On the Theoretical and Experimental Contributions to the Process Systems Engineering

Multi-Scale Experimental Analysis, Robust Optimisation and Explicit Model Predictive Control of Fuel Cell Energy Systems

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Outline

- Introduction and Control Objectives

- Multi-Scale Research Overview and Outcome
  - Micro Scale – Unit Cell
  - Meso Scale – Integrated System
  - Macro Scale – Automotive Propulsion System

- Conclusion and Discussions
Introduction and Background

Fuel cell is an electrochemical device that converts hydrogen or hydrogen rich fuel directly into electricity. Fuel cells are ideal power source in many areas of transport and stationary applications offering wide range of tangible environmental, economic and operational benefits. **Control is critical for the robust operation of the fuel cell system**—ultimately essential for maintaining:

(a) uninterruptable power demand under load variations

(b) high efficiency and performance affected by uncertainty

(c) reliability and longevity of the system, and

(d) economic profit margins
Advantages of PEM Fuel Cell

- Quick Start
- Low Operating Temperature
- High Efficiency
- Lower Corrosion Rates
- High Power Density
Fuel Cell Vehicular Applications

1. Cylinders hold hydrogen sourced from natural gas
2. Fuel cell supply unit - the cells have a gross power of 250kW
3. Fuel cell stacks
4. Fuel cell cooling units
5. Air conditioning unit
6. Water vapour from exhausts are the buses’ only emissions
7. Electric motor, can give a top speed of 80kph

http://news.bbc.co.uk/1/hi/england/london/3391507.stm

http://www.element-energy.co.uk/2011/02/hydrogen-buses-enter-service-in-london/
Transport for London: First Fuel Cell Bus RV1 running between Covent Garden and Tower Gateway Station since January 2011
Multi-Scale Fuel Cell Research

Eikerling, Kornyshev, Kucernak, *Driving the hydrogen economy*, Physics World, 2007
Multi-Scale Fuel Cell Research Focus

Kucernak et al, 2007

Manthanwar et al, 2014
Multi-Scale Fuel Cell Research Focus

Structure of the ionomer - hydrophobic polymer backbone surrounded by water phase

A platinum particle attached to a carbon particle substrate surrounded by ionomer

A single catalysed coated carbon particle

Catalyst layer showing pores and agglomerates of catalysed carbon particles

Catalyst layer and membrane

Gas transport layer, Microporous diffusion layer, composite catalyst layer and membrane

A MEA/bipolar plate combination showing feed channel and diffusion layer

Fuel cell stack composed of multiple electrode/flow-field plate combinations

Distance scale / m

Kucernak et al, 2007

10^{-3} 10^{-2} 10^{-1} 10^0 10^1 10^2

distance scale (m)

Unit Cell

Integrated Power Plant

Vehicular Propulsion System

Manthanwar et al, 2014
Energy System Challenges
Energy Systems Research Objectives

PEM Fuel Cell

- Theory

ESE

- Laboratory
- Applications

Key Questions

- What happens inside fuel cells?
  - In-situ and Ex-Situ Experiments
  - Observable and Unobservable Information

- What happens with BOP integration?
  - Hardware-In-the-loop System Integration
  - Optimisation and Control Algorithms

- What happens in real world?
  - Deployment and Testing on Prototypes
  - Development of Microcontroller Platform
Brief Introduction to Control Theory
Brief Introduction to Control Theory
Multivariable Control Structure
What is Advanced Process Control?

Advanced Process Control asks the much sought after control objective question, how to attain desired profit margins from a plant operating under uncertainty while at the same time satisfy all the following conditions?

- Process Feasibility
- Process Stability
- Operational Safety
- Equipment Reliability
- Consistent Product Quality
- Overall Process Efficiency and Performance

Technology of Model Predictive Control gives the answer
Model Predictive Control Algorithm

Robust Control Policy

\[
\Gamma(x(0)) = \min_{u(.)} \left\{ x(N)^T P x(N) + \sum_{k=0}^{N-1} x(k)^T Q x(k) + u(k)^T R u(k) \right\}
\]

s.t. \( x(k + 1) = A(\theta)x(k) + B(\theta)u(k) + Gw(k); \ x(0) = x_0 \)

Constraints

\[
\begin{align*}
x(k) & \in \mathcal{X} \subseteq \mathbb{R}^n \\
u(k) & \in \mathcal{U} \subseteq \mathbb{R}^m \\
w(k) & \in \mathcal{W} \subseteq \mathbb{R}^p ; \ \mathcal{W} \equiv \{w_{lb} \leq w(k) \leq w_{ub}\} \\
\theta & \in \Theta \subseteq \mathbb{R}^q ; \ \Theta \equiv \{\theta_{lb} \leq \theta \leq \theta_{ub}\} \\
x(N) & \in \mathcal{O}_\infty \subseteq \mathcal{X} ; \ \forall k = 0, 1, \ldots, N - 1
\end{align*}
\]

Analogy of Chess Moves: Compute Robust Control Policy above, Implement First Set of Actions and Repeat
Model Predictive Control – Predict
Model Predictive Control – Implement
How to Control Fuel Cell* System?

- Need Accurate Models of
  - Unit Cell
  - Stack
  - Balance of Plant
  - Application (e.g. Automotive Powertrain Dynamics)

- Control Objectives
  - Heat Management
  - Electricity Management
  - Water Management
  - Energy, Environment and Economics

*All the work in this research refers to the Polymer Electrolyte Membrane Fuel Cell and can be extended to other types
Implementation Strategy

**Design and Modelling Toolbox (D1)**
- **Task 1**: System Modelling
- **Task 2**: Optimal Model-Based Design of Experiments

**Optimisation and Control Toolbox (D2)**
- **Task 3**: System Optimisation
- **Task 4**: System Control

**Online Hardware-in-the-Loop (D3)**
- **Task 5a**: System Analysis and Diagnostics
- **Task 5b**: Validation, Characterisation and Benchmarking
New Unit Cell Model - Open Cathode

\[ \Delta H_{\text{fus}}^{\circ} = 241.81 \text{ kJ/mol} \]

\[ T \Delta S_{\text{fus}}^{\circ} = -13.24 \text{ kJ/mol} \]

\[ \Delta G_{\text{fus}}^{\circ} = -228.57 \text{ kJ/mol} \]
New Unit Cell Model – Liquid Cooled
Fuel Cell Electrochemistry

\[ E_{cell} = E_{ner} - E_{act} - E_{ohm} - E_{con} \]

\[ E_{ner} = E^o - \frac{RT}{nF} \ln \left( \frac{C_{H_2O}}{C_{H_2} \sqrt{C_{O_2}}} \right) \]

\[ E_{act} = \frac{RT}{\alpha nF} \ln \left( \frac{j + j_{loss}}{j_o} \right) \]

\[ j_o = \kappa nFe^{(-\beta nFE^o/RT)} \]

\[ E_{ohm} = jR_{ohm} \]

\[ R_{ohm} = \gamma_1 + \gamma_2 T + \gamma_3 j \]

\[ E_{con} = \frac{\zeta RT}{nF} e^{\theta j} \]
Complex Dynamics of Fuel Cell

\[
\begin{align*}
V_c \frac{dC_{O_2}}{dt} &= C_{O_2}^{\text{in}} F_c^{\text{in}} - C_{O_2} F_c^{\text{out}} - \frac{1}{2} r_{H_2O} A_m \\
V_c \frac{dC_{H_2O}}{dt} &= C_{H_2O}^{\text{in}} F_c^{\text{in}} - C_{H_2O} F_c^{\text{out}} + r_{H_2O} A_m \\
V_c \frac{dC_{N_2}}{dt} &= C_{N_2}^{\text{in}} F_c^{\text{in}} - C_{N_2} F_c^{\text{out}} \\
V_c \frac{dT}{dt} &= F_c^{\text{in}} T_a - F_c^{\text{out}} T + \frac{Q_h A_m}{\rho_a C_{p_a}} - \frac{U_c A_c}{\rho_a C_{p_a}} (T - T_s) \\
V_s \frac{dT_s}{dt} &= \frac{U_c A_c}{\rho_s C_{p_s}} (T - T_s) - \frac{\rho_a C_{p_a} F_c^{\text{in}}}{\rho_s C_{p_s}} (T_s - T_a) - \frac{U_s A_s}{\rho_s C_{p_s}} (T_s - T_a) \\
\frac{dP_e}{dt} &= j E_c N_c - \frac{1}{\eta_c} P_e
\end{align*}
\]
Algebraic Relationships

