F.A. Coutelieris

Modeling of transport phenomena in a fuel cell

Department of Engineering and Management of Energy Resources, University of Western Macedonia, Bakola & Sialvera, 50100 Kozani, Greece,
Tel: +302461056751; Fax: +302461021731; e-mail: fcoutelieris@uowm.gr

National Center for Scientific Research “Demokritos”, 15310 Aghia Paraskevi Attikis, Greece,
Tel: +302106503447; Fax: +302106525004; e-mail: frank@ipta.demokritos.gr

NATIONAL CENTRE FOR SCIENTIFIC RESEARCH "DEMOKRITOS"
153 10 AG.PARASKEVI ATTIKIS POB 60228 THA. 6513111-9 6518911-9 TLX 216199

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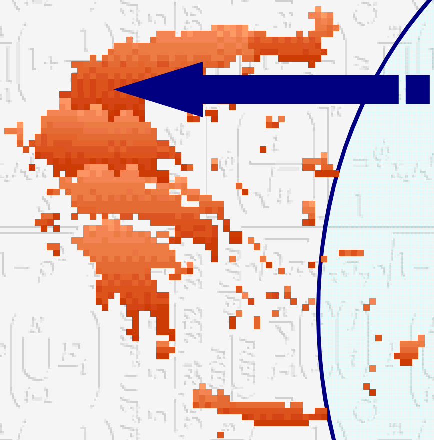
General:



KOZANI-UOWM

PUBLIC POWER CORP. (THE MAJOR ELECTRICITY PRODUCER IN GREECE)

>60% of Greek electrical power is produced **here**

General:

Electricity is produced by **COAL**

Serious environmental impact

Research on **RENEWABLE** and **ALTERNATIVE** energy sources

Energy research …

.. is actually focus on:

- Energy sources (fuels, wind, solar, etc)
- Conversion efficiency
- Emissions (sources, dispersion in atmosphere, etc)
- Fuel utilization (devices, technologies, etc)
- Heat waste management
- … and more

Utilization …

.. can be treated by several points of view:

- Reaction kinetics
- Thermodynamics
- Material science
- Devices used → FUEL CELLS
- Technologies applied
- … and more

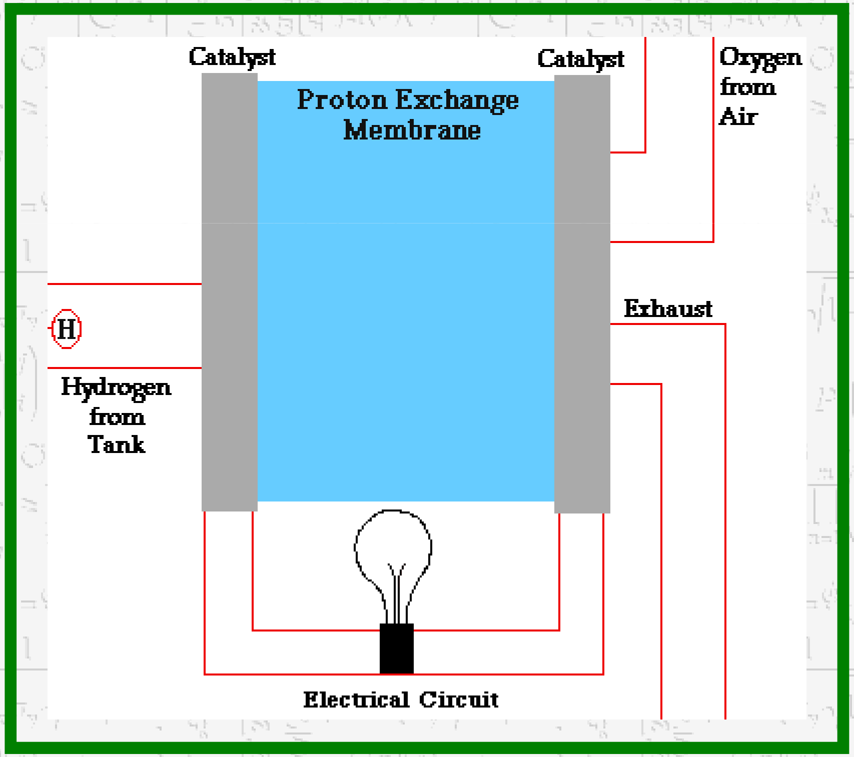
Fuel Cells…

… are energy devices that directly convert the chemical energy of the feeding fuel into electricity

