# Abstracts for Poster Presentations

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**SOFCs**

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Model Predictive Control to Balance Renewable Energy Fluctuations Using Hydrogen Technology
Yousif Al-Sagheer

University of Birmingham

The advantage of model predictive control (MPC) algorithms over conventional controllers, like PID’s, is the ability to interpret pre-defined operational objectives and to guide a system to operate within or at some defined constraints. Furthermore, MPC has a built-in noise compensation feature as it updates its input data over some prediction horizon at each successive time step and then recalculates the optimal control actions over some control horizon. For a system of renewable energy generation units integrated with hydrogen technology (Electrolyser, fuel cell, H2 storage unit) there is the need to control the energy flow among system components. The most important benefit behind this integration is balancing energy fluctuations due to uncertainty in the solar and wind energy generation, and sometimes due to demand side uncertainty. The control objective of keeping the zero net power difference between generation and demand is considered here. The net power balancing can be attained through turning-on electrolyser or fuel cell according to energy surplus or deficiency levels, respectively, taking into account hydrogen inventory status. Thus, control variables will be the power set points assigned to the electrolyser and fuel cell units, these set points have to be implemented and tracked by low level controllers of these two units.

A cost function is formulated that expresses control objectives and performance indices over a finite prediction horizon, which is extended to capture system dynamics along an entire day of system operation (24 h). Sampling time is determined according to the most detailed time series data of prediction, in the current study it is 10 minutes. Hence, the number of independent variables will be (24x6x2 = 288). Another essential task is formulating operational constraints in terms of the control variables. The Matlab symbolic math toolbox is used to construct the cost function and constraints.

A non-linear cost function subjected to system constraints is solved using the Matlab optimization toolbox to find the optimal future control action along the prediction horizon. However, only the first optimal control actions that have the highest certainty are implemented on the next adjacent sampling interval. Afterward, the entire process is repeated for the next time step applying the concept of receding horizon and updating the predictions to capture system uncertainty.

The MPC controller shows very good results in keeping the net power difference between generation and demand to zero value by absorbing energy surplus events through the electrolyser and by compensating energy deficiency events through the fuel cell, taking into account H2 storage. Updating future predictions continuously led the implemented control actions to have a high degree of certainty and consistent with surplus and deficiency events.

Updating the predictions and solving the optimization problem have to be accomplished within one sampling time in order to synchronize control actions with real time operation. Otherwise, a compromisation among sampling time, prediction horizon and uncertainty would be necessary. Although there is a high degree of freedom in designing a cost function, this would be at the expense of retracting of energy management objectives.
Solid oxide fuel cells offer a high efficiency, fuel-versatile solution to our current and future energy needs and are beginning to provide a commercially viable alternative to the combustion of fossil fuels. One of the impediments to full-scale viability has long been the issue of durability, for a range of cell components. Of these, the anode presents serious challenges such as volume expansion on redox cycling, problematic coking and sulfur deposition as well as microstructural changes throughout operation.

A pathway of anode degradation that is currently under-characterised is known as nickel agglomeration; the thermally driven capillarity effect that leads to the metallic component of the anode cermet to coarsen as a means to reduce its surface area-to-volume ratio. This leads to a loss of triple-phase boundary (TPB) density concomitant with a loss in fuel cell performance, and sometimes a breakdown in nickel percolation and hence diminishing electronic conductivity.

The mass transport mechanisms that support this process at high temperature are thought to include an evaporation and re-precipitation pathway, as well as bulk and surface diffusion routes. The extent to which each of these play a role in the degradation in a variety of operating conditions and at various length and time-scales is not well-understood. Similarly, the impact of the original microstructure and the effect of the agglomeration phenomenon on electrochemical performance is yet to be fully explored.

A variety of approaches are used to inspect the transport mechanisms, kinetics and microstructural changes involved in this process. Through dry and humid annealing of patterned nickel samples prepared by photolithography, the relative importance of each of the transport routes is under investigation. Via 3D tomographic techniques such as FIB-SEM slice-and-view and X-ray nano-CT, the microstructural evolution of nickel is monitored. Key microstructural parameters can be extracted from these datasets which inform on the kinetics and shape changes involved in SOFC anode materials. It has been demonstrated that FIB-SEM tomography is well-suited to monitoring the difference in nickel morphology before and after annealing, due to good solid-phase contrast from low-energy SEM imaging. Correlation is found between the porosities extracted from this and from X-ray nano-CT reconstructions. This, coupled with increasing evidence of solid-phase contrast with X-rays, suggests a non-destructive lab-based imaging tool for the dynamics of nickel agglomeration is imminent.
Biomass-based carbon aerogels for oxygen reduction reaction in polymer membrane fuel cells

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Polymer electrolyte membrane fuel cells (PEMFCs) are considered as a promising sustainable technology for automotive and stationary applications, however, have many challenges to overcome for mass commercialization. One of the main challenges is associated with the oxygen electrode where carbon supported platinum is used as the catalyst for oxygen reduction reaction (ORR), giving rise to high cost (because of Pt), degradation of performance related to the migration, agglomeration and dissolution of Pt particles, and carbon corrosion during start-up/shut down cycling which may be induced by the presence of Pt [1-2].

This paper reports our research on using biomass-derived N-doped carbon aerogels (N-CA) as next generation ORR catalysts in the oxygen electrode of PEMFCs. N-doped carbons recently appear to be attractive catalyst/electrode materials in low temperature alkaline and PEMFCs, and have shown prolonged stability and low cost promise [3-6]. The N-CA materials are derived from biomass using inexpensive process (i.e. Hydrothermal Carbonisation). They can be easily tailored to have different physicochemical functionalities and micro (< 2 nm), meso (2-50 nm), and macro (> 50 nm) porosity [3, 4]. In this work we optimise the N-CA materials to achieve high ORR performance in acidic environment. The optimised materials are then taken into real PEMFC single cells to test the electrochemical performance (e.g. the polarisation curves and electrochemical impedance spectroscopy (EIS)) to elucidate materials effects on the electrochemical performance.

Acknowledgement : We are grateful for the financial support from H2FC SUPERGEN Hub.