\[ r_{H_2O} = \frac{j}{nF} N_c \]

\[ F_{c}^{out} = \frac{(C_{O_2}^{in} + C_{N_2}^{in} + C_{H_2O}^{in}) F_c^{in} + \frac{1}{2} r_{H_2O} A_m}{C_{O_2} + C_{N_2} + C_{H_2O}} \]

\[ C_{p_a} = \frac{C_{N_2} C_{p}^{N_2} + C_{O_2} C_{p}^{O_2} + C_{H_2O} C_{p}^{H_2O}}{C_{N_2} + C_{O_2} + C_{H_2O}} \]

\[ C_{p}^{\psi} = c_1^{\psi} + c_2^{\psi} T + c_3^{\psi} T^2 + c_4^{\psi} T^3; \quad \forall \psi = \{H_2, O_2, N_2, H_2O\} \]

\[ \Delta H_{f_{H_2O_g}} = \Delta H_{f_{H_2O_g}}^{o} + \sum_{i=1}^{4} \left\{ \frac{1}{i} \left( c_{i}^{H_2O} - c_{i}^{H_2} - \frac{1}{2} c_{i}^{O_2} \right) (T_i^o - T_i^o) \right\} \]

\[ Q_e = \gamma_1 j + \gamma_2 jT + \gamma_3 j^2 \]

\[ Q_h = -\Delta H_{f_{H_2O_g}} r_{H_2O} - P_e + Q_e \]

\[ E_c = \left( \frac{\alpha - \beta}{\alpha} \right) E^o - \frac{RT}{nF} \left[ \ln \left( \frac{1}{\sqrt{C_{O_2}}} \right) + \frac{1}{\alpha} \ln \left( \frac{j}{\kappa nF} \right) + \zeta e^{\theta j} \right] - Q_e \]
Unit Cell Experimental Objectives

- Why hot spots Occur?
- Where do they occur?
- Can we develop in situ experimental temperature map?
  - spatially and temporally resolved
- Can we minimise number of sensors to achieve the same?
  - how many and where do we place them?
- Can we control the hot spots?
Novel In Situ Experimental Technique

Design of fully automated 50 cm\(^2\) Test Unit fitted with total 140 Thermocouples on both Sides of MEA
Thermocouple Locations
MEA Assembly
**Thermocouple Static Characterisation**

\[ y_o = 92.3187x \]

![Calibration Curve](image)

\[ y = 92.13x + 0.27 \]
Static and Dynamic Characterization

Accuracy with 95% Confidence: 0.3 C
Accuracy with 100% Confidence: 0.5 C
Resolution: 0.5 C
Offset at 0 C: (-) 0.0394 mV
Minimum Reading: (-) 10 C
Maximum Reading: 80 C
Dynamic Settling Time: 300 ms
Dynamic Time Constant: 75 ms
Response Time: 100 ms
Thermal Bath Controller at 80 C
Experimental Setup

Scribner Fuel Cell Test Station

In house built Data Acquisition
Fully Assembled Unit Cell
Thermocouple Locations

Thermal Map

1 2 3 4 5 6 7 8 9
16 15 14 13 12 11 10 9
17 18 19 ... 36 37 38 39 40
48 47 46 45 44 43 42 41
49 50 51 52 53 54 55 56
64 63 62 61 60 59 58 57
10
20
30
40
50
60
70
80
Thermal Map Result
Unit Cell Conclusions

- Measured Spatially and Temporally resolved Temperature distributions due to reaction along the single serpentine channel flow path and across the MEA
  - Steady State Profiles
  - Developed Dynamic Movie

- Collected data is undergoing further analysis with ultimate goal to combine simultaneous measurements of
  - Local Temperature, Current Density and Flow Distributions