Several types of Fuel Cells:

- Solid Oxide FCs
- Polymer Electrolyte Membrane FCs
- Direct Fuel FCs
- Molten Carbonate FCs
- … and more

How a fuel cell works:



Fuel electrode:

$$\frac{1}{2}H_2 \rightarrow H^+ + e^-$$

Air electrode:

$$\frac{1}{4}O_2 + H^+ + e^- \rightarrow \frac{1}{2}H_2O$$

Strong/Weak points:

- Zero emissions
- The flue gas is steam
- Fuel flexibility
- High costs
- Low efficiencies
- Small life-cycle

The efficiency of a fuel cell…

… strongly depends on the transport phenomena occurred and on the materials used

Difficulties in improvement:

- Description of transport processes in micro-level (too many phenomena to be taken into account)
- Up- & Down-scaling (micro-⇔ meso-⇔ macro-scale)
- Complicated geometries (porosity, etc)

Application:

The investigation of transport phenomena (momentum, heat, mass, charge) occurred in a SOFC and a PEM fuel cell.

Scope:

The development of a model which **must**

- adequately simulate the microscopic transport phenomena in a fuel cell
- be simple enough
- be transferable from one FC type to another
- be easily applicable

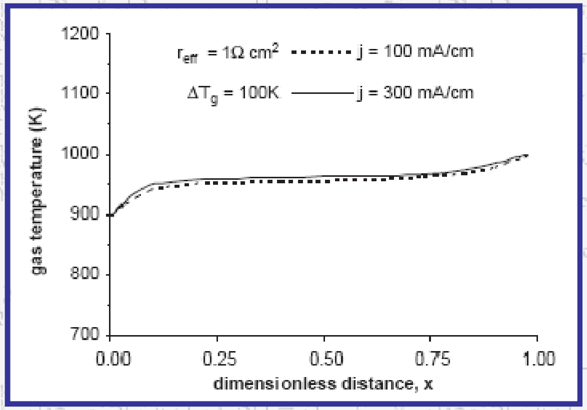
To start with…

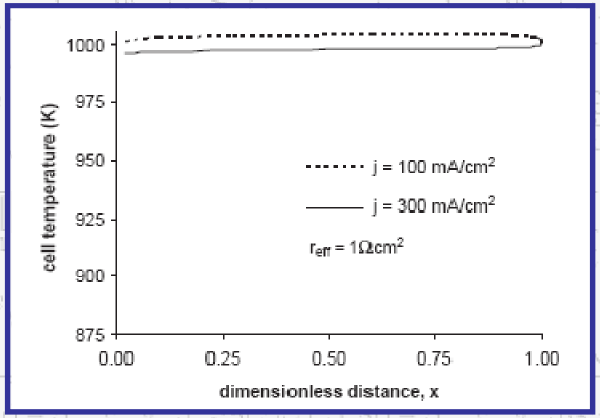
… some general assumptions have to be made:

- feed stream is a mixture very rich in hydrogen (H_2 >90%)
- hydrogen reacts only partially in the catalyst/electrolyte interface
- pressure in both the anode and cathode compartments is equal to 1 atm be simple enough

One-dimensional model:
Assumptions/Considerations

- Mass transport mainly occurs at the direction parallel to the cell axis
- Isothermal conditions