References


Effect of a Ti interlayer on hydrogen sorption behaviour of a Mg thin film
Yuan Cao, Shahrouz Nayeboossadri, David Book

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Mg-based powders are promising materials to store hydrogen due to their relatively high gravimetric hydrogen storage capacity (7.6 wt % for pure Mg). However, these powders need to be heated to about 300 °C in order to absorb and desorb hydrogen, and the sorption rate tends to be slow.

Therefore, there is a need to better understand the hydrogen sorption mechanisms in Mg and Mg-based materials. Compared with Mg-based powders, Mg thin films may exhibit lower hydrogen absorption temperatures and faster absorption kinetics. Hence, thin film may be used as a convenient model system, to investigate hydrogen sorption mechanisms.

In this work, Mg thin films were deposited onto glass substrates using a magnetron sputtering technique known as (CFUBMSIP). A Pd top layer was deposited in order to try to prevent oxidation of the Mg, and also to enhance hydrogen dissociation and recombination (Ares et. al, 2010).

The hydrogen absorption properties of these Pd (60 nm)-Mg (150 nm) thin films were investigated by in-situ XRD. Pd reacted with H₂ to form PdH0.6 at room temperature which was later dehydrogenated during heating process at 175 °C. While the Mg layer was shown to absorb H₂ at 150 °C to form MgH₂. Mg₅Pd₂ phase was also observed at 300 °C, which agrees with the Mg-Pd binary phase diagram (Makongo et.al, 2006).

In order to try to avoid alloying between Pd and Mg layers, a Ti interlayer was then sputtered between the Mg and Pd layers. The effects of this Ti interlayer on the micro-structure and hydrogen absorption temperature will be discussed.

References


Mixed Matrix Porous Materials for High Pressure Gas Hydrogen Storage Tanks
Robert Dawson, Leighton Holyfield, Andrew Burrows and Tim Mays
University of Sheffield

Hydrogen from renewables is seen as one potential source of sustainable energy, for example in fuel cells to power vehicles in order to reduce the demand on fossil fuels. One of the technical challenges for the use of hydrogen as a fuel is its storage. Storage of hydrogen at low temperatures (e.g. at 33 K) has been suggested, while the storage of hydrogen at high pressures (up to 700 bar at ambient temperatures) has been proposed for commercial vehicles. However, to store hydrogen at such high pressures investment into materials is required to maintain the storage conditions. Furthermore, there are safety considerations when working with tanks at such high pressures. The heavy and bulky system required for such high pressures are a particular problem for mobile applications. If the storage pressure can be reduced lighter, less demanding systems can be utilised. Storing hydrogen using porous materials could offer way of achieving this aim for example by providing tank liners to reduce the pressure of the tank while maintaining the capacity.

The use of mixed matrix porous materials (MMPMs) with high surface areas provide a practical solution to the processability of porous materials which are often insoluble powders. PIM-1 a soluble microporous polymer\(^1\) which can be cast into self-standing films can be used as a support in which to disperse other porous materials such as: microporous organic polymers,\(^2\) metal-organic frameworks\(^3\) silicas\(^4\) and zeolites. Here two further microporous organic polymers have been introduced into a film of PIM-1. The characterisation of the MMPMs by both low pressure and high pressure gas sorption will describe the relationship between the porosity of the soluble porous polymer and the dispersed porous materials and how it affects the surface areas and pore sizes of the MMPMs.

References


HYDROGEN PRODUCTION THROUGH SORPTION-ENHANCED STEAM REFORMING OF ETHANOL USING CaO-BASED SORBENT MIXED WITH IRON OXIDE CATALYST

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A novel synthetic CaO-based sorbents for carbon dioxide (CO$_2$) capture in sorption enhanced steam reforming (SESR) were prepared by the co-precipitation method. Magnesium oxide (MgO) and cerium oxide (CeO$_2$) were mixed with calcium oxide (CaO) in different molar percentages in order to obtain the optimum percentage which provide high CO$_2$ uptake capacity and cyclic stability. The TGA results for CO$_2$ uptake, revealed that for the molar ratio of CaO, MgO and CeO$_2$ of (6:2:1) and (4:2:1), the sorbents had CO$_2$ capture capacity of 29 and 25 wt. % respectively. The fresh sorbents were characterized using X-ray diffraction, mercury porosimetry, N$_2$ physisorption and scanning electron microscopy. It was found that the sorbents with higher CO$_2$ uptake capacities had relatively high porous surface structure with porosity percentage (>66%). Modelling of CO$_2$ uptake kinetics showed that JMA (Johnson-Mehl-Avrami) fits best the first and second stages except for the molar ratio of CaO, MgO and CeO$_2$ of (4:2:1) sample where surface chemisorption (SC) fits the initial stage and JMA fits the second stage. While contracting volume model (CV2/3) fits the final stages of all the studied sorbents. The stability of sorbents at high temperatures was examined over multiple cycles of carbonation/de-carbonation reactions. After 45 cycles, the sample with a molar ratio of CaO, MgO and CeO$_2$ of (6:2:1) remained as high as 25 wt.% (0.43g CO$_2$ /1g CaO) with only 25% decrease from its CO$_2$ uptake capacity as a fresh sample. Therefore, the later sample was selected to be mixed with iron oxide catalyst and used for the SESR. The study of ethanol steam reforming employing iron oxide as a catalyst with and without in-situ CO$_2$ removal has been investigated. The results confirmed that iron oxide exhibited catalytic activity for hydrogen (H$_2$) production from ethanol steam reforming/decomposition reactions. Furthermore, the CaO-based sorbent had successfully decrease the amount of CO$_2$ produced until 70 min of reaction time. Ethanol reforming with in-situ CO$_2$ removal was investigated at 550-700 °C. The maximum H$_2$ yield achieved was 3.5 mol (H$_2$) /mol (EtOH) at 600°C. GC results revealed that there was no evidence of CO and C across the studied temperature range. The results showed an enhancement in reaction reactivity by increasing the Gas hourly space velocities (GHSV). The amount of H$_2$ produced remained stable within 10 cycles which is equivalent to 30 hours of reaction time.
Plasma-etched MoS$_2$ and WS$_2$ nanosheets for the hydrogen evolution reaction (HER): influence of morphology and degradation in electrocatalytic activity

