Modelling & Control of PEM Fuel Cells

Research Activities at IIT Madras

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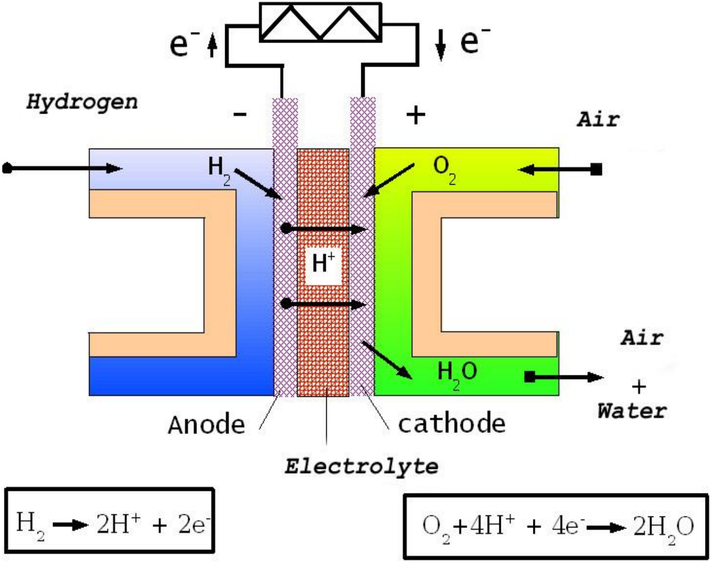
PEMFC Systems Research at IIT Madras

Outline

1. Introduction
2. Modelling of PEMFC System
    - Challenges in Fuel Cell Control & Modelling
    - Models for Thermal and Water Management
3. Control of Fuel Cells
    - Overview
    - Control of stack temperature
    - Continuous humidication and control of RH
4. Research at IIT Madras by the Fuel Cell Group

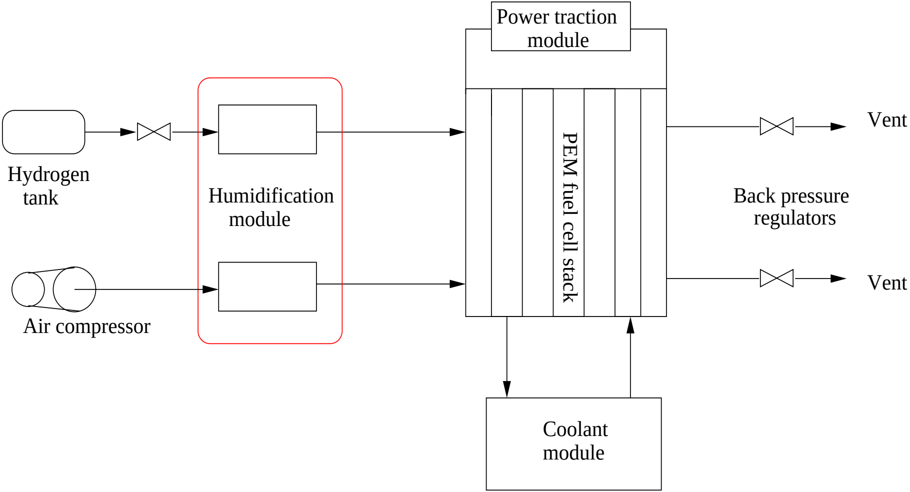
Schematic diagram of PEM fuel cell



$H_2 \rightarrow 2H^+ + 2e^-$

$O_2 + 4H^+ + 4e^- \rightarrow 2H_2O$

Schematic diagram of PEM fuel cell stack system

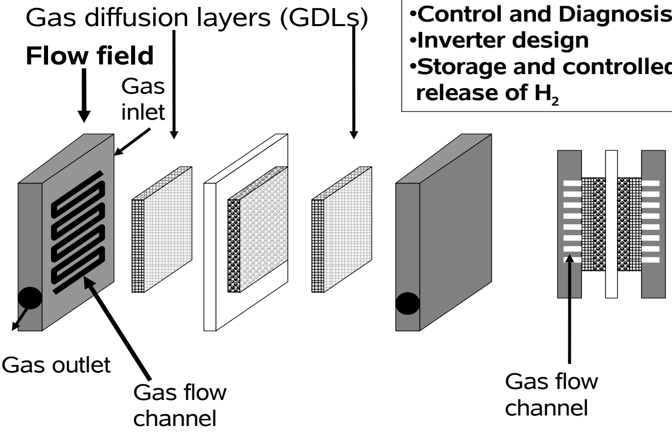


Sectional view of a stack

Different components of a stack

Research Issues

- **Reformer**
- **Control and Diagnosis**
- **Inverter design**
- **Storage and controlled release of H_2**



Objectives of study

- Evaluate the merits and demerits of first-principles models vs. data driven models for control and understanding of fuel cell behaviour.
- Develop control-oriented models.
- Compare and evaluate different control algorithms for different control configurations.
- Develop and build data-driven models of PEM fuel cells.
- Develop a full-scale diagnostic scheme for monitoring key performance variables in a PEM fuel cell.
- Implement control and fault diagnostic schemes on a real-time basis.
- To optimize the energy utility such that parasitic losses are minimized and generated energy is recycled.

Challenges

Interaction

Dynamic models that quantify the inter-relationships of various physical quantities of a fuel cell system hold the key to the successful control & monitoring of a fuel cell system. FCS poses challenges in several aspects

Interaction: The changes in the control parameters of an FCS are not independent. For e.g., stack temperature also affects the humidity of the air and hydrogen inside the stack, since the vapour saturation pressure is strongly dependent on the temperature. Interactions dictate the pairing in control schemes and can limit the performance of a control system.

Challenges

Non-linearities

Non-lineariities The relationships between the variables can be extremely non-linear depending on the variations in the operating conditions. For e.g., the magnitude and sign of the gain of power density w.r.t power density and current density changes with the operating conditions.

A linearized model is typically a starting point for the control analysis of fuel cell systems. Non-linearities can limit the predictability of such models

Challenges

Multiscale phenomena

Multiscale phenomena: Different phenomena occur in a fuel cell system at different timescales. In an automotive propulsion-sized PEM fuel cell.

- Electrochemistry $O(10^{-19}$ sec)
- Hydrogen and air manifolds $O(10^{-1}$ sec)
- Flow control/supercharging devices $O(10^{0}$ sec)
- Cell and stack temperature $O(10^{2}$ sec)

Multiscale analysis of the fuel cell system may be necessary to enhance the understanding of the process behaviour as well as to design the control system.

Challenges

Spatial and Temporal Variations

Distributed Parameter System: The parameters (physical quantities) of a fuel cell system not only vary temporally but also spatially. The temperature, hydration, reactant pressure can vary significantly across the space between the electrodes. Thus, lumped parameter system based analysis of these systems can be of limited use when a precise operation is required.

Coupled PDEs may have to be solved.

Analytical Models

- Analytical models are only approximate and do not include an actual mode of transport process with in the cell, they are useful for quick calculations of simple systems.
- F. Standaert et al. [1998] developed an analytical model with many simplified assumptions to predict cell voltage analytically for various current densities for isothermal and non-isothermal conditions. This model also predicts the water management requirements.

Semi-empirical & Mechanistic Models

- Semi empirical models combine theoretically derived differential and algebraic equations with empirically determined relationships.
- In mechanistic models differential and algebraic are derived based on the physics and electro-chemistry governing the phenomena internal to the cell.

PEMFC model categorization

Semi-Empirical Models

Features / Authors	Polarization	Transport Phenomena	Thermal effects	Water Management	Concentration effects	CO Kinetics	Flow field effects	Membrane conductivity
Springer et al. (1991)	■							■
Amphlett et al. [1995]	■							
Lee et al. [1998]	■							
Ronald et al. [2000]	■							
Maggio et al. [2001]	■				■			
Ronald et al. [2002]	■							■
Pisani et al. [2002]	■							
Chan et al [2003]	■				■			
Maxoulis et al [2004]	■							
Yu et al. [2005]	■		■	■				

PEMFC model categorization

Mechanistic Models

Features / Authors	Dim.	Polarization	Transport Phenomena	Thermal effects	Water Management	Conc. effects	CO Kinetics	Flow field effects	Membrane conductivity
Bernardi & Verbrugge [1992]	1	■							■
Fuller et al. [1993]	2	■							
Gurau et al. [1998]	2	■							
Ticainelli et al. [1998]	3	■							
Um et al. [2000]	3	■				■			
Nguyen et al. [2000]	3	■							■
Baschuk & Li [2000]	1	■							
Dutta et al. [2001]	3	■				■			
Berning et al. [2002]	3	■							
Wang et al. [2003]	3	■		■	■				

PEMFC model categorization

Control-oriented Models

Features / Authors	Lumped Model	Distributed Parameter Model	Controlled Variables			
			Air Flow	H_2 Flow	Temp.	Power
Pukrushpan et al . [2004]	■		■			
Golbert and Lewin [2004]		■				■
Ardalan et al. [2005]			■			
Caux et al . [2005]	■		■	■		■
Li et al. [2006]					■	
Chengbow et al.	■		■	■		

Pukrushpan et al (2004) model

- Reactions at electrode/catalyst surface are instantaneous.
- Temperature of stack is maintained constant (80 ^{o}C)
- Relative humidity(RH) of gas(fuel/air) is 100%.
- Hydrogen supply from high pressure tank considered to be static due to its fast dynamics (a proportional controller is in place).
- Flooding does not occur at the cathode or anode side.
- Membrane is completely hydrated.
- Activity of the catalyst is constant over a long period of time.
- Control: Focus on air flow control by manipulating compressor motor voltage.

First-principles Modelling
Thermal and Water Management

Assumptions

- The product water generated at the cathode is assumed to be in liquid state
- The water vapour and liquid is assumed
- Ideal gas law was employed for gaseous species
- Stack temperature is uniform due to high thermal conductivity and sufficient no of cooling plates.
- The water transport across the membrane assumed to be in vapour phase.
- The liquid water at the surface of the channels assumed to be neglisible.
- The H_2 gas entering into the stack on anode side is saturated.
- No liquid water at anode side

Fuel cell total energy balance

Based on fundamental energy balance for a fuel cell the lumped model has been developed as follows

$$\begin{aligned} Q_{theo} &= Q_{elec} + Q_{sens} + Q_{latent} + Q_{loss} \\ W_{out} &= W_{in} + W_{gen} \end{aligned}$$

where

Q_{theo}: Theoretical energy of the electrochemical reaction

Q_{elec}: Electrical energy generated from the stack ($V_{stack}I$)

Q_{sens} : Sensible heat of fuel and oxidant on anode and cathode side and coolant water

Q_{latent}: Energy due to phase phase change

Q_{loss} : Energy loss due to convection to the surroundings

Energy loss due to natural convection

$$Q_{loss} = hA(T_{stack} - T_{atm})$$

Thermal loss by convection to the surrounding is given as

$$\frac{hL}{K} = \left[0.825 + 0.387 \frac{Ra^{0.1333}}{[1 + \frac{0.492}{N_{pr}}^{0.56}]^{\frac{8}{27}}} \right]$$

where

h : Film heat transfer coefficient (W/m^2.K)

A : Area of perimeter (m^2)

L : Length of the stack(m)

Sensible heat

Sensible heat of cooling water:

$$Q_{sens,W} = N_W C_{p,W} (T_{Wout} - T_{Win})$$

Sensible heat at anode side:

$$\begin{aligned} Q_{sens,a} &= N_{H_2,a,out} C_{p,H_2} (T_{aout} - T_0) + N_{W,g,a,out} C_{p,H_2O,g} (T_{a,out} - T_0) \\ &\quad - N_{H_2,a,in} C_{p,H_2} (T_{a,in} - T_0) - N_{W,g,a,in} C_{pH_2O,g} (T_{a,in} - T_0) \end{aligned}$$

Sensible heat at cathode:

No liquid water enters at cathode inlet.