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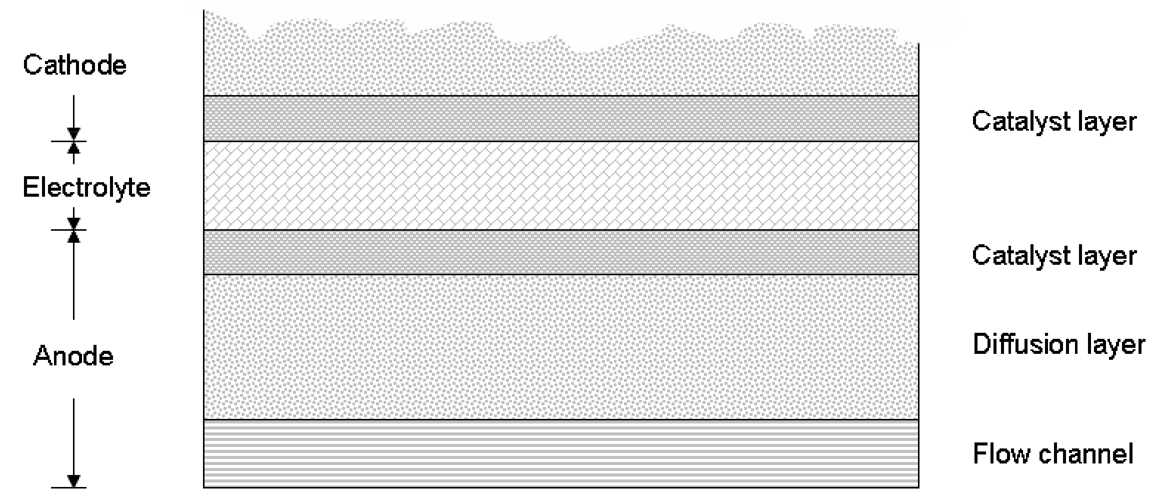
One-dimensional model:

Area of interest



One-dimensional model:

Differential equations

$$D_f^{eff}\frac{d^2C_f}{dx^2}=\left(\frac{I-i}{4F}+\lambda_W^d\frac{I}{F}\right)\frac{dC_f}{dx}+\frac{I}{4F}\left(1-C_f\right)\frac{di}{dx}$$

PEM

$$D_f^{eff}\frac{d^2C_f}{dx^2}=\frac{I-i}{4F}\frac{dC_f}{dx}+\frac{I}{4F}\left(1-C_f\right)\frac{di}{dx}$$

SOFC

Mass transport

$$\frac{d^2i}{dx^2}=\left\{\frac{\gamma}{C_f}\frac{dC_f}{dx}+\frac{4a_aF}{RT}\left[\left(R_m+R_s\right)i-R_sI\right]\right\}\frac{di}{dx}$$

All

Current density

One-dimensional model:

Downgrade technique

$$\frac{dC_f}{dx} = C_f^* \qquad \frac{di}{dx} = i^*$$

transformation

$$\frac{dC_f^*}{dx} = \frac{1}{4FD_f^{eff}}\left[\left(I - i + 4\lambda_W^d I\right)C_f^* + I\left(1 - C_f\right)i^*\right]$$

PEM mass transport

$$\frac{dC_f^*}{dx} = \frac{1}{4FD_f^{eff}}\left[\left(I - i\right)C_f^* + I\left(1 - C_f\right)i^*\right]$$

SOFC mass transport

$$\frac{di^*}{dx} = \left\{\frac{\gamma}{C_f}C_f^* + \frac{4a_a F}{RT}\left[\left(R_m + R_s\right)i - R_s I\right]\right\}i^*$$

current density

One-dimensional model:

Boundary conditions

$$C_f\left(x=0\right)=C_f^{ref}$$

$$C_f^*\left(x=0\right)=0$$

$$i\left(x=0\right)=0$$

$$i^*\left(x=0\right)=0$$

One-dimensional model:
Numerical solