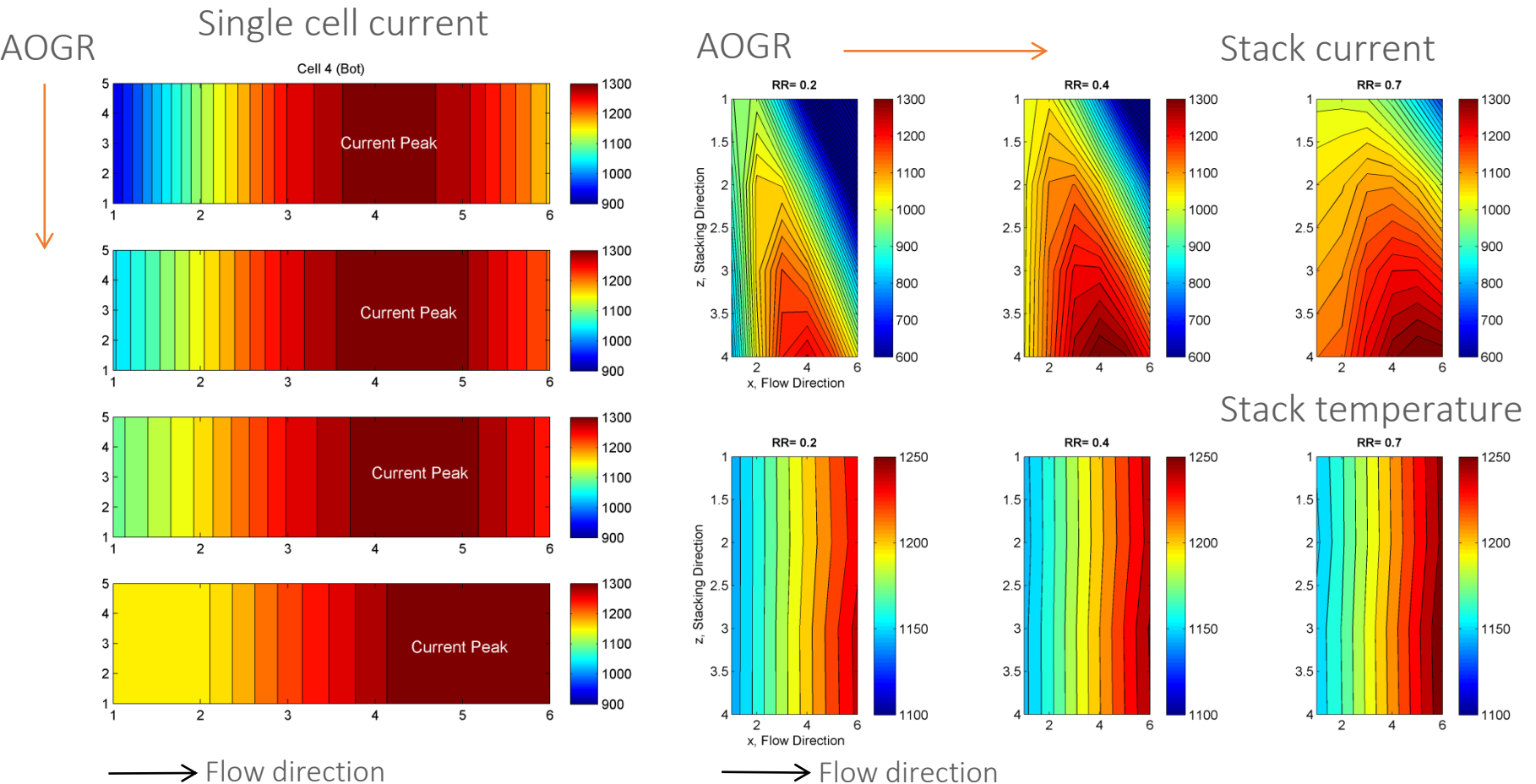


Stacking direction gradients as a function of anode off-gas recycle (AOGR)



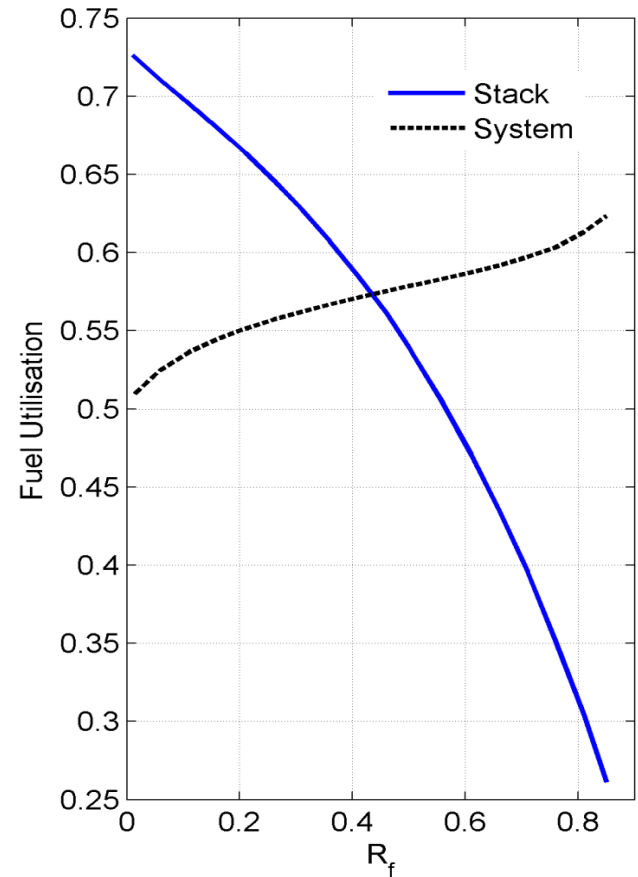
- AOGR rate has different effect on cells in stack depending on their fuel share;
- AOGR influences the gradient in stacking direction making room for optimization works for thermal management
- AOGR should be limited to due sizing and cost issues.

Counters for single cell unit and multi-cell stack under varying AOGR



Process performance: Effect of recycle fraction on stack and system fuel utilisation

- AOGR reduces the fuel utilization in stack while increases that for whole system;
- This is technically desired because overall efficiency will be improved while stack/cell fuel starvation and hot spot formation can be avoided;
- Optimization of AOGR must be conducted through a detailed stack model integrated in a system level model such as this work.
- This optimization task is certainly a multi- objective one that leads in a so called “effective operation” not “most optimum operation” as it ultimately results in a compromised strategy.



Thank you for your attention!

References

- Amiri, A., S. Tang, P. Vijay and M. O. Tadé (2016). "Planar Solid Oxide Fuel Cell Modeling and Optimization Targeting the Stack's Temperature Gradient Minimization." Industrial & Engineering Chemistry Research **55**(27): 7446-7455.
- A. Amiri, P. Vijay, M.O. Tadé, K. Ahmed, G.D. Ingram, V. Pareek, R. Utikar, Solid oxide fuel cell reactor analysis and optimisation through a novel multi-scale modelling strategy, *Comput. Chem. Eng.* 78 (2015) 10-23.
- Tang, S., A. Amiri, P. Vijay and M. O. Tadé (2016). "Development and validation of a computationally efficient pseudo 3D model for planar SOFC integrated with a heating furnace." Chemical Engineering Journal **290**: 252-262.
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