Sensible heat ...Contd

$$\begin{aligned} Q_{sens,c} &= N_{O_2,c,out}C_{p,O_2}(T_{cout} - T_0) + N_{W,g,c,out}C_{p,H_2O,g}(T_{c,out} - T_0) \\ &+ N_{W,l,c,out}C_{p,H_2O,l}(T_{c,out} - T_0) + N_{N_2,c,out}C_{p,N_2}(T_{cout} - T_0) \\ &- N_{O_2,c,in}C_{p,O_2}(T_{cout} - T_0) + N_{W,g,c,in}C_{p,H_2O,g}(T_{c,out} - T_0) \\ &+ N_{N_2,c,in}C_{p,N_2}(T_{cout} - T_0) \end{aligned}$$

Latent heat at cathode:

The amount latent heat on cathode side is depends on where the gas can be saturated due to formation of water on cathode side.

$$Q_{latent} = (N_{W,g,c,out} - N_{trans} - N_{W,g,c,in})H_{vapourisation}$$

Flow rates

$$
\begin{aligned}
N_{a,H_2,in} &= \frac{\alpha I \times N_{cells}}{2F} \\
N_{c,air,in} &= \frac{\beta I \times N_{cells}}{4F \times 0.21} \\
N_{W,g,a,in} &= N_{H_2,a,in} \frac{P^{sat}_{W,g,a,in} RH_{in}}{P_{a,in} - P^{sat}_{W,g,a,in} RH_{in}}
\end{aligned}
$$

Water transfer across the membrane is the sum of electro-osmatic drag, diffusion flux and convection flux

$$
N_{trans} = N_{drag} + N_{diff} + N_{conv}
$$

Temperatures of stack and outlet flows

From law of energy: Energy accumulation = Energy in - Energy out

$$
\begin{aligned}
\frac{dT_{stack}}{dt} &= \frac{Q_{theo} - Q_{elec} - Q_{sens} - Q_{latent} - Q_{loss}}{M_{stack} C_{p,stack}} \\
T_{a,out} &= 2\left[T_{stack} - \frac{Q_{sens,a} + Q_{mass,a}}{(hA)_a}\right] \\
T_{c,out} &= 2\left[T_{stack} - \frac{Q_{sens,c} + Q_{latent,c} - Q_{mass,c}}{(hA)_c}\right] \\
T_{W,out} &= \frac{(2T_{stack} - T_w in)hA_w + 2N_W C_p T_{Win}}{hA_W + 2N_W C_p T}
\end{aligned}
$$

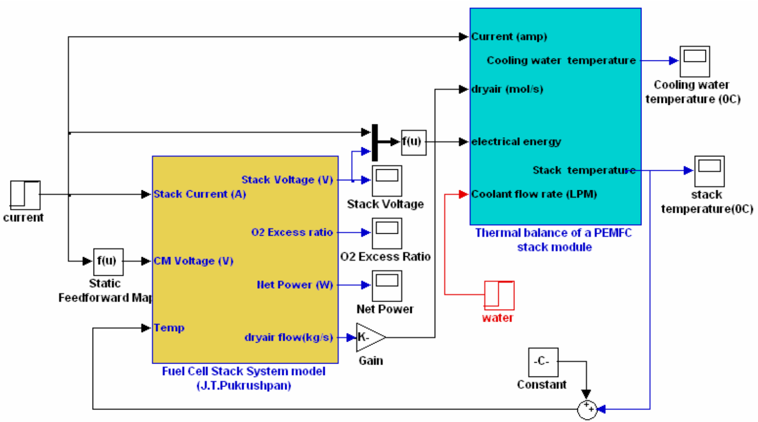
Temperatures of stack and outlet flows Contd..

where

$$
\begin{aligned}
Q_{mass,a} &= N_{trans} C_{p,H_2O,g}(T_{stack} - T_0) + N_{H_2,con} C_{p,H_2,g}(T_{stack} - T_0) \\
Q_{mass,c} &= N_{trans} C_{p,H_2O,g}(T_{stack} - T_0) + N_{H_2,con} C_{p,H_2O,l}(T_{stack} - T_0) \\
&\quad - N_{O_2,con} C_{p,O_2,g}(T_{stack} - T_0) \\
Q_{sens} &= Q_{sens,a} + Q_{sens,c} + Q_{sens,W} \\
Q_{latent} &= Q_{latent,c}
\end{aligned}
$$

Integrated Model

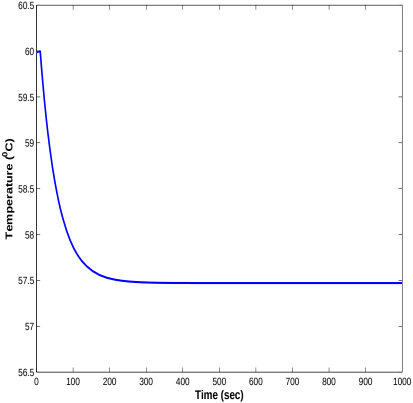
Temperature loop is open



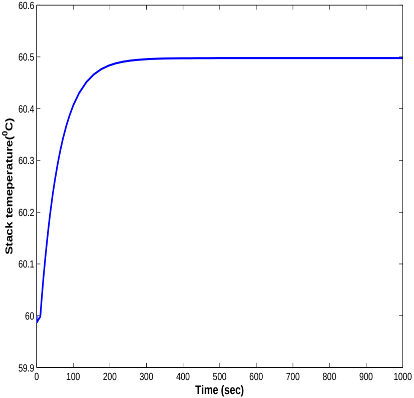
Open-loop simulation of integrated model

Unit step response to coolant flow & load change

Response to change in coolant flow



Response to a change in load



Performance of fuel cells

Fuel Cell Stack

A typical fuel cell system comprises a fuel cell stack integrated with several auxiliary components such as fuel and air supply systems, humidifiers, coolers, valves, *etc*.

Efficient fuel cell system power response depends on

- Air and hydrogen feed
- Flow and pressure regulation
- Heat and water management

Several auxiliary actuators such as valves, compressor motors, pumps, fan motors, expander vanes, humidifiers and condensers are involved in the control system

Control Issues

Parameters in the FCS

- Reactant flow rate control
- Maintenance of proper temperature
- Control of membrane hydration (to avoid membrane degradation and to prevent drying/flooding of the fuel cell)
- Control of total and partial pressures of the reactants across the membrane (to avoid detrimental degradation of the stack)
- Humidity of the air flow
- Power conditioner (to account for the significant variations in the fuel cell stack voltage) to condition the power supplied by the stack to the traction motors and auxiliary components.

Control Issues

Fuel Processor System (FPS)

The FPS is used to produce H_2 from natural gas using a catalytic partial oxidation reactor (CPOX). The amount of hydrogen created in the FPS depends on both the catalyst bed temperature and the CPOX air-to-fuel ratio.

In general, the control objectives are:

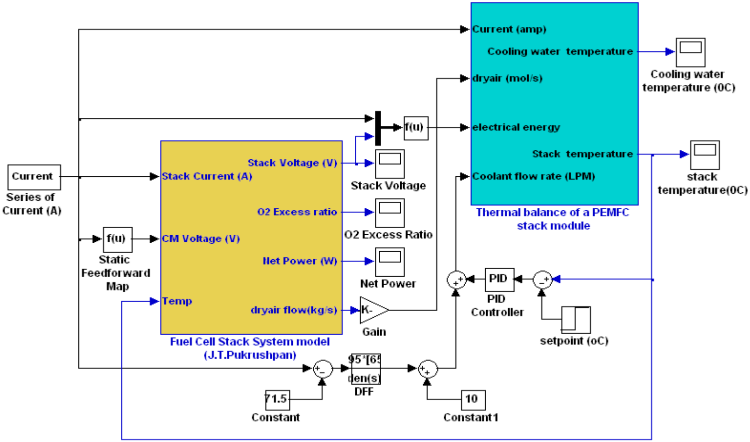
- To protect the fuel cell stack from damage due to fuel starvation
- To protect the CPOX from overheating
- To keep overall system efficiency high

The key performance variables are thus (*i*) the Oxygen-to-Carbon ratio, (*ii*) the CPOX temperature, (*iii*) the FPS exit total flow rate and (*iv*) the FPS total hydrogen flow rate.

Stack temperature control

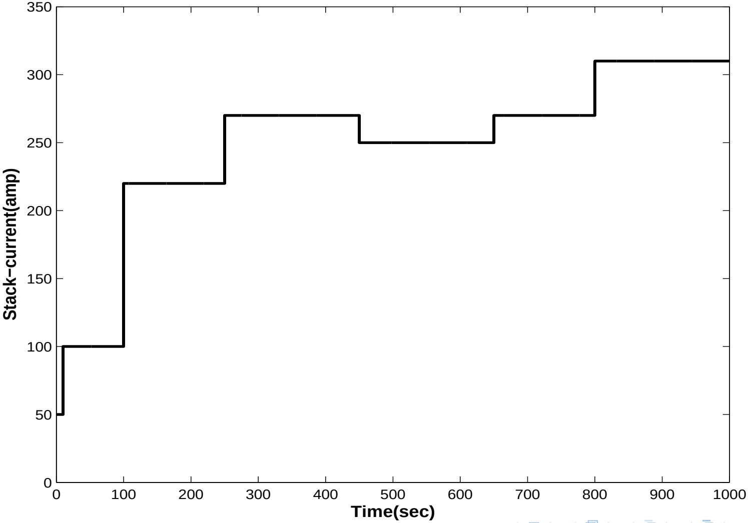
Integrated Model

Temperature loop is closed



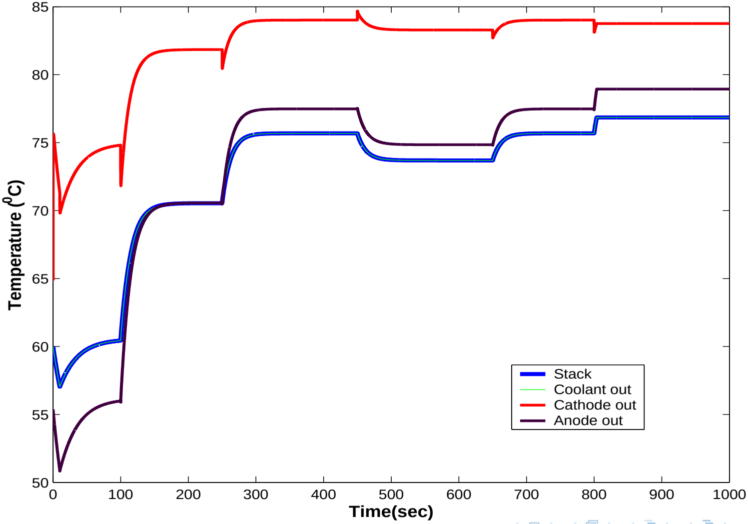
Load profile

Response without controller



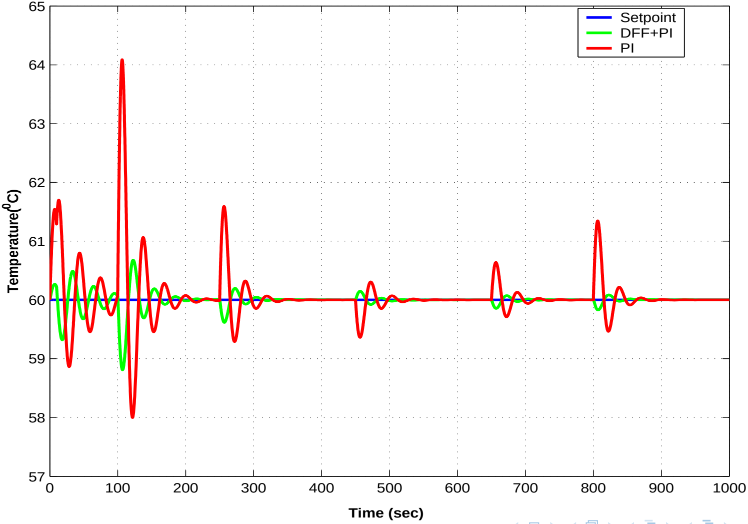
Temperature profiles

Response without controller



Stack temperature control

Comparison of control schemes



Continuous humidification of a PEMFC system: Design and Control

Why is humidification required?

- Water management is essential to efficient performance of a PEM fuel cell, because the proton conductivity depends on hydration of polymer membrane.
- The net power of a stack is higher when hydrogen alone is humidified than both the reactants are being humidified and fed into the fuel cell stack.

Since the performance of the fuel cell is dependent more on hydrogen humidification than on oxygen humidification, the scope of the work is restricted to the hydrogen humidification.

Types of humidification

The existing humidification systems are classified under the following types which are

External Humidification

The gases are heated and humidified externally in external humidification, thereby allowing us to maintain the %RH of gas at the desired value.

Internal Humidification

The gases are preheated before introducing into electrochemical active area of fuel cell. In internal humidification, %RH of gas can not be maintained at desired value.