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The layered transition metal dichalcogenides (TMDs) have been traditionally utilized because of their tribological properties as well as for their catalytic activity in hydrodesulphurization processes$^1$. However, since earth-abundant MoS$_2$ was reported to exhibit electrocatalytic activity for the hydrogen evolution reaction (HER) to a degree linearly dependent on the number of edge sites$^2$, burgeoning interest has resulted. The pursuit of a high density of 1T metallic phase active edge sites on MoS$_2$ has resulted in the preparation of several nanostructures by chemical methods: nanowires$^3$, mesoporous double-gyroid thin films$^4$ and graphene-supported nanoparticles$^5$, amongst others. Physical methods such as mechanical cleavage$^6$ and vapour transfer growth$^7$ have managed to obtain 2D TMDs crystals, but the absence of surface defects (steps, kinks) with S-rich Mo active sites$^8$ hamper their electrocatalytic activity for HER. One feasible strategy to address this problem is the application of nanolithography principles and, in particular, the production of reproducible nanostructured arrays with high surface areas. This report focuses on the design and optimisation of a novel methodology to nanopattern MoS$_2$ and WS$_2$ crystals by plasma etching, and further analysis of the electrocatalytic response. Monodisperse nanospheres ordered on the TMDs surface by means of solvent-based methods act as nanolithography masks, creating an array of nanocolumns/nanopillars upon plasma etching with appropriate parameters. Electrochemical measurements show a significant improvement in HER onset overpotential with respect to bare MoS$_2$ and WS$_2$ samples, giving a steady-state voltammetric profile similar to that obtained for microelectrodes. Finally, degradation studies are presented to evaluate how morphological variations affect the electrocatalytic properties of the materials investigated. The methodology reported opens up a new approach to the nanopatterning of TMDs.

References:

Experimental and CFD study into cross-flow passive venting in small Fuel Cell enclosures
Tara Singh Ghatauray, Dr James Ingram, Dr Paul Holborn
London South Bank University

An experimental and Computational Fluid Dynamics (CFD) study is presented on Helium dispersion in a $0.216 \text{ m}^3$ ‘cross-flow’ passively ventilated enclosure at low release rates (1-5 L/min), to simulate a Hydrogen leak in a small fuel cell (FC) enclosure. The Helium, (a safe analog for Hydrogen), was released from a centrally positioned vertical 5mm diameter nozzle. Observations of Helium dispersal behaviour and concentration were made, subject to variations in vent area and leak rate. SolidWorks ‘Flow Simulation’ CFD, studies, of the scenarios were undertaken, with the empirical data used to validate the CFD model.

Hydrogen as a primary energy carrier with FCs powering vehicles, domestic CHP and static commercial applications underpins a ‘Hydrogen economy’. However, Hydrogen’s flammable range (4-74%) poses safety concerns. FC deployment in small enclosures will become common; however Hydrogen leaks could readily create flammable mixtures. This research is motivated by accident prevention and better understanding of hydrogen’s behaviour in small enclosures. Mechanical ventilation to control hydrogen is not favoured as it drains FC output. Passive ventilation can purge enclosures, but relies upon small driving forces, with size, shape and position of ventilation openings critical for predictable flow and maintaining low concentrations. Determining a relationship between leak rate, ventilation inlet/outlet area and internal hydrogen concentration will inform enclosure safety design. CFD model reliability will speed development and reduce costs.

The experimental rig comprised a 600mm square enclosure with opposing vents and a network of four XEN-TCG3880 (mini-kathorometer) Helium sensors, with concentration data retrieved via a USB link (for LabVIEW processing). Sensors were repositioned to obtain data across the enclosure. Three vent heights were tested (20mm, 40mm, and 60mm) at various release rates (1, 2, 3, 4, 5 L/min). A simplified CAD model was developed for CFD modelling. Isothermal and adiabatic conditions were assumed, environmental boundary conditions attached to openings and the experimental release rates were applied to the leak feature. Mesh sensitivity was tested and an optimal arrangement determined. I-L or k-ε turbulence models were applied and simulations run.

A comparison of CFD (Figure 1) and experimental results was undertaken. As anticipated, flow rates through the enclosure increased with larger vents and were more effective at keeping Helium concentrations below 4% across the range of nozzle release levels. Flow Simulation models replicated the flow behaviour with k-ε simulations more convincing across the range. Cross-flow arrangements provide effective displacement ventilation, with flow in through lower vents and out through upper vents. ‘Flow Simulation’ output with the k-ε model is closer to experimental findings. Further work is required for robust validation with investigation of thermal and environmental pressure variations.
Figure 1 Examples of SolidWorks ‘Flow Simulation’ CFD output
**Amorphous Zr-based Thin-Films as Potential Hydrogen Purification Membranes**  
Carmel Greenwood*, Shahrouz Nayebossadri, John D. Speight, David Book  
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PEM fuel cells are sensitive to gas impurities and, for long exposures, ideally require an ultra-pure hydrogen gas feed. One method of doing this is to pass hydrogen through a crystalline PdAg23 alloy foil heated at about 300 °C; however, the prohibitively high cost of palladium, has limited the wider application of these membranes.

Amorphous alloys (based on transition metals) are under investigation as alternative hydrogen separation membranes due to their lower cost, resistance to hydrogen embrittlement, and superior mechanical properties compared to their crystalline counterparts.

This study investigates the effects of deposition conditions and heat treatment on composition and crystallisation characteristics of Zr-based thin-films synthesized using Closed Field Unbalanced Magnetron Sputter Ion Plating (CFUMSIP). Sputtering allows good control of film thickness and composition. Zr-based alloys, including ZrCu, ZrCuTi, ZrCuY, and ZrNi, were investigated due to their high predicted hydrogen permeability. CFUMSIP seems to be an effective method for producing dense, amorphous Zr-based thin-films of approximately 5 μm thick. It was found that low Ar flow during deposition produced crystalline films, whereas others found low chamber gas flow encouraged the glass-forming ability. The optimum flow rate to produce amorphous films was 25 sccm Ar. Films were deposited onto glass substrates using a series of 10 minute coatings with intermediate cooling periods to avoid excessive heating and crystallisation. A comparison of crystallisation temperatures and activation energies of nucleation and growth of films produced by CFUMSIP and melt-spinning was made. Sputtered Zr39Ni61 thin-films showed the most promise with regards to stability under hydrogen, crystallising at the relatively high temperature of 438.8 °C.

However, further investigations into hydrogen solubility and permeability will need to be carried out, in order to fully assess this alloy’s potential as a hydrogen purification membrane.

**References**

Lab-based micro and nano XCT investigations of two solid oxide fuel cell geometries and detailed imaging of anode specific materials
Thomas M.M. Heenan, D. J.L. Brett, P. R. Shearing

Electrochemical Innovation Lab, Department of Chemical Engineering

Solid oxide fuel cells (SOFCs) offer the capability of combined heat and power integration, allowing for very high overall efficiencies. Although the high temperature operation of such devices does not come without limitations, particularly the thermal stresses associated with start-up and shut-down.

Various works have been conducted on the characterisation of SOFC microstructures with the use of techniques such as focused ion beam scanning electron microscopes (FIB-SEMs), synchrotron and laboratory X-ray computed tomographies [1,2,3]. Increasing our understanding of microstructural developments on the nano and micrometre scale has aided in the development of improved electrode and electrolyte materials and operating conditions.

With the use of two lab-based X-ray computed tomography techniques, SEM, high precision thermal imaging and electrochemical impedance spectroscopy (EIS) we are able to investigate the effects of such geometries on microstructural degradation after exposure to thermal cycling and carefully characterise anode material microstructures on the nanometre scale.

References

[1] 3D reconstruction of SOFC anodes using a focused ion beam lift-out technique PR Shearing, J Golbert, RJ Chater, NP Brandon Chemical Engineering Science 64 (17), 3928-3933 2009


Near Surface Structure and Composition of Acid Leached Pt Alloys for Use as Fuel Cell Catalysts

David W. Inwood, A. E. Russell, A. M. Bonastre, and J. Sharman

University of Southampton

Catalysis of the O$_2$ reduction reaction (ORR) at the cathode of PEMFCs remains a limiting factor in their performance, and requires several times more Pt than required for the anode. Pt alloyed with other transition metals has shown increased activity for ORR due to modifications of the electronic structure of the catalyst surface. Altering the structure allows further optimisation in terms of stability and activity, for example de-alloying PtM/C allows the formation of porous and non-porous core-shell nanoparticles. The Pt-rich shell protects the Pt alloy core from further dissolution of the non-noble element, whilst retaining the benefit to catalytic activity$^1$.

The work presented here focusses on the effect of degradation on the surface structure of the core-shell catalysts. To mimic typical fuel cell operation, Pt/C and Pt$_3$Co/C catalysts are immersed in 1 M HClO$_4$ at 80°C whilst the potential is cycled between 0.6 – 1.0 V vs. RHE up to 1000 times$^2$. After 0, 50, 100, 200, 500, 750, and 1000 cycles the catalyst was characterised based on its electrochemical surface area, and analysed using XRD (x-ray diffraction) and ex-situ XAS (x-ray absorption spectroscopy). Surface sensitive XAS measurements were attempted by poisoning the catalyst with I to provide a heavy neighbour atom to distinguish Pt atoms found at the surface from those Pt atoms in the core.


Studies of nickel electrodeposition on different silver coated substrates for fuel cell and gas separation applications
Zadariana Jamil, Enrique Ruiz-Trejo, Milla E Puolamaa and Nigel P Brandon

Imperial College London

Electrodeposition of Ni has been extensively developed especially in decorative, functional and electroforming industries. This work investigates Ni electrodeposition on Ag foil and Ag-coated substrates particularly, GDC scaffolds, Ag/GDC composites and YSZ pellets. This deposition is required for the fabrication of solid oxide fuel cell (SOFC) electrodes and oxygen separation membranes. Firstly, the Ag substrates have been prepared by coating the ceramic substrates (GDC and YSZ) with Ag by an electroless method to provide a conductive surface for Ni electrodeposition. Using potentiostatic and voltammetric techniques, Ni electrodeposition mechanisms on Ag substrates have been studied in the function of nickel concentration (Watts bath), temperature, stirring rate, wetting agent and deposition potential. The cyclic voltammetry (CV) analysis has been performed to understand the deposition and the dissolution processes of Ni. Scanning electron microscope has been used to test the uniformity and the microstructure of the electrodeposited layers.
Electrochemical devices such as solid oxide fuel cells (SOFCs) are one of the most promising ways of producing energy cleanly and efficiently via oxidising fuel without going through an intermediate combustion process. Conventionally screen-printed SOFC anodes are therefore highly complex porous microstructures. While most studies try to link performance and lifetime of the produced electrodes through measurements of bulk parameters, recent developments in 3D imaging have made it possible to tie the internal microstructure of these anodes to aspects of their performance, such as their electrochemistry and their mechanical strength. By examining two different electrode structures with different compositions, the three different phases commonly associated with SOFC electrodes were identified and the triple-phase boundaries (TPBs) between metal, ceramic and porosity as well as the uninterrupted network of each phase were imaged and measured. Subsequent nanoindentation and electrochemical conductivity testing allowed the correlation of bulk measurements to aspects of the porous structure of the electrode, such as neck-neck areas between the Ni metal phase, the ceramic ScSZ phase, and the ceramic-metal Ni-ScSZ phases. The results from advanced quantification show it is possible to link particular microstructural features and phases with performance attributes. In doing so the work enables better understanding of how microstructure affects electrode performance, and thereby the design of electrodes.
Vanadium-Hydrogen flow battery for energy storage applications - a feasibility study

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Increasing the penetration of renewable energy generation contributes significantly to reducing emissions and is one of the most effective routes to a secure and sustainable energy supply. However, renewable sources (e.g. solar and wind energy) are intermittent, unreliable and put stress on the electricity grid. Energy storage systems at scale can compensate for this, enabling greater deployment of renewables at lower system cost than grid reinforcement.

Redox flow batteries are an attractive device for grid scale energy storage across a wide range of power and energy, from kW/kWh to MW/MWh due to their ability to decouple power and energy, site-independence, rapid response time of few milliseconds, ability to operate at high depth of discharge and long cycle life. This project assesses a new hybrid redox flow battery, invented at Imperial College London, which combines key features of the conventional Vanadium/Vanadium flow battery with key features of PEM fuel cell technology to create a Vanadium-Hydrogen Flow Battery (VHFB). This novel VHFB technology can potentially offer a significant cost reduction compared to existing flow battery technologies.

The project is a collaboration between Imperial College, Arcola Energy and Alstom Power. The main goal is to build a 250 W / 500 Wh proof of concept system by adapting existing fuel cell stack technology developed by Arcola Energy, and to assess the techno-economic viability of VHFB systems for a range of grid scale storage applications.

Initial results of this study will be presented.
Numerical simulations of flow field in PEMFCs with metal foam gas distributor
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Hambat

It is important to uniformly supply the fuel gas into the active area in polymer electrolyte membrane fuel cell (PEMFC). Recent studies have shown that the cell performance can be significantly improved by employing metal foam gas distributor as compared with the conventional bipolar plate types. The metal foam gas distributor has been reported to be more efficient to fuel transport. In this study, three-dimensional computational fluid dynamics (CFD) simulation have been performed to examine the effects of metal foam flow field design on the fuel supply to the reaction site. Darcy's law is used for the flow in the porous media. By solving additional advection equation for fluid particle trajectory, the gas transport has been visualized and examined for various geometrical configuration of metal foam gas distributor. Figure 1 shows the variation of pressure drop in the gas flow field as a function of flow rate for different types of flow field design. It is observed that the metal foam gas distributor results in less pressure drop as well as more homogenous flow distribution as compared with the conventional serpentine flow channel.

Figure 1 Pressure drop in the flow field as a function of volume flow rate
1D Modelling of Open-Cathode Air-Breathing Proton Exchange Membrane Fuel Cells and its extension to 3D modelling

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Proton Exchange Membrane Fuel Cells (PEMFC) offer clean energy generation for a range of applications, including the automotive sector. However, to accelerate large scale commercialisation further development work is required that will benefit from improved understanding of the processes occurring within the fuel cell. In addition to current and voltage, thermal and water management are key parameters to be considered in deciding the optimal operating point for fuel cell systems. In order to extend the in-situ understanding of PEMFC operation, robust PEMFC computational models are required.

This project aims to develop a 3D model of open cathode air breathing fuel cell predicting current distribution, species transport and water management. This model will be validated against experiments that provide current, temperature and water distribution results.

![Figure 1](image.png)

Figure 1. (a) Single channel model. (b) Current density profile at the membrane with varying load. (c) Species concentration at 0.5 V, Cathode water (d) Validation techniques- Neutron Imaging spectroscopy[1], [2], (e) Validation Technique – Electrochemical impedance spectroscopy [3].
This paper presents 1 + 1 dimensional computational model of an open-cathode air-breathing PEMFC that captures the species and charge transfer through the fuel cell layers and along the channel length. These results are further extended to 3D analysis of PEM FC layers explaining, the 7-layer single channel 3D computational model for solving species transport processes and electrochemical reaction for an air-cooled polymer electrolyte fuel cell in steady state condition, (Figure 1).

This paper also explains the novel experimental methods to build and validate the PEFC computational model such as X-ray tomography, EIS, and Neutron Imaging.

References:


For last decades, plastics materials have been key enablers for innovation and have contributed significantly to the development of society. However, large amounts of waste plastics have been produced due to the increasing demand of plastic materials. At the moment, around 38 wt. % of waste plastics ended up as landfill in 2012 in the EU, causing big environmental problems and waste of energy stored inside the plastics. In this work, we focus on converting plastic waste into clean hydrogen-rich synthesis gas and high value carbon nanotubes (CNTs). Catalyst development is one of the key factors for this process to improve hydrogen production and quality of CNTs. Ni/SiO$_2$ and Fe/SiO$_2$ catalysts with controlled metal particle sizes will be reported in this work about their performance on productions of hydrogen and CNTs from catalytic gasification of waste polypropylene, using a two-stage fixed-bed reaction system. The influences of the types of metals and the crystal size of metal on product yields and quality of CNTs in terms of purity and homogeneity will also be studied, using gas chromatograph, X-ray diffraction, scanning electron microscopy, transmission electron microscopy etc.
Hydrogen Production by Chemical Looping Using Iron-Oxide-Perovskite Composite Material

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Chemical looping involves a sequence of cyclic redox reactions of a solid oxygen carrier material (OCM). Theoretically, the OCM at the end of the cycle will remain unchanged. Whilst the products from the reduction and the oxidation step are separated, it is an alternative technique that can produce hydrogen without any separation technique such as pressure-swing adsorption to remove carbon containing impurities. Iron oxide is widely used as the OCM in the steam-iron process for hydrogen production as it is thermodynamically favourable [1], however it loses its activity due to sintering and agglomeration during redox cycles [2]. Perovskites, such as $\text{La}_{0.7}\text{Sr}_{0.3}\text{FeO}_{3-\delta}$ (LSF731), have been proposed as the OCM in chemical looping process [3]. It has good oxygen transport properties that provide a very high stability and a constant productivity under long-term redox cycling. However, it has a small oxygen capacity and the hydrogen production per cycle is lower than iron oxide with a similar weight.

Two methods, the modified Pechini method and mechanical mixing, were used to prepare the composite materials with different iron oxide weight fractions and different particle sizes. As a result, the embedded iron oxide within LSF731 matrix provides a high oxygen capacity whilst the oxygen transport properties of LSF731 prevent agglomeration of iron oxide.

The hydrogen productivity and the stability of the composite OCMs were analysed by a micro-reactor feeding carbon monoxide and water alternatively to produce carbon dioxide and hydrogen in a separate stream. Two hundred redox cycles were performed for each OCM. The hydrogen productivity for all tested composite OCMs were higher than iron oxide on its own over two hundred redox cycles. The hydrogen production from OCM prepared by mechanical mixing was relatively constant throughout two hundred redox cycles, while an increase in hydrogen production was observed for OCM prepared by the modified Pechini method.