- Developed Mathematical Model for two types of Unit Cells

- Dynamic Model is validated for use in Control Study
PEM Fuel Cell System

H₂ → MassFlow → Hydrator

N₂ → MassFlow → Hydrator

Air → MassFlow → Hydrator

Water → H₂O

H₂Recycle Pump

Electronic Load

Radiator
Pilot Plant Design
Mass Flow Controllers
Test Facility During Construction

Design to Reality

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Fully Automated Power Plant
Power Plant Conclusions

- Test Facility is Fully Commissioned and Ready to Operate

- Developed High Fidelity Dynamic Model for
  - Stack and Balance of Plant Equipment

- Robust Model Predictive Control Algorithms are Designed

- Planned Experimentation is underway with ultimate goal to
  - Validate Dynamic Model of the whole system
  - Deploy in Real Time Robust Control Policies for Efficient
    - Water, Heat and Electricity Management
    - Under varying operating scenarios that affect parameters of the model
Framework for Vehicle Propulsion
Automotive Control System

Source: Clemson University Vehicular Electronics Laboratory
PEM 30 W Fuel Cell

Horizon Fuel Cell Technologies
Transmission Control Objectives

- Speed Control
- Location Control
- Battery Management
- Fuel Cell Power Management

Electric Motor

Transmission System and Gearbox
Vehicle Architecture
Vehicle Kinematics
30W PEM - Model Validation

Fuel Cell Stack of 14 Unit Cells

- Voltage (V)
- Power (W)
- Current (A)
30W PEM - Dynamic Profiles
Motor Model Validation
Model Predictive Control Policy
Demonstration of Explicit MPC

20 ft = 1 ft
6 m = 0.3 m
1 km = 50 m
100 km = 5 km
### Key Contributions

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<tr>
<th>Unit Cell</th>
<th>Plant</th>
<th>Applications</th>
<th>Theory</th>
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<tr>
<td>• Built Novel Test Platform</td>
<td>• Designed Pilot Plant</td>
<td>• Developed Smart Home</td>
<td>• Tuning of MPC</td>
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<tr>
<td>• Developed Thermal Map</td>
<td>• Developed Fuel Cell Lab</td>
<td>• Developed Fuel Cell Vehicle</td>
<td>• MPC with State Estimation</td>
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<tr>
<td>• Developed Dynamic Model</td>
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<td>• Validated Vehicle Model</td>
<td>• MPC with Move Suppression</td>
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<tr>
<td>• Validated Model</td>
<td>• Designed Controller</td>
<td>• Deployed MPC on a Chip</td>
<td>• MPC with Integral Action</td>
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<tr>
<td>• Built Control Hardware</td>
<td>• Validate Model: in progress</td>
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<td>• Robust Invariant Sets</td>
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<tr>
<td></td>
<td>• Deploy Controller: in progress</td>
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<td>• Robust MPC (RMPC)</td>
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<td>• RMPC - additive uncertainty</td>
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<td>• RMPC for Polytopic System</td>
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Conclusion and Future Outlook

- Robust Parametric Model Predictive Controller
  - Guarantees feasibility and stability
  - Achieves closed-loop operational performance

- Advantages of Multi-Parametric Controller
  - Provides complete road-map of optimal solution
  - Provides accuracy of solution
  - Provides insight into the model-based control structure

- Implementation and Future Extension
  - Controller Deployment on the plant
  - Development of fast onboard control automation architecture
  - Development of Application Prototypes
Future Vehicle Prototype

- 1/10 Model of a Real Vehicle
- Top Speed: 60 km/h
- Power: 30 W
- Battery Management & Transmission Control
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  - Stratos Pistikopoulos, Department of Chemical Engineering
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- Research Team (Thermal Map)
  - Thiago Lopes, Stephen Atkins

- UG Students (Vehicle Prototype)
  - Aksat Shah, Jubeda Khatun, and Akachukwu Ifeobu

- Design and Development Team (Pilot Plant)
  - Centre for Process Systems Engineering (Redesign and Full Development)
  - Chemical Engineering Workshop (Plant Assembly and Manufacturing)
  - Chemical Process Engineering Research Institute (Initial Design)

- Sponsors

![EPSRC Logo]

![PSE Logo]

![ARM Logo]
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