Literature review

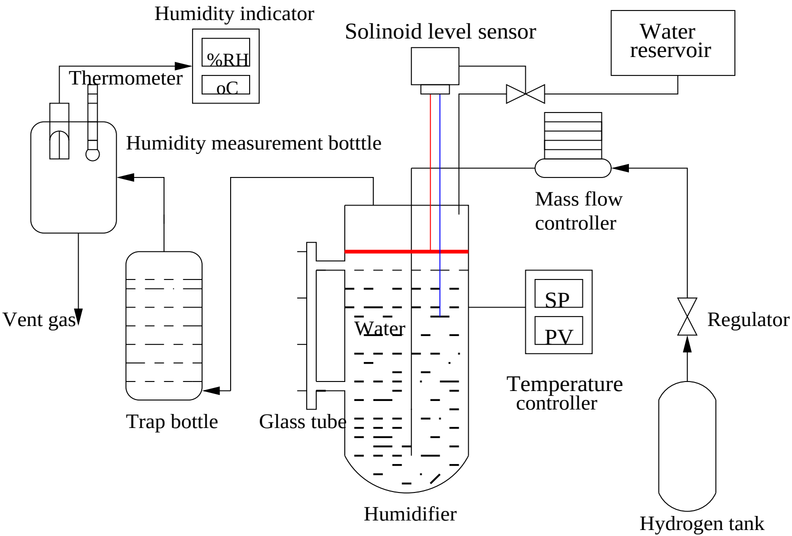
- Sridhar *et.al*[2001] have shown that the rate of water pick-up of H_2 gas at various flow rates in bubble humidification is lower when compared to membrane humidification. Hence they studied the effect of membrane thickness, area of membrane, gas flow rate and temperature of hot water on water pick up of H_2 in a membrane humidification.
- Rajalakshmi *et.al*[2002] have studied the effect of design parameters such as sparger diameter, number and diameter of sparger holes on relative humidity of H_2 besides the effect of gas flow rate and temperature of humidifier in a bubble humidifier. In their studies significant water carry over was observed at higher gas flow rates (above 15 lpm).

Literature review Contd...

- Duksu and Junbom [2004] have shown that the performance of PEM fuel cell is dependent more on H_2 humidifier temperature than the oxidant humidifier temperature.

To the best of authors knowledge the continuous humidification of H_2 gas has not been studied using a external or stack coolant water circulation in a bubble humidifier.

Existing bubble humidification system



Issues in the existing H_2 humidifier setup

- Water level has been maintained with solenoid level control.
- The running stack has to be stopped frequently for liquid water injection into the humidifier.
- Humidifier bottle has been heated with electrical jacketed heater.
- Water carry over occurs at high gas flow rates (above 5 lpm).

Issues in the existing H_2 humidifier setup Contd..

Disadvantages

- Water reservoir should kept at high elevation (10m) for operating the stack at 1 atm pressure (gauge). Therefore, it cannot be implemented in real time applications.
- Water level cannot be adjusted dynamically to avoid water carry over during high gas flow rates.
- External heat supply is needed for heating the humidifier bottle though the heating source is available in the form of stack coolant water.

Main features of proposed design

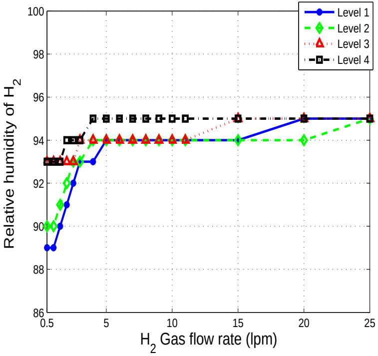
- It can be used for continuous humidification of H_2 gas.
- Water level can be maintained automatically between level 1 and level 4 at higher and lower gas flow rates respectively.
- Water-carry over can be avoided over a wide range of gas flow rates.

Scale-up: The proposed design can be scaled-up to a specified gas flow rate and stack operating pressure using the principles of geometric and kinematic similarity.

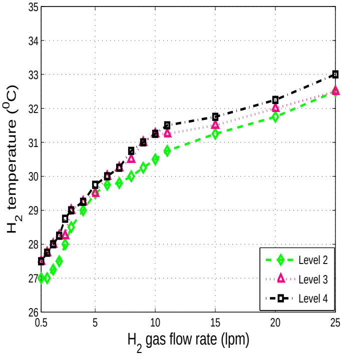
Studies required for a proposed design

- Effect of water level (gas residence time)
  - To determine the gas flow rate at which the water carry-over occurs
  - To study the effect of gas residence time on RH at constant humidifier temperature
- Effect of humidifier temperature
  - To study the relation between the humidifier and exit gas temperatures
  - To study the effect of humidifier temperature on relative humidity of H_2

Effect of water level (residence time)



RH of H_2 at $T_{humidifier}$=40^0C

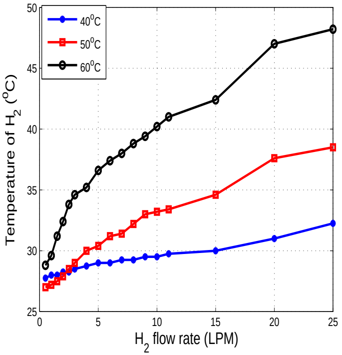


Temperature of H_2 gas

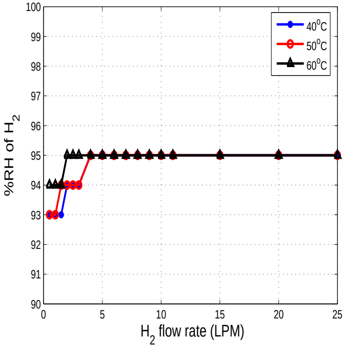
Effect of water level (residence time) Contd..

- The experiments were conducted for different levels of liquid volume (320 cc, 580 cc, 800 cc, 1000 cc) at humidifier bottle temperature 40°C.
- The relative humidity of H_2 is dependent on gas residence at lower gas flow rates and is independent at higher gas flow rates.
- The variation in gas temperature at the exit of the humidifier bottle at any gas flow rate is due to changes in the gas residence time in the humidifier.

Effect of Temperature

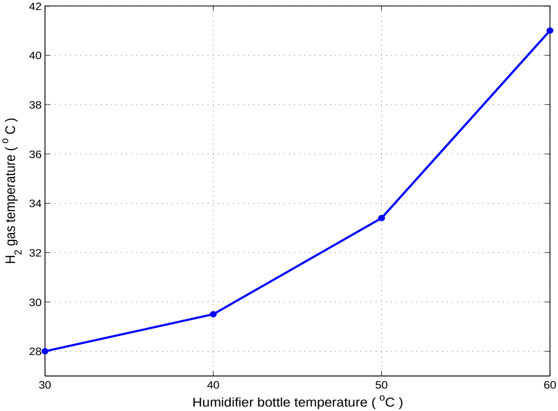


Relative humidity of H_2 gas



Temperature of H_2 in hygrometer

Effect of Temperature Contd...

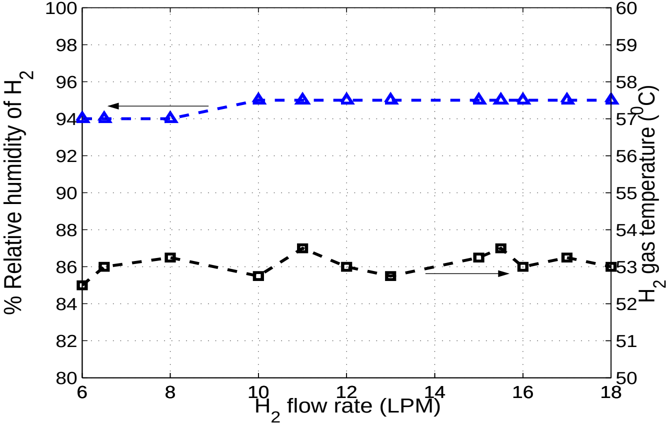


T_{H_2} at different temperatures of humidifier bottle, level 1 and gas flow rate 10 lpm

Effect of Temperature Contd...

- To study the effect of temperature, experiments were conducted at level 1 (lower) to avoid water carryover and thereby %RH was considered to be less dependent on liquid level at higher (4-25 lpm) gas flow rates.
- The relative humidity of H_2 is constant at higher gas flow rates for a wide range of gas flow rates.
- The temperature of H_2 gas increases exponentially with an increase in humidifier temperature. Using this chart, one can determine the humidifier temperature to achieve a desired exit temperature.

Results with continuous humidifier



Relative humidity of H_2 at exit temperature; Humidifier temperature 55°C

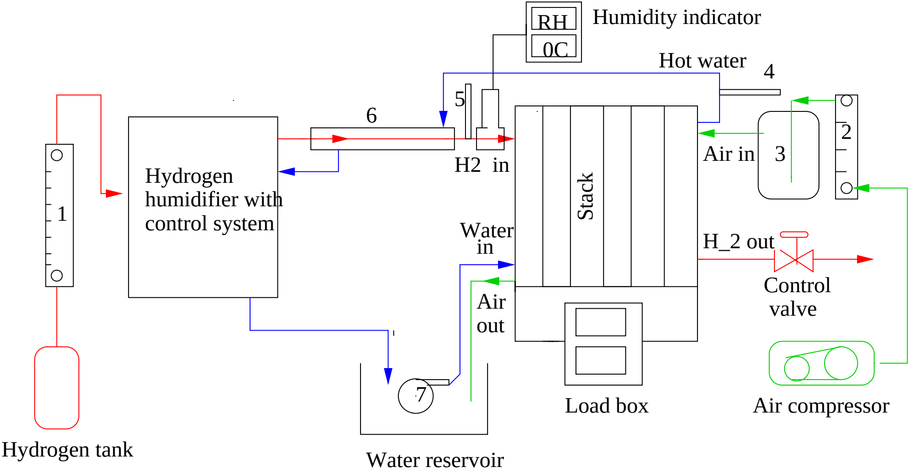
Design operating pressure of level control bottle

In order to know the design operating pressure of level control bottle, two types of float balls have been tested in the present experiments and the results obtained from Eq. 2 are compared.

Float ball type	Type of material	Diameter/ Height (cm)	Mass (grams)	Design pressure (mbar)	
				Experimental	Model
Hollow sphere	HDPE	Dia = 6.1	28.62	60	62
Cylinder	Thermo coal	Dia= 6.1 Height = 6.1	27.25	120	123

The cylindrical float ball is preferred to a hollow spherical ball since it gives a higher limiting pressure for the same diameter of the float ball.

Implementation on a 1 kW stack



1,2 Rotameters 3. Air humidifier 4,5 :Thermometers 6. Exit gas heating section 7. Water pump

Results with 1 kW stack Contd....

H_2 flow (lpm)	P_{H_2} (mbar)	current I (amp)	voltage (V)	$\triangle h_{water}$ (cm)	stack outlet T_{H_2O} (^{0}c)	Stack inlet T_{H_2} (^{0}c)	%RH
17.5	120	20	23.6	0.6	58	53.5	94
16	100	18	24.6	0.8	56	53	94
15	85	16	26.5	1.3	56	52.5	94
14	75	14	27.2	2.1	54	51	94
12	65	12	29.2	2.7	52	50.5	94
10	55	10	32	3.1	51	49.5	94
8	45	8	32.4	3.3	50	48.5	94
5	30	6	34	4.0	50	48	94
4	15	4	35.2	4.9	49	47	93
3	10	2	37.7	5.3	48	45.5	93

Summary

- The condensation of water vapour is avoided at electrode/flow field interface during the start up of stack when the gas is humidified with recirculated stack coolant water.
- H_2 gas is being humidified continuously without water carry over by the gas.
- Constant relative humidity of H_2 is maintained over a wide range of gas flow rates.
- External heating is not required for continuous humidification H_2

Main contribution:

The conventional bubble humidifier has been converted to a continuous humidifier and designed to control the %RH of H_2 at the stack temperature without the water carry-over.

Fuel Cell Activities at IITM

Dept. of Chemical Engg., Dept. of Chemistry,
Dept. of Electrical Engg., Dept. of Physics,
Dept. of Mechanical Engg.,
Dept. of Metallurgical and Materials Engg.,
IDRG Energy, and IDRG Materials

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Technology Issues

- System integration
- Robustness
- Modularity
- Scalability
- Locally available fuels
- Turndown ratio
- Load following capability
- Serviceability

Experience and Expertise - Catalyst

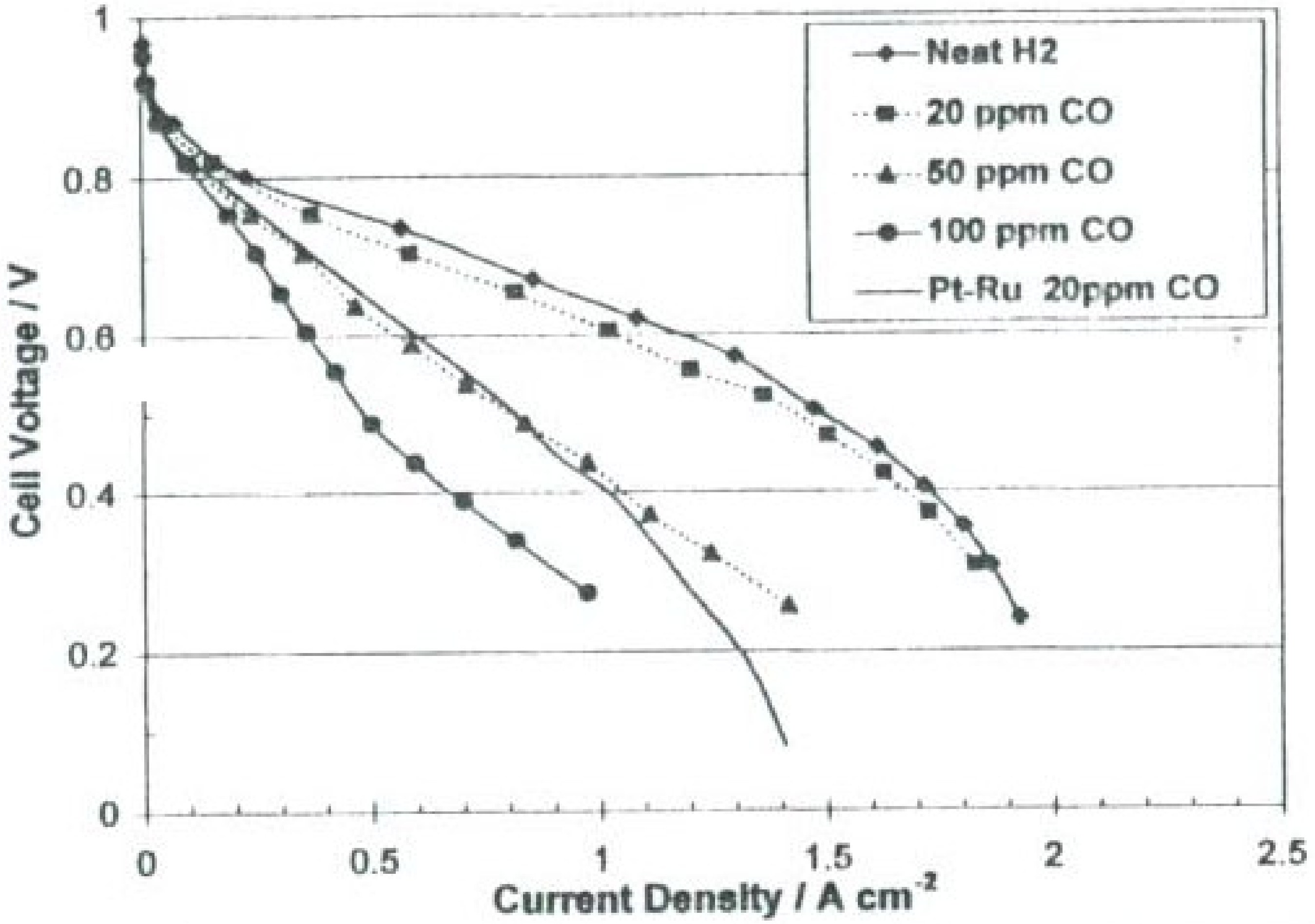


Figure 1: Fuel cell performance with PtMo anode catalyst exposed to various levels of CO in H_2. A polarization curve obtained for PtRu exposed to 20 ppm CO is included for comparative purp_____ Test conditions: Pt loadings 0.3 mg/cm^2 for anode and cathode of all cells; T_{cell}= 80°C, anode and cathode back pressure = 30 psig; 2 stoich anode flow rate.

Experience and Expertise - Catalyst

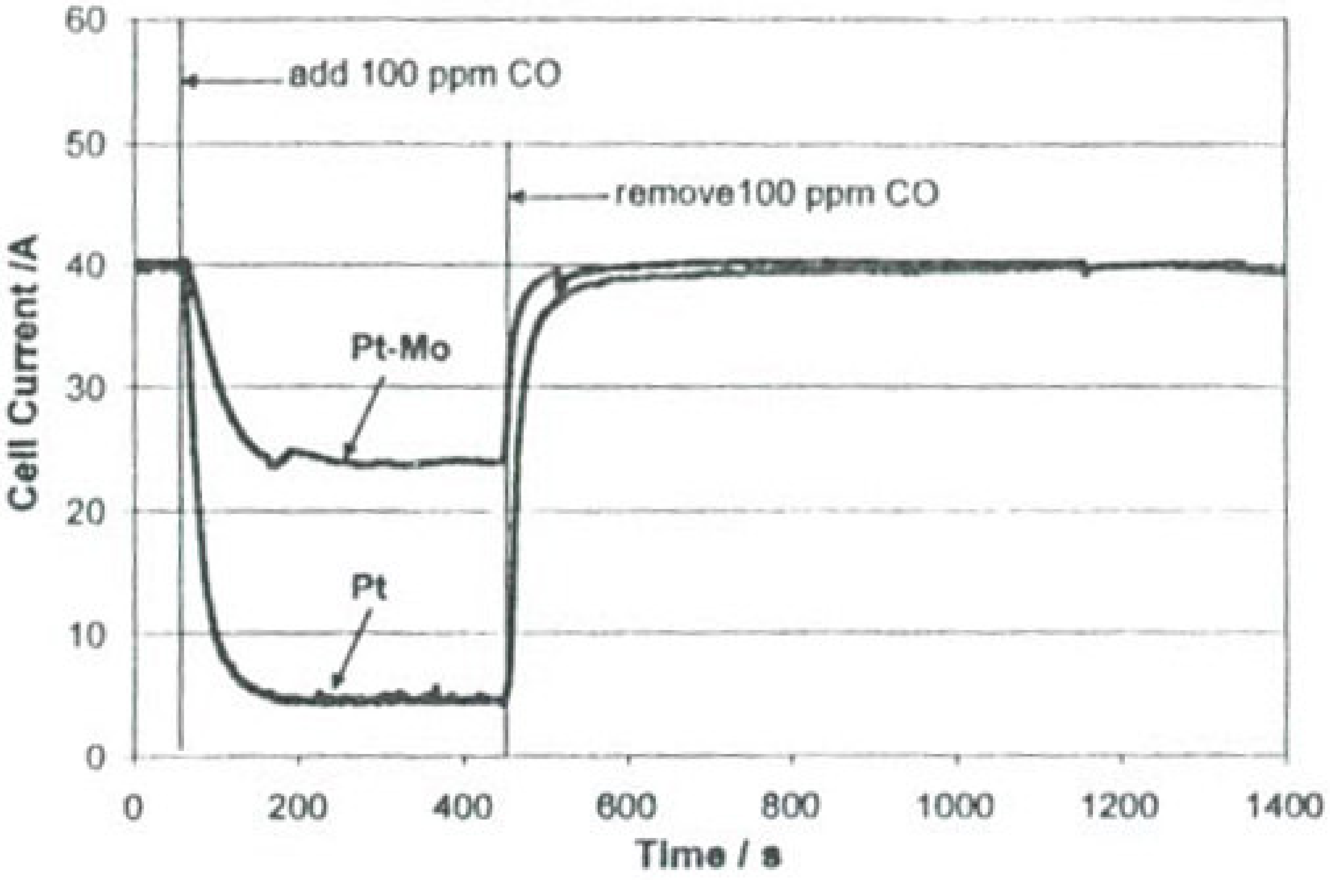
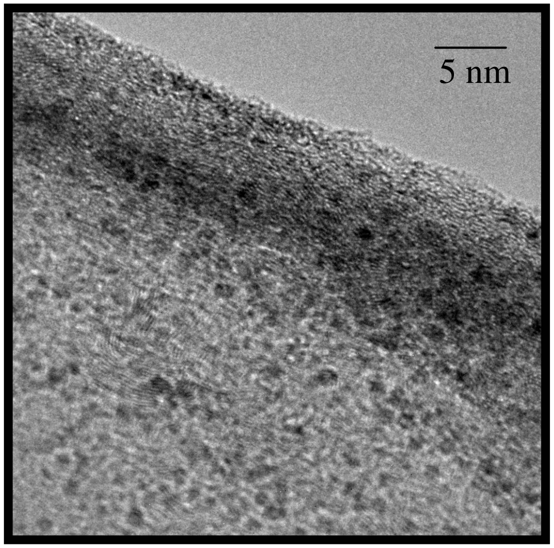


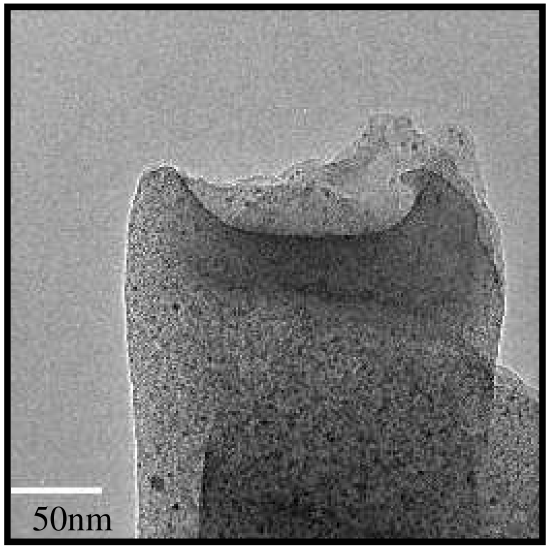
Figure 7: Transient response of cells with PtMo and Pt anodes. For t < 60 sec, cells are exposed to simulated reformate containing 20 ppm CO with a 2% airbleed. At t = 60 sec, CO level is increased to 100 ppm. At t = 450 sec, CO level is returned to 20 ppm. Test conditions: Pt loadings 0.3 mg/cm^2 for anode and cathode of all cells; T_{cell}= 80°C, anode and cathode back pressure = 30 psig; 2 stoich anode flow rate.

(a)



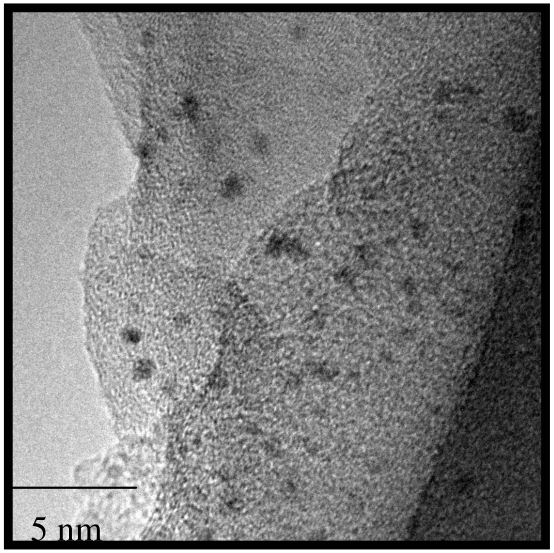
Carbon nanotube based electrodes demonstrate one to two orders of magnitude higher activity than conventional catalysts

(b)

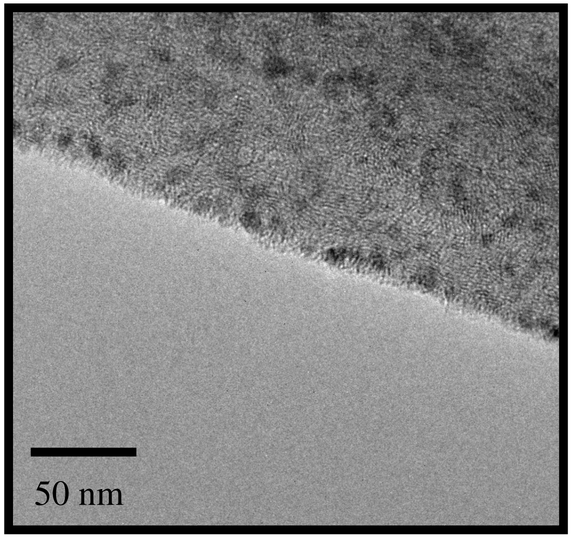


(a) Pt filled CNT (1.2 nm)

(c)

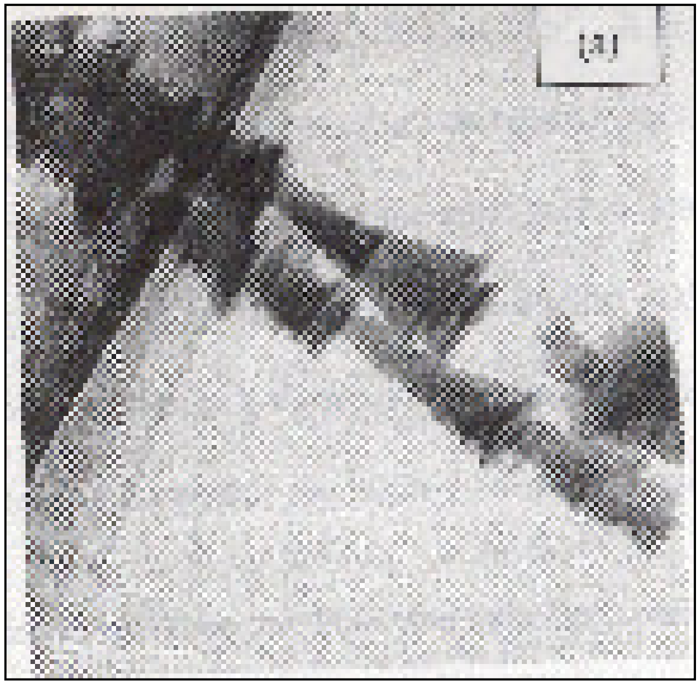


(d)