References


Improvement of the Hydrogen Desorption Properties of the LiBH4–LiNH2 System
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The xLiBH4−yLiNH2 system has been the subject of much recent research as potential hydrogen storage and delivery material. A LiBH4−2LiNH2 mixture was reported to release 10 wt% hydrogen from 250°C. However, this system has the drawbacks of an evolution of ammonia (2-3 mol%) and a lack of reversibility of the main product Li3BN2 [1–2]. Zhang et al. reported that the addition of small amount of CoO could help to reduce the onset hydrogen desorption temperature of a LiBH4−2LiNH2 mixture to 100°C and more importantly, the majority of the hydrogen release occurred at the melting temperature of the product mixture obtained around 220°C [3]. The melting point of borohydride-rich mixtures was informed to be lower than that of the LiBH4−2LiNH2 mixture [4].

Therefore, the effects of a CoO catalyst on the products and dehydrogenation properties of reactions between LiBH4 and LiNH2 in a 1:1 molar ratio were examined. The results showed that on addition of CoO, the decomposition of LiBH4 was also enhanced. The products of reactions of LiBH4−LiNH2−nCoO, where n ≤ 0.05, at 400°C were a mixture of P21/c and I41/amd polymorphs of Li3BN2, LiH, and amorphous phase of BN which is consistent with the work reported by Anderson et al. [4]. With an amount of 0.1CoO, only the P21/c phase was observed alongside LiH. A remarkable reduction in temperature of hydrogen evolution was observed, showing hydrogen release from 135°C, peaking around 250°C, and also a depression in ammonia discharge was achieved. In ball-milled sample the amount of hydrogen desorbed from this ratio was greater than 10 wt%.

References

PtIr Alloy Dendritic Nanostructures for Oxygen Reduction and Ethanol Oxidation Reactions

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Dendritic Pt-based alloy nanostructures have been known to exhibit improved electrocatalytic properties due to their particularly modulated surface and electronic structures favorable for alcohol oxidation and oxygen reduction reactions. We prepare the PtIr alloy nanoparticles NPs with a dendritic shape as a three-dimensional structure for enhanced ethanol oxidation reaction (EOR) and oxygen reduction reaction (ORR) by thermal-decomposition in the presence of cetyltrimethyl-ammonium chloride (CTAC) as a surfactant agent. The PtIr alloy dendritic nanostructures show a well-defined alloy nanostructure with three-dimensional structures analyzed using TEM, XPS, and XRD. In particular, the PtIr alloy nanostructures exhibit 2.74 times higher electrochemical active surface areas (EASAs) than commercial Pt/C. Also, in EOR, the PtIr alloy dendritic electrocatalyst indicates excellent electrochemical properties, including high \( I_r/I_s \) ratio and current density, great negative on-set potential, and good electrochemical stability compared to commercial Pt/C electrocatalyst. In addition, the PtIr alloy dendritic electrocatalyst exhibits enhanced electrochemical activity and stability i.e., 3.19 times higher specific mass-kinetic activity than commercial Pt/C electrocatalyst, and a reduction of 8 mV of half-wave potential in ORR. The improved electrochemical activity and stability of the PtIr alloy dendritic electrocatalyst in EOR and ORR are ascribed to dendritic structures, the surface state of the electrocatalyst, and the controlled electronic structure due to the Ir atoms in the alloy phase.
Development and modeling of a PEM fuel cell/super capacitor hybrid drive train system for cost and efficiency optimization of a fuel cell bus

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The aim of the project is to assess the use of super-capacitor energy storage systems in a scaled fuel cell drive train for application on a bus. Through development of a laboratory based drive train and various Simulink/PSCAD models of hybrid drive trains the performance of the FC/Super-capacitor system can be analysed and compared to other hybrid propulsion systems. Control strategies will be developed to allow for the downsizing of the fuel cell whilst still meeting the systems performance requirements. This will allow the system to be optimized in terms of cost and efficiency for any given duty cycle of the system.

Thus far the basic fuel cell drive train, consisting of the PEM fuel cell, DC-DC converter and the induction motor and controller, has been installed and coupled to the load system. A computer based Simulink/PSCAD has been simultaneously developed to be validated by experimental results. Performance data from a UCL diesel hybrid bus in operation on a London bus route has been collected to disseminate the impacts of various parameters, such as road gradient and traffic conditions, on the performance of the hybrid drive train system.

The efficiency and operation of the basic drive train will be tested under various load conditions before the super-capacitor system is added. This will allow for the validation of the Simulink/PSCAD model and the development of various control strategies to optimise the performance of the FC/Super-capacitor hybrid propulsion system. Additionally various Simulink/PSCAD models of full-scale hybrid propulsion systems are being developed. The data collected from the UCL bus will act to both validate these and provide a power profile from which these models can be compared.
Effects of surface area of patterned membrane on the MEA Performance for Polymer Electrolyte Fuel Cell

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In this study, in order to increasing MEA performance, electrode reaction area and utilization of catalysts, surface of membrane has been patterned with different shapes. The MEA with patterned membrane were investigated using polarization curve of cells, SEM and EIS(electrochemical Impedance spectroscopy).

The patterned membrane was fabricated with the Nafion resin and meshes by hot-pressing process. The fabricated patterned membrane was changed from F⁻ form to H⁺ form using chemical process with NaOH and H₂SO₄. Platinum catalyst supported on carbon (JM, Hispec4000), Nafion ionomer(30 wt%), and solvents were mixed thoroughly to prepare the catalyst ink. The prepared catalyst ink was coated on the patterned membrane by spraying to spread the catalyst. A gas diffusion layer (GDL) was used with SGL 10BC. Surface and cross section of the patterned membrane and MEAs were observed by SEM. The surface area of the patterned membrane was increased. Therefore the reaction area of the MEA was also increased. The performance of MEA for PEMFC was increased, due to the increasing the surface area and reaction area of membrane and MEA. The fabrication process for MEA with patterned membrane can be a method to increase the performance of MEA for PEMFC.