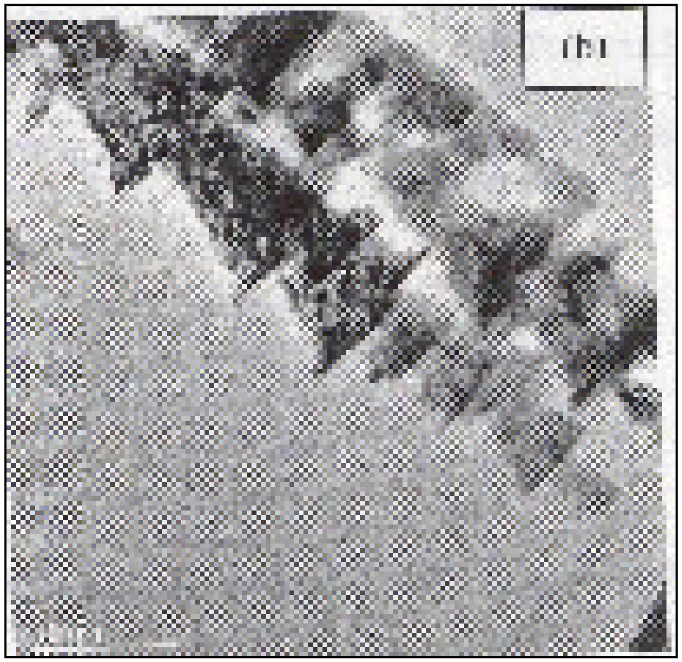


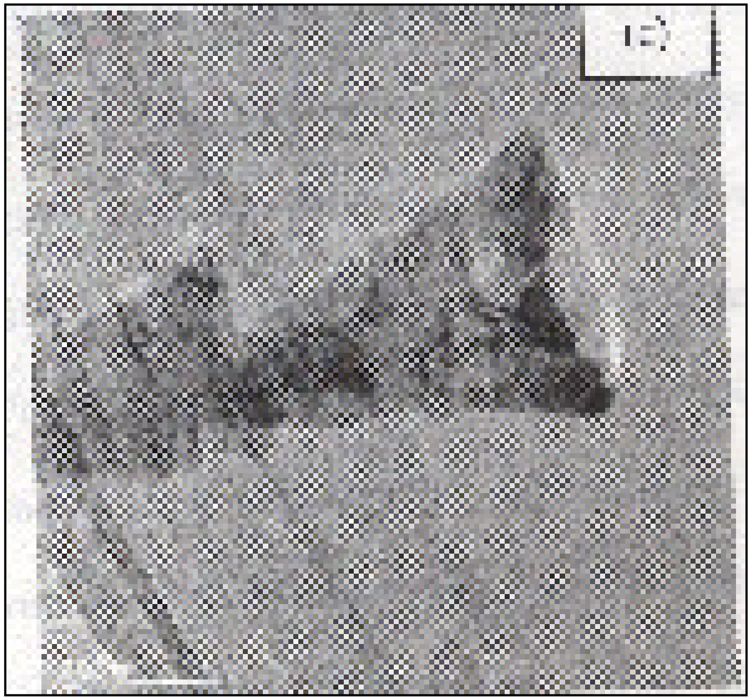
(b-C) Pt-Ru filled CNT (1.6 nm)

(d) Pt-WO_3 filled CNT (10 nm)



Template Synthesized Conducting Polymer Support



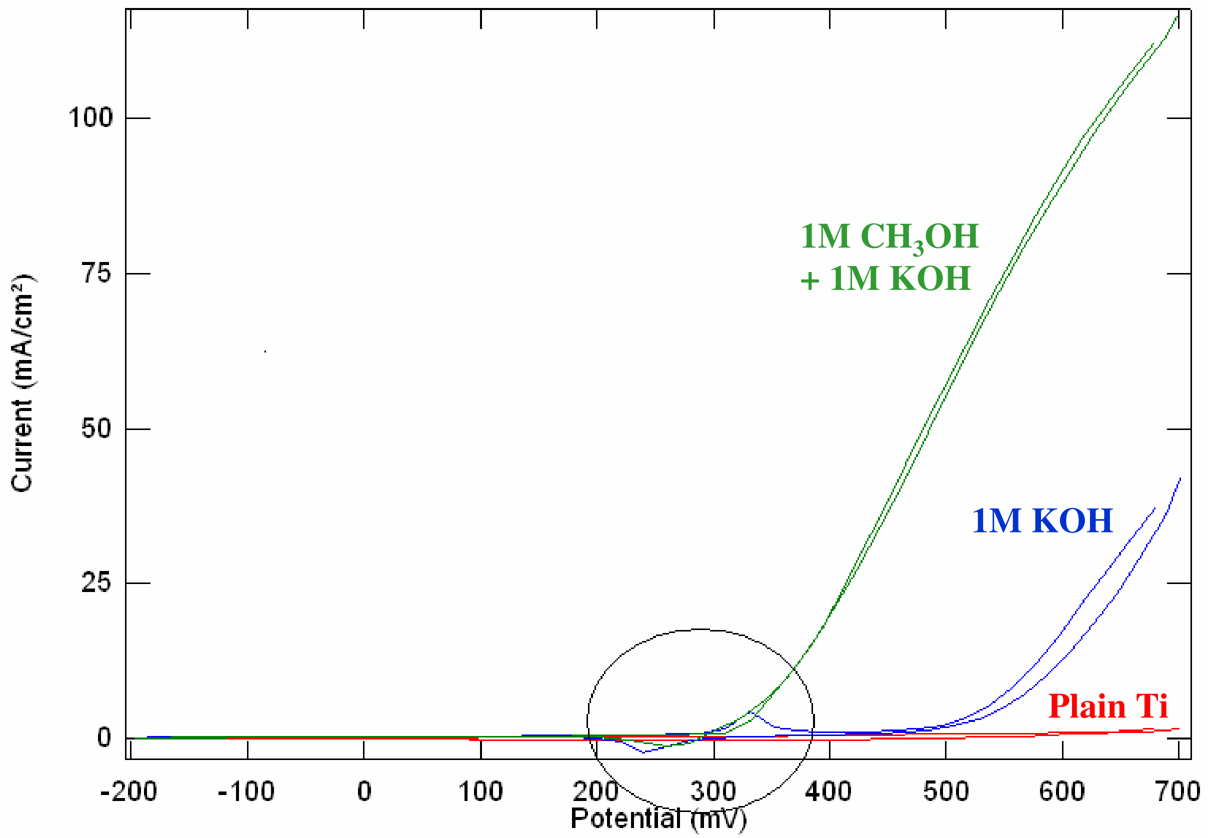


Template synthesized material demonstrates an order of magnitude higher activity

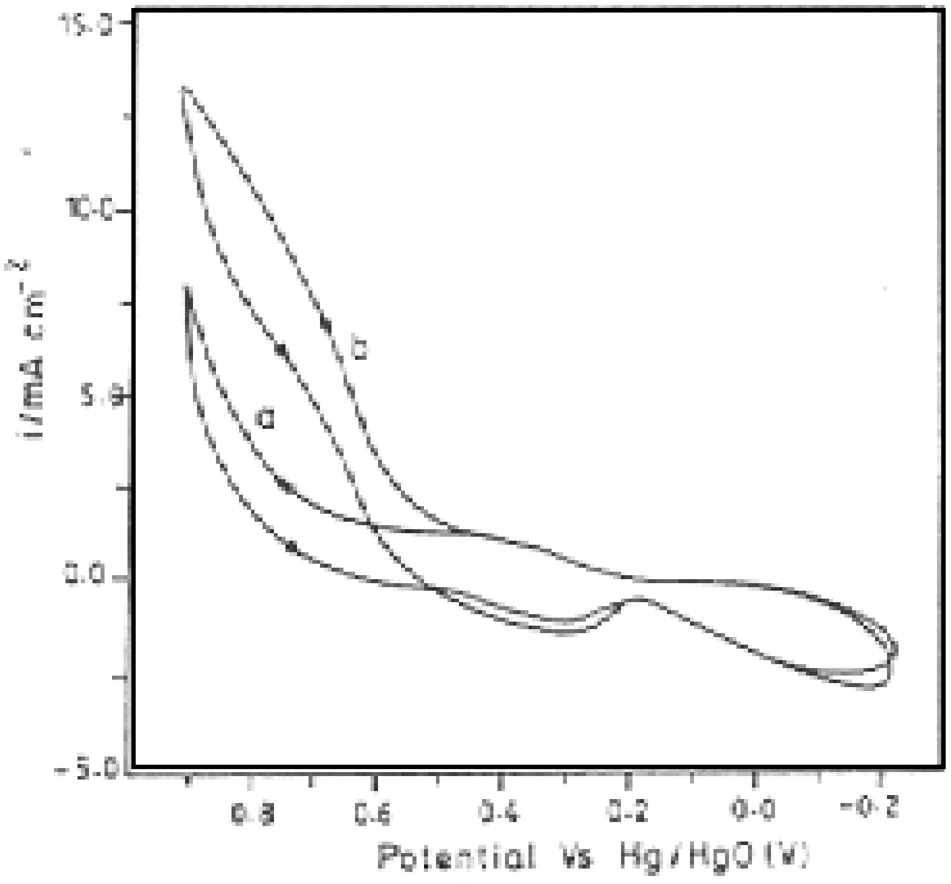
HR-TEM Images of (a-c) template- syntheisized poly(3-methyl)thiophene.

Electrodeposited Ni-Pd anodes

- High rate of Palladium surface segregation in the alloy
- Segregation found to enhance catalytic activity of Ni-Pd alloy compared to pure Pd



Electrochemical studies on bulk Sr substituted Lanthanum cuprates



- **Anodic peak between +0.26 V - +0.5 V**

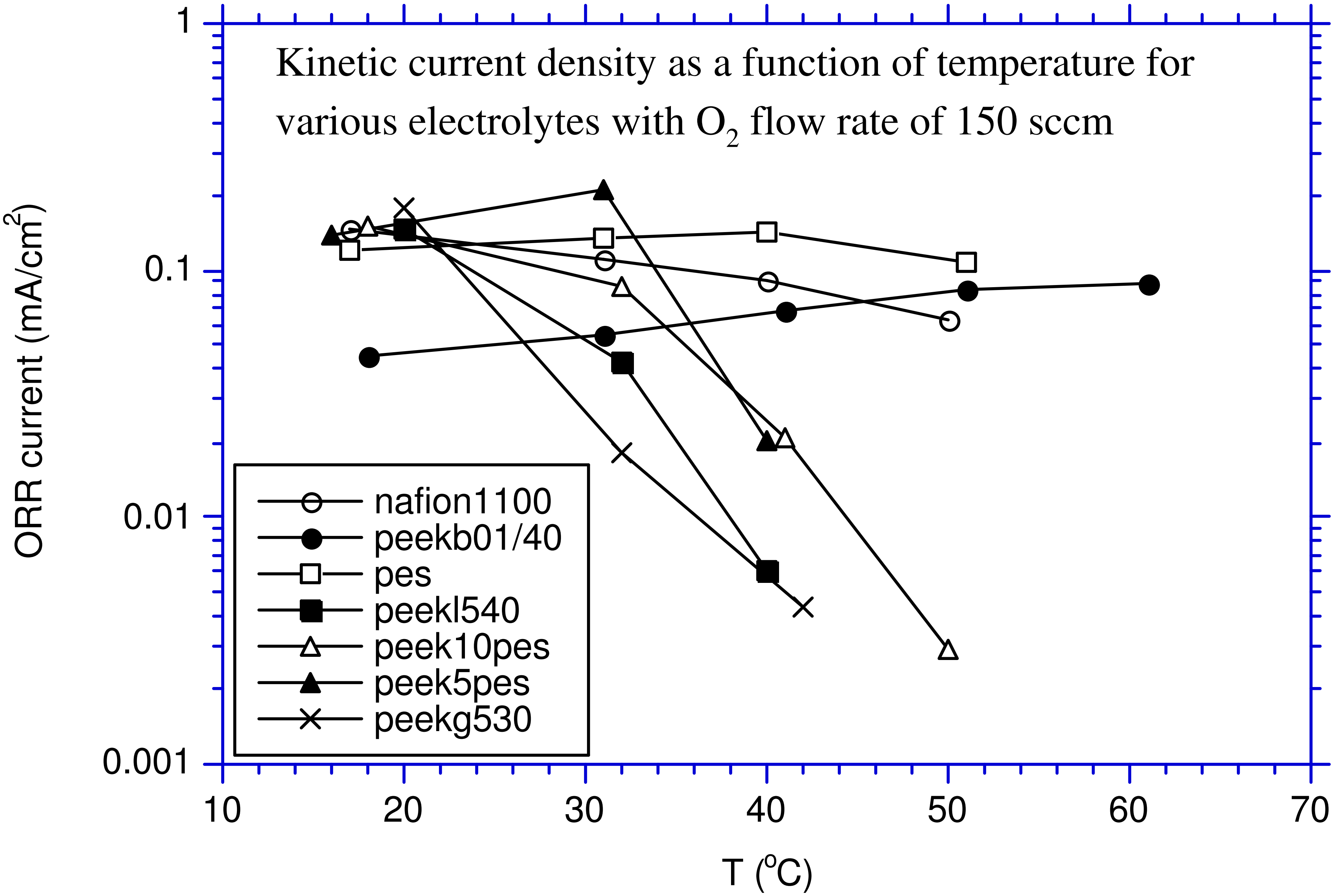
  ⇒ Cu(2+) →Cu(3+)

- **Methanol oxidation starts at ~0.46 V vs Hg/HgO**

V.Raghuveer, K.R. Thampi, N. Xanthapolous, H.J. Mathieu and B. Viswanathan, Solid State Ionics 140 (2001) 263

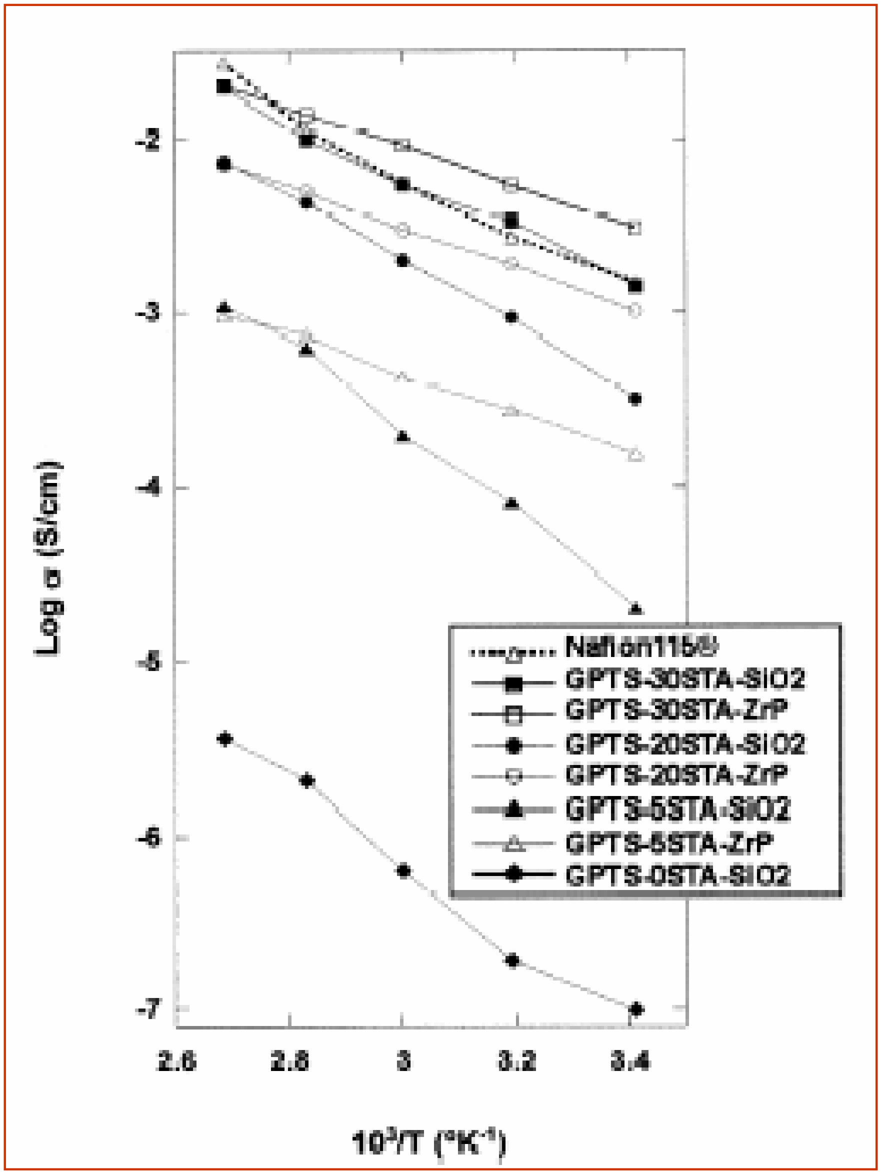
Cyclic Voltammogram of bulk cuprate in (a) 3 M KOH and (b) 1 M CH_3OH at a scan rate of 25 mVs^{-1}

Experience and Expertise - Membrane



Prathap Haridoss, Guido Bender, Francisco A. Uribe, and Thomas A. Zawodzinski Jr.
Electrochemical Materials and Devices Group, Los Alamos National Laboratory, Los Alamos, NM 87545
Unpublished

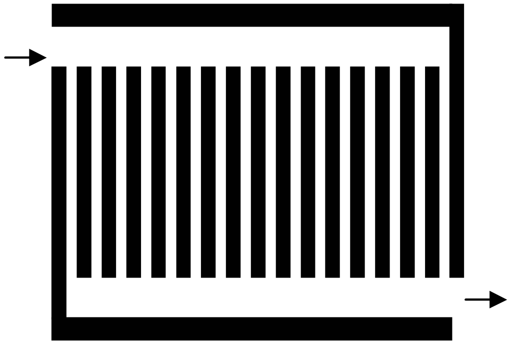
- GPTS-0%STA-SiO_2 shows conductivity 10^{-7}S/cm
- Increasing temp 20 to 100° C – conductivity increases largely – 1×10^{-7} to 3.6×10^{-6} S/cm
- Introducing 5 % STA – conductivity increases up to 2.1×10^{-5} at 20 ° C and 1.1×10^{-3} at 100 ° C
- STA increases – 30 % - conductivity reaches to 1.4×10^{-3} to 1.9×10^{-2} S/cm
- Showing almost equal to Nafion-115



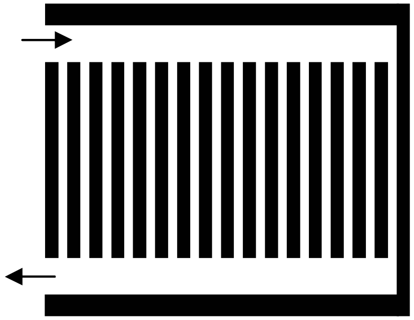
Conductivity of GPTS–*x*STA–SiO_2 and GPTS–*x*STA–ZrP composites *x*=0–30

Experience and Expertise - Modelling

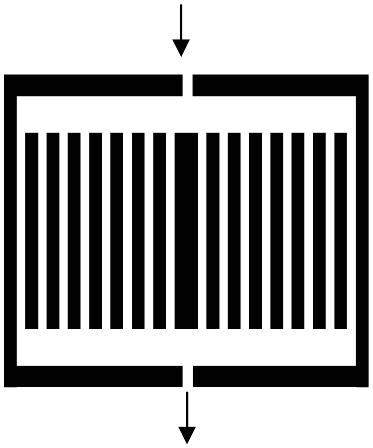
Parallel channel configurations



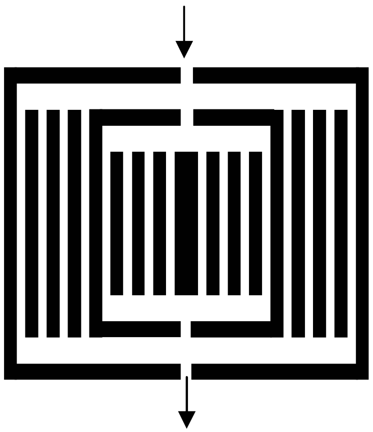
Z-type



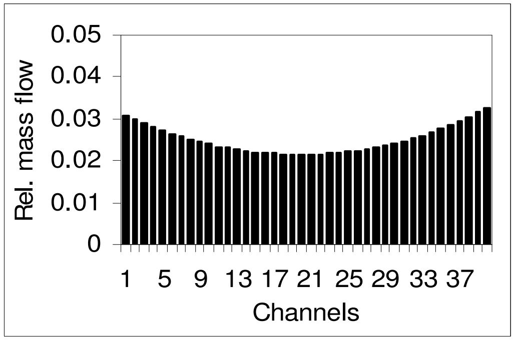
U-type

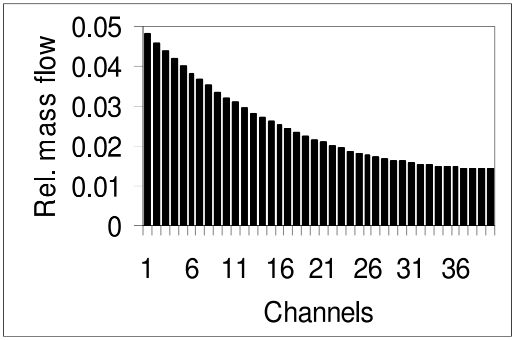


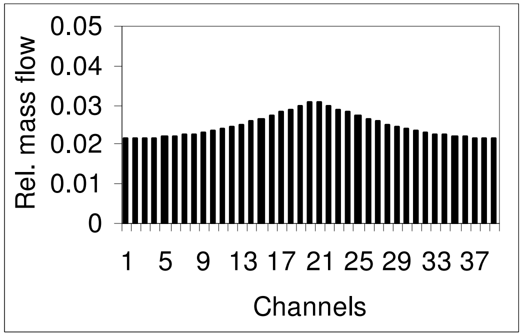
2U-type

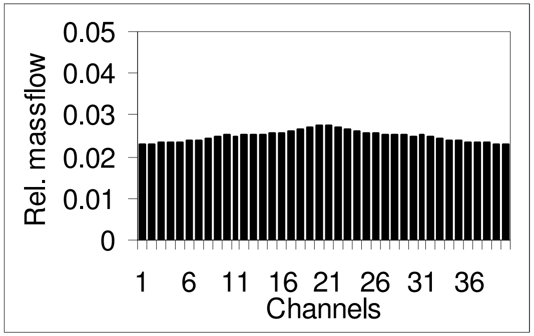


4U-type

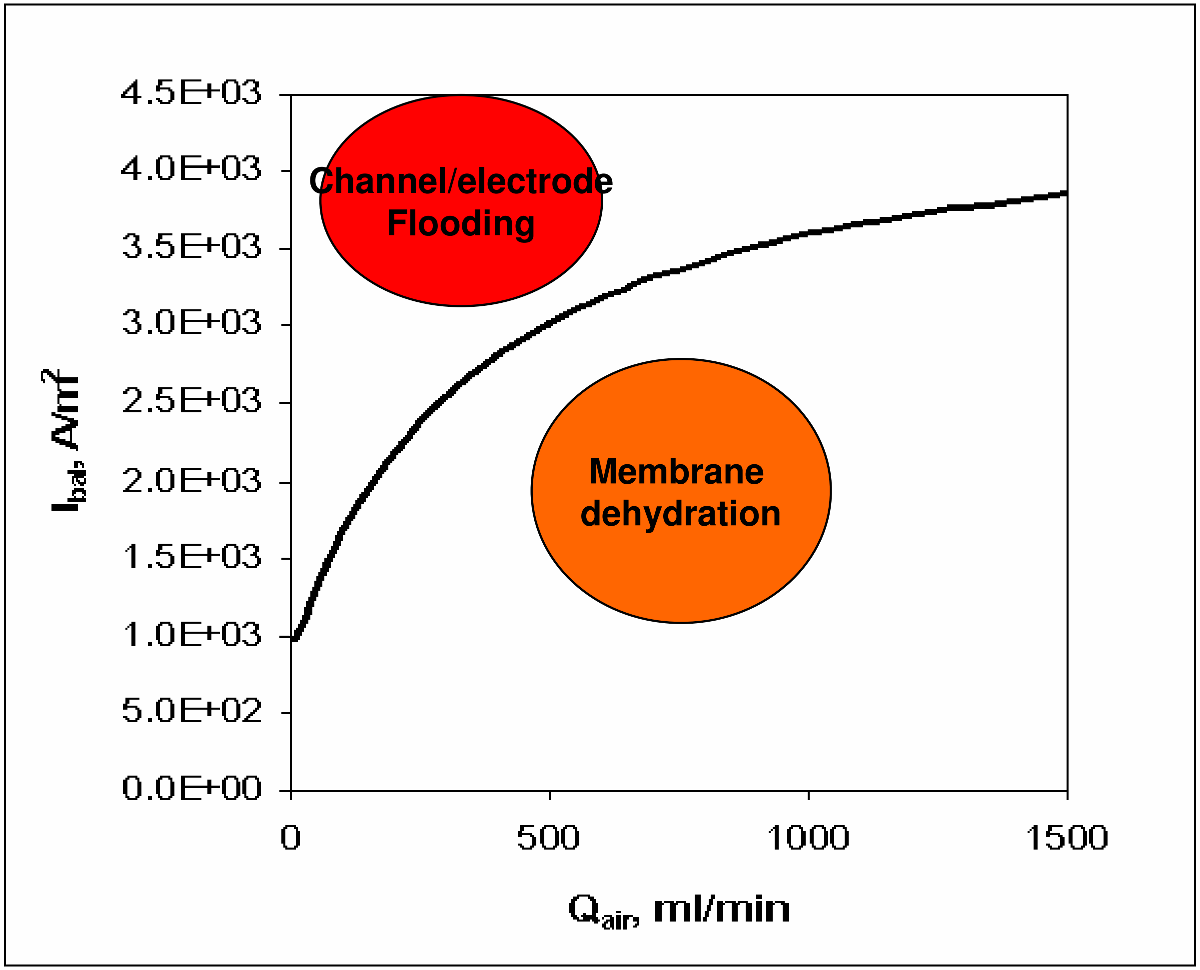








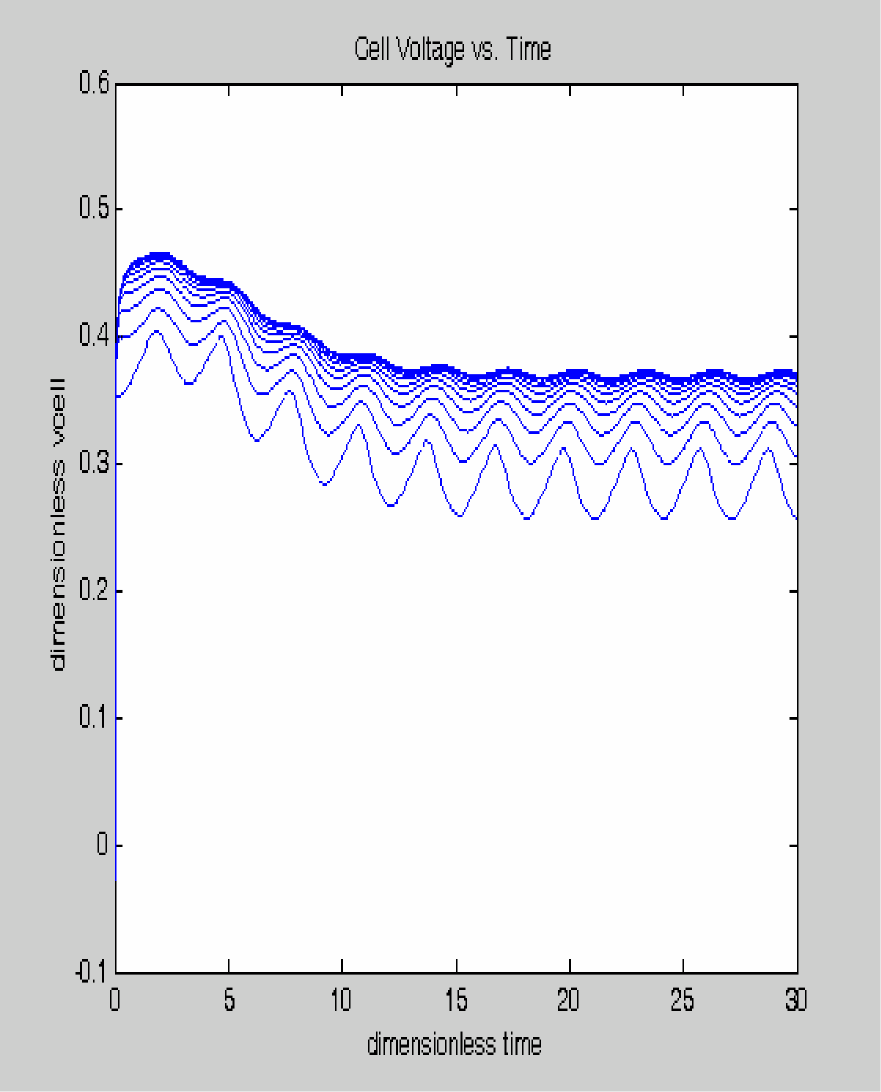
Typical variation of balance current density



$I < I_{bal}$ – Membrane dehydration

$I > I_{bal}$ – Electrode/channel flooding

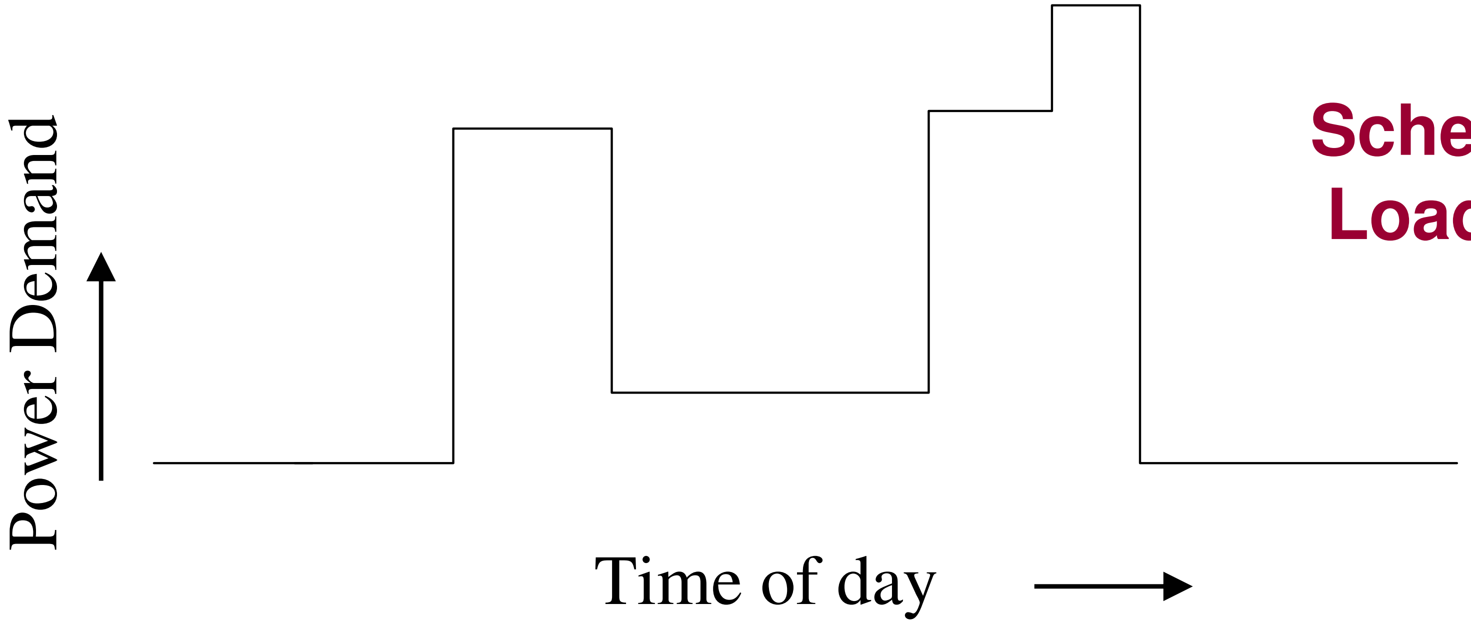
Pulsing feed strategy



The pulsing strategy of feed every 150 s yields a sustained 10% increase of the average cell voltage

Experience and Expertise – Controls and Diagnostics

- **Qualifying a fuel cell stack**
- **Systematic diagnostic scheme implemented**
- **Load following and reformer response time**
- **Fuel starvation issue resolved using appropriate control scheme**



Schematic of Load Profile

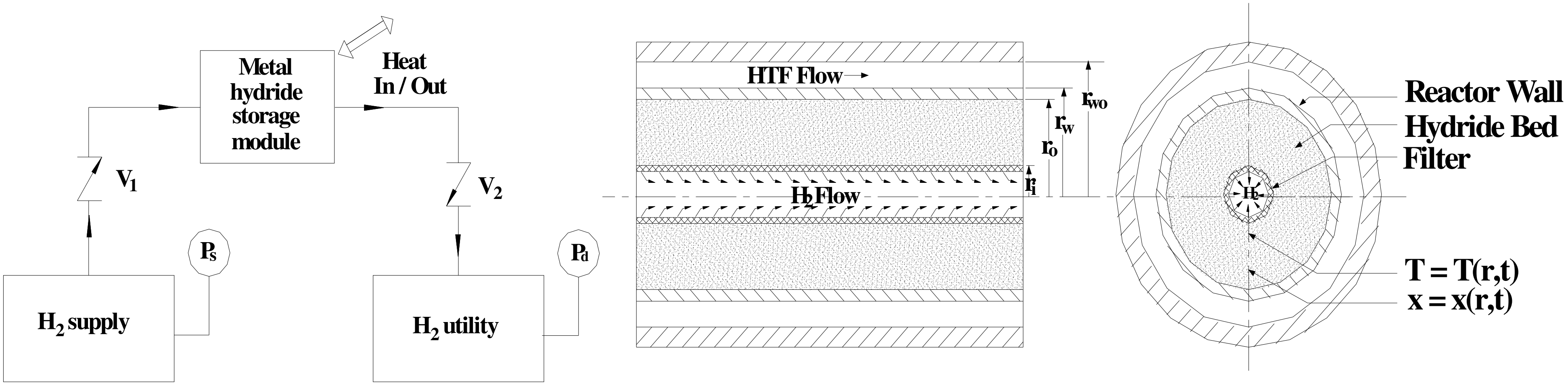
IITM: Experience and Expertise – Hydrogen Storage

Variation in Dissociation Energy

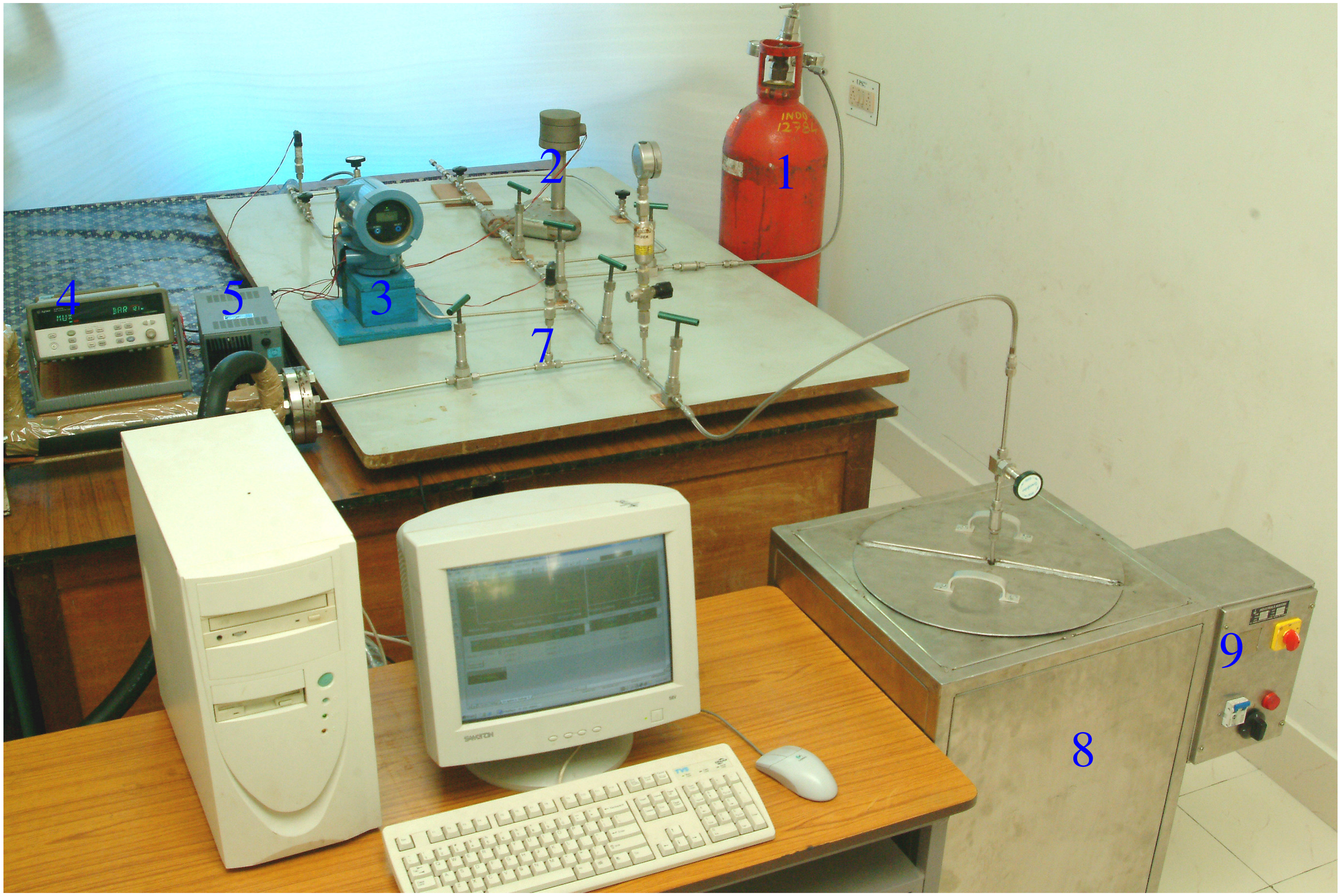
Heteroatom	Mode of substitution	H_2 Dissociation energy (eV)
Hydrogen	-	4.74
Un substituted CNT	-	4.76
Nitrogen substituted CNT	$1 N + 1 H_2$	0.31
(Each ring 1N)	$3 N + 1 H_2$	0.32
	$3 N + 3 H_2$	0.33
(Each ring 2N)	$6 N + 1 H_2$	0.56
	$6 N + 3 H_2$	0.50
Phosphorus substituted CNT	$1 P + 1 H_2$	2.06
(Each ring 1P)	$3 P + 1 H_2$	1.36
	$3 P + 3 H_2$	1.51
Sulphur substituted CNT	$1 S + 1 H_2$	0.27
(Each ring 1S)	$3 S + 3 H_2$	1.03

WORK DONE AT R&AC LABORATORY

- Thermodynamic Studies on Various Metal Hydride Based Thermal Devices
- Coupled heat and mass transfer analysis of metal hydride beds
- Heat and mass transfer recovery in single and multistage metal hydride systems
- Performance studies on different engineering applications such as metal hydride based hydrogen compressor, heat storage, hydrogen storage modules, cold storage and water pumping systems
- Screening of alloys for different engineering applications

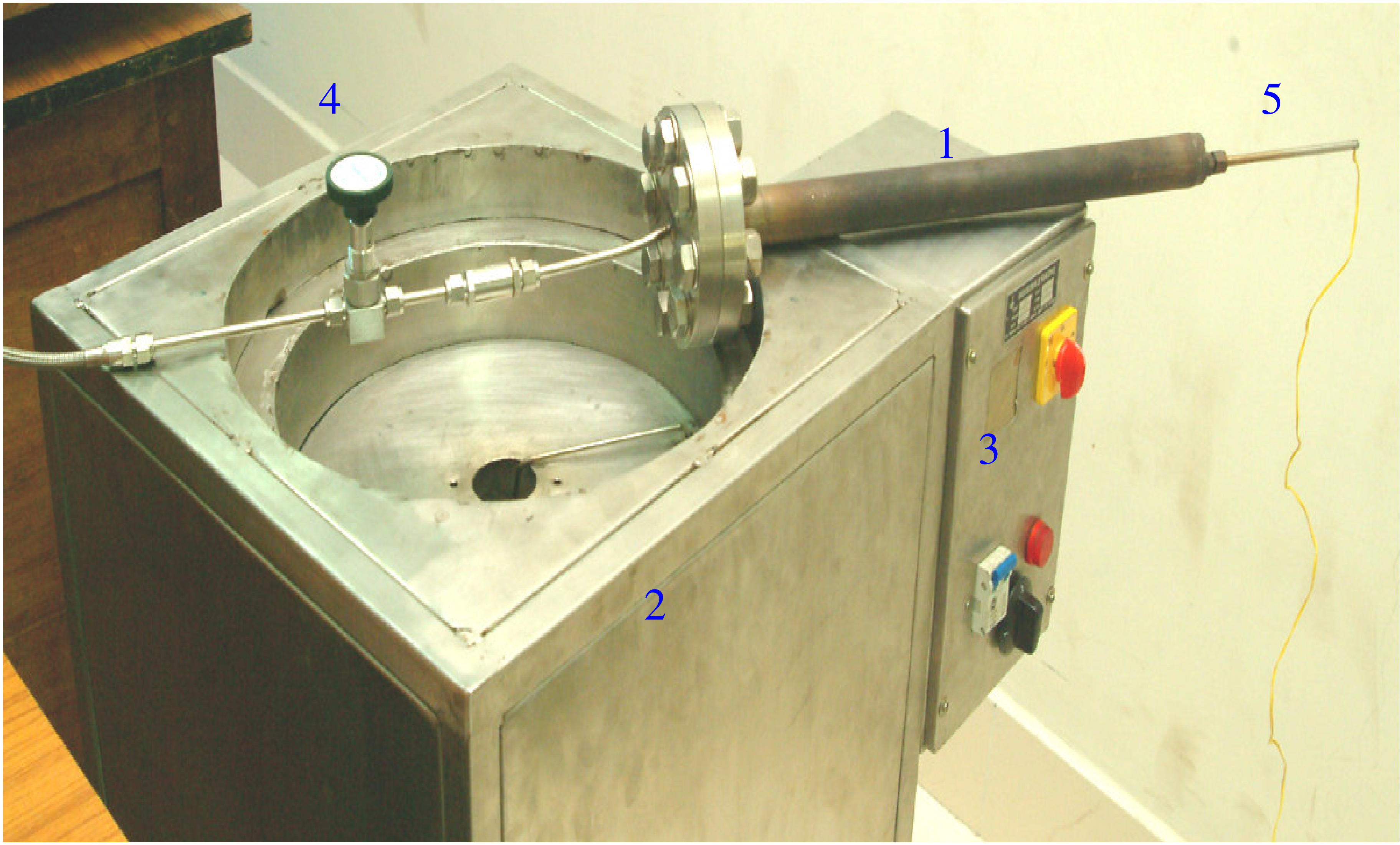


Physical model of cylindrical hydrogen storage reactor



Hydrogen storage experimental set up for Mg_2Ni alloy

1. Supply cylinder 2. Mass flow meter sensor 3. Mass flow meter transmitter
4. Data logger 5. Constant voltage source 6. Reactor 7. Pressure transducer
8. High temperature oven 9. PID Controller



Rector used for hydrogen storage with Mg_2Ni

1. Reactor 2. High temperature oven 3. PID Controller
4. Packless metallic bellow valve 5. Thermocouple

Comparison of Hydrogen storage capacities

Sl. No	Supply pressure, bar	Hydrogen storage capacities (%wt)		
		Mg_2Ni *(300 °C)*	$MmNi_{4.6}Fe_{0.4}$ *(25 °C)*	$MmNi_{4.6}Al_{0.4}$ *(25 °C)*
1	5	-	-	0.678
2	10	3.01	-	1.09
3	15	3.25	-	-
4	20	3.69	-	1.18
5	25	-	0.785	1.248
6	30	-	1.18	1.3
7	35	-	1.438	1.308

IITM: Experience and Expertise

Accomplishments

US Patents:

6,821,661 Hydrophilic anode gas diffusion layer; P. Haridoss, C. Karuppaiah, and J. McElroy

6,774,637 Method of qualifying at least a portion of a fuel cell system and an apparatus for the same; R. Hallum, C. Comi, Y. Wu, P. Haridoss, and C. Karuppaiah

6,696,190 Fuel cell system and method; P. Haridoss

US Patent applied for:

20030031916 Fuel cell electrode; P. Haridoss, C. Karuppaiah, J. McElroy, and G. Eisman

Indian Patents:

187590: A process for the preparation of FCC catalyst for use in petroleum refining (Process I); Prof C N Pillai
Dr B Viswanathan & Others

IITM: Experience and Expertise

Accomplishments

Indian Patents (Contd.)
187611: A process for the preparation of FCC catalyst for use in petroleum refining (Process II); Prof C N Pillai
Dr B Viswanathan & Others

Supported Metal catalysts and a method of manufacture thereof; Prof. B. Viswanathan, Prof. T. K. Varadarajan, Mr. S. Shanmugam

A process for the manufacture of an inorganic-organic membrane for use interalia in Fuel Cells, Lithium Batteries, and Electrochromic displays; Prof. B. Viswanathan, Prof. T. K. Varadarajan, Mr. S. Shanmugam

A method for manufacture of Carbon Nanotubes and such tubes whenever so manufactured; Prof B. Viswanathan, Mr. B. Rajesh

IITM: Experience and Expertise

Accomplishments

Indian Patents Pending:
159 / MAS/ 95: A process for the preparation of FCC catalyst for use in petroleum refining (Process III); Prof C N Pillai
Dr B Viswanathan & Others

384 / MAS / 2001: A Method of Manufacture of Carbon Nanotubes and such tubes whenever so manufactured; Prof B Viswanathan Sri B Rajesh

Patent application under progress:

Continuous humidification of H_2 gas in a bubble humidifier using external / stack cooling water recirculation: Design and control
A.K. Tangirala, V. Gollangi, B. Viswanathan, K.S. Dhathathreyan

IITM: Experience and Expertise

Accomplishments

Some Recent Publications:

Catalyst

B. Rajesh, K. Ravindranathan Thampi, J.M. Bonard, N. Xanthopoulos, H.J. Mathieu, and B. Viswanathan, Template Synthesis of Conducting Polymeric Nanocones of Poly(3-methyl thiophene) *J. Phys. Chem. B. ;* 2004; *108*(30); 10640-10644

Ch.Venkateswara Rao and B.Viswanathan**,** Oxygen reduction by FeN_4 – a density functional study, Indian Journal of Chemistry (November 2004.).

B. Rajesh, K. Ravindranathan Thampi, J.M. Bonard, N. Xanthopoulos,H.J. Mathieu, and B. Viswanathan , Pt particles supported on conducting polymeric nanocones as electro-catalysts for methanol oxidation, Journal of Power Sources 133, 155-161(2004).

B.Rajesh, K.Ravindranthan Thampi, J.M.Bonard, H.J.Matheu, N.Xanthopoulos and B.Viswanathan, Nano structured conducting polyaniline tubules as catalysts support for Pt particles for possible fuel cell applications, submitted to Electrochemistry and Solid State Chemistry Letters.7(11)A404-A407(2004).

Membrane

S. Shanmugam, B. Viswanathan and T. K. Varadarajan, Synthesis and characterization of silico-tungstic acid based organic-inorganic nano-composite membrane, solid state Ionics (communicated).

IITM: Experience and Expertise

Accomplishments

Some Recent Publications:

Flowfields

S. Maharudrayya, S. Jayanti, A.P. Deshpande, Flow distribution and pressure drop in parallel-channel configurations of planar fuel cells, *Journal of Power Sources*, 144, p 94–106 (2005)

S. Maharudrayya, S. Jayanti, A.P. Deshpande, Pressure losses in laminar flow through serpentine channels in fuel cell stacks, *Journal of Power Sources*, 138 p 1–13, (2004)

Hydrogen storage

M.Aulice Scibioh and B.Viswanathan, Hydrogen storage in carbon nano materials – possibilities and Challenges, Chapter 2 in Photo/Electrochemistry & photobiology in Environment, Energy and Fuel 65–100(2003).

M.M. Shaijumon and S. Ramaprabhu ; Synthesis of carbon nanotubes by pyrolysis of acetylene using alloy hydride materials as catalysts and their hydrogen adsorption studies; *Chemical Physics Letters, 374 513–520 (2003)*

M.M. Shaijumon and S. Ramaprabhu ; Synthesis of carbon nanotubes by pyrolysis of acetylene using alloy hydride materials as catalysts and their hydrogen adsorption studies; *Chemical Physics Letters, 374 513–520 (2003)*

M. Aulice Scibioh and B. Viswanathan, Hydrogen Future: Facts and Fallacies; Bulletin of the catalysis society of India Vol 3 Pages 72–81(2004).

M. Sankaran, K. Muthukumar, B. Viswanathan, Boron Substituted Fullerene Can They be One of the Option for Hydrogen Storage, Fullerenes, Nanotubes and Carbon Nanostructures 13, 43–52 (2005).

IITM: Experience and Expertise

Accomplishments

Some Recent Publications:

Hydrogen storage

R.VIJAY, R.SUNDARESAN, M.P.MAIYA & S.SRINIVASA MURTHY
Comparative evaluation of Mg-Ni hydriding materials prepared by mechanical alloying
Int. J of Hydrogen Energy, Vol.30, 2004, pp.501-508

R.VIJAY, R.SUNDARESAN, M.P.MAIYA, S.SRINIVASA MURTHY, Y.FU, H.P.KLEIN and M.GROLL
Characterization of Mg-xWt% FeTi (x=5-30) and Mg-40% FeTiMn mechanically alloyed hydrogn absorbing materials
J of Alloys and Compounds, Vol.384, 2004, pp. 283-295.

P.MUTHUKUMAR, M.PRAKASH MAIYA and S.SRINIVASA MURTHY
Experiments on a metal hydride based hydrogen compressor
Int. J of Hydrogen Energy, Vol.30, 2005, pp. 879-892

P.MUTHUKUMAR, M.PRAKASH MAIYA and S.SRINIVASA MURTHY
Experiments on a metal hydride based hydrogen storage device
Int. J of Hydrogen Energy, Article in Press (Available on line), Science Direct, Elsevier, 2005.