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Fig.1. SEM images: cross-sectional view of the patterned membranes and the MEA.
Freeze-Dried Ammonia Borane-Polyethylene Oxide Composites: Phase behaviour and Hydrogen Release
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Ammonia borane (AB, NH₃BH₃) is a highly promising candidate material to meet the US Department of Energy’s targets for portable hydrogen storage systems owing to its excellent gravimetric hydrogen storage capacity of 19.6 wt% H₂, low dehydrogenation temperatures (compared to other candidates), and encouraging progress in recycling the material ¹. Combining AB with polymers into composites can advantageously modify its hydrogen release and, polymers are a particularly attractive choice since they tend to be cheap and lightweight.

A solid-state hydrogen storage material comprised of ammonia borane (AB) and polyethylene oxide (PEO) has been produced by freeze drying from aqueous solutions across a full range of compositions from 0% to 100% AB by mass. The focus of this work is to relate the hydrogen release mechanisms of these composites to the phase mixing behaviour between AB and PEO.

The mixing behaviour of AB and PEO was investigated using x-ray diffraction which showed that a new crystal phase, distinct from both AB and PEO, is formed. The space group and lattice parameters of this new crystal structure have been calculated. It was found that hydrogen bonding interactions between the ethereal oxygen atom (–O–) in the PEO backbone and the protic hydrogen atoms attached to the nitrogen atom (N–H) of AB molecules play a significant role in improving the dehydrogenation properties of these materials. A temperature-composition phase diagram has been produced for the AB-PEO system using nuclear magnetic resonance and thermal techniques to explicate the close relationship between the phase mixing behaviour and hydrogen release properties of these promising hydrogen storage materials.

References

Hydrogen Fuel Production from Renewable Sources and its Role in Balancing the Grid in Libya

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The rapid growth of renewable energy sources and their integration into the grid has been motivated by the depletion of fossil fuels and environmental issues. Unfortunately, the grid is unable to cope with the forecasted growth of renewable energy which would lead to its instability. In order to solve this problem and to support such integration, it is recognised that energy storage should be utilised. In this research demand side management provided by electrolytic hydrogen production will be studied.

Exploration of surplus power (solar or wind) to produce a clean hydrogen (zero emission) is the main core of the research. This study will take place in the east part of Libya since the forecast there is promising in terms of the production of renewable energy from wind and solar power regarding wind speed and solar irradiation already registered (some projects have been installed in this area).

The assumption in this research is that the hydrogen will be sold from many garage forecourts of different sizes and with different operational regimes.

Our research will involve the relation between surplus power (high or low), price (high or low) and storage tank (full or empty).

In this stage of the research, the comparison of 100% of renewable energy scenario and the demand to have surplus power has been applied and we are now only dealing with one garage forecourt to see the effect of the capital expenditure (CapEx), operational expenditure (OpEx) and the electricity price (which is the core of the study).

The study at this stage is only dealing with the variation from day to day (the price will change daily depending on the surplus power quantity). In the future it might include hourly variation depending on the time permitting of the research. The sizing and optimization of all parts of the system from the supply to the load will also be covered.
NITROGEN DOPED CARBON AS CATHODIC CATALYST FOR MICROBIAL FUEL CELL

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Oxygen reduction reaction (ORR) is very important in order to develop unconventional energy sources such as fuel cells (e.g., enzymatic biofuel cells, microbial fuel cells). Microbial fuel cell is a promising technology for pretreatment of wastewater with simultaneous generation of electricity. However, there are still limitations for the commercial application on a large scale. Up to now, platinum (Pt)-based materials are the most common catalysts for direct ORR. Carbon materials can be used either as a catalyst on its own or as a catalyst support [1-4].

In our studies, N-doping (~3\% mas.) has been successfully introduced into carbon structure in order to receive a metal-free catalyst. Our results confirm that the type of nitrogen group (pyridinic or graphitic) and the surface roughness strongly influence the ORR activity. Further, these materials exhibit efficient electrocatalytic activity (the onset potential of 0.76 V vs. RHE) for oxygen reduction reaction (ORR) in alkaline media.

The beneficial properties of our system might be exemplified by their application as well as catalysts for oxygen reduction at the cathode surface of microbial fuel cells.

References

FEA modelling and experimental validation of stress and strain in SOFCs during steady state and cycling operations
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FEA models of cells and short stacks using the anode supported flat-tube SOFC design developed by our Korean partners POSTECH and HK Oil have been created using the finite element analysis software ABAQUS. Stress and strain values were evaluated during the simulation of steady state operation and simple thermal and redox cycles, resulting in high stress levels during heat-up and cool-down phases especially in the electrolyte, exceeding 350 MPa.

The results of the models were experimentally validated using SOFC cells and stacks assembled from materials provided by HK Oil. The validation of strain and displacement caused by thermal stress and creep is achieved with a high resolution 3D video gauging system observing the operating cells and stacks through quartz windows in a modified laboratory furnace.

Understanding the thermal and mechanical environment of cells and stacks during operation and cycling steps is a key factor for the improvement of the design leading to higher life time expectancy and lower probability of critical failure, because mechanical issues are most likely to cause rapid failure and step change deterioration of performance during the life cycle of SOFCs.
Impact of redox cycling on microstructure related mechanical property change in solid oxide fuel cells

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One of the main limitations to the nickel-ceramic based anode is shown a large volume change upon Ni reoxidation, which could lead to surface crack, microstructure break and loss conductivity to anode. In this poster, there will be reviews of Ni reoxidation effects on the anode of the electrolyte supported fuel cell. And then, the early stage working plan will be presented, which includes using SEM and Nano-indentation techniques to have a systematic analysis on the anode microstructure and mechanical property with the different redox cycles.

The fine microstructure for the Ni-YSZ anode

The microstructure failure due to Ni expansion and shrinkage
In recent SOFC and SOEC electrode design experiments, all-ceramic electrodes have shown increasingly promising performance under testing. The perovskite group La1-xSrTi1-yMyO3 with an A-site deficiency has been proven to have the potential to electronically conduct upon reduction and can ex-solve the M dopant as shown previously with metals such a nickel (ref Irvine in Nature Mat).

By ex-solving the metal from the perovskite, capitalising on an A site deficiency, the agglomeration of the Nickel on the surface of the material – an occurrence that plagues conventional Ni-YSZ anodes- is avoided, allowing for greater catalytic activity and thus increasing the working life of the system. Further ex-solution of other metals may lead to resistance to coking and or exhibit sulphur tolerance.

Preliminary results on the synthesis of these materials by co-precipitation/combustion and characterization of ceramic scaffolds based in the family La1-xSrTi1-yMyO3 (M = Ni) by SEM, XRD and conductivity will be presented. Images will consist of SEM and optical microscope captures of materials.
Design and Development of an Ontology-based Framework for Providing Intelligent Support to Fuel Cell Stacks’ Operation Monitoring Tasks

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The key focus of this research is to develop a dynamic and adaptive application using semantic modelling techniques such as RDF (Resource Description Framework), OWL (Web Ontology Language) and SWRL (Semantic Web Rule Language) to facilitate the fuel cell design process and ensure prolonged optimal operation. The main intent is to optimise the health management capability throughout the fuel cell service lifecycle. The presented methodology aims to manage and interrogate large amounts of sensor data to enable system level intelligent decision making in dynamically changing situations.

This research puts forward an innovative ontology-driven proposal within the scope of the applied hydrogen and fuel cell technology area. Ontologies are basically used to capture widely distributed knowledge resources within some domain of interest in the form of concepts and semantic relationships among them. While the ontology-based system development in various science and engineering domains is an active research area, its concerns towards modelling the fuel cells’ domain knowledge and operational behaviour are not yet well covered. In this proposal, a modular hierarchy of a PEM (Proton Exchange Membrane) fuel cell’s constituent elements as well as auxiliary stack devices has been constructed, and ontology classes are populated with specific instances and corresponding attribute values. Furthermore, the failure-mode analysis of some desirable parameters and factors that might influence the runtime operation of the fuel cell system such as temperature, relative humidity, demand load, pressure etc, has been performed. In this regard, the fault-state causal reasoning models are formulated (based on a-priori knowledge of probable occurring anomalies) for efficiently predicting and diagnosing the performance decline of a fuel cell stack. A knowledge acquisition/representation tool Protégé has been utilised for developing the fuel cells’ domain ontology. Incorporation of several fault prediction scenarios has been done within the designed ontology executing multiple mathematical modelling expressions. Initial experimental results regarding the electrochemical degradation test, effectively confirm the applicability of our proposed method for semantic reasoning within the fuel cell’s stack failure detection and problem solving sessions.

Keywords: Fuel Cell, Low Carbon Energy, Domain Ontology, Knowledge Representation, Decision-support System, Semantic Reasoning and Diagnosis, Knowledge-based System

References:

Modelling and Measuring Multiphase Flow in GDLs
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Better PEFC performance and cost savings can be achieved by improving the current density produced by the cells at lower voltages by countering mass transport losses. At high current density water is produced in greater quantities and must be managed in order to keep supplying the reactant gases. The electrodes of the fuel cell are porous and so understanding how water is transported through porous material is key to improving performance.

Firstly a CFD model of liquid transport through an idealised fibrous structure will be presented representing a gas diffusion layer (GDL).

Secondly a pore network model (PNM) created as part of an open source collaborative project (www.openpnm.org) will be presented. The PNM examines fluid flow in porous material and accurately represents the geometry and topology of GDLs. The influence of structural changes on fluid transport will be presented.

Finally experimental results measuring the in-plane relative diffusivity and permeability of air through a partially saturated commercial GDL is presented with details of the experimental procedure including manufacture of the custom sample holder with a 3D printer.
Thermal Coupling of SOFC and Plate Heat Exchanger desorber
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SOFCs are a potential candidate for use as Auxiliary Power Units (APU’s) on board heavy duty trucks. Heat from the SOFC exhaust is generally used either for cabin heating or for recuperative heat exchange and even after that there is still a considerable amount of high quality heat available. The unique selling point of an SOFC is the availability of both electricity and high quality heat. Not using the heat from an SOFC stack is tantamount to using only half the available useful energy from the fuel.

The ongoing research work focuses on the design & development of a compact Solid Oxide Fuel Cell –Vapour Absorption Refrigeration System (SOFC-VARS) unit for refrigerated truck applications. Within the broader framework this work presents a numerical model and simulation for thermal integration of an SOFC stack with a plate heat exchanger desorber via a specially designed tube in tube heat exchanger with internal fins.

The sizing of the heat exchanger and desorber has been carried out to fit a small refrigerated van, to cater to a 1 kW cooling load. The modelling focuses on the heat transfer aspects at the SOFC and heat exchanger end and on both heat & mass transfer aspects at the desorber end.

The results show that a plate heat exchanger desorber is able to produce the required quantity of refrigerant needed for a 1 kW cooling load. A thorough sensitivity analysis on the plate heat exchanger desorber has also been carried out to identify the parameters that affect desorption performance the most and the parameters that have least effect on the desorption performance.

The use of plate heat exchangers as desorbers not only gives a high heat transfer surface needed for desorption but also leads to considerable reduction in desorber volume when compared to conventional falling film desorbers. Based on the results obtained from modelling, appropriate design maps have been drawn which showcase the sizing of the plate heat exchanger desorber and the SOFC stack and also the mass flow rate of thermal oil needed.
Development of the graphite-metal hybrid bipolar plate

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Composited bipolar plates have been considered as the PEFC because of its high conductivity and excellent corrosion resistance as compared with metal bipolar plate. Metal bipolar plates have been used the stack for automotive application because of its lightweight, low permeability and shock resistance. Both composite and metal bipolar plate have been limited to gas flow field at the bottom of the material properties. To improve the performance of PEFC, some candidates of metal with a porous flow field were considered as the gas distributor instead of present gas flow channels. The metal provided fuel cell stacks with efficient catalyst reaction and advanced electrical contact in micro-scale. We are planning to study the manufacturing technology to replace the gas flow channels with the graphite-metal hybrid bipolar plate. This graphite-metal hybrid (GMFH) bipolar plate seems to provide the PEFC with improved cell performance by combining the advantages of both a porous flow field and a graphite-composite bipolar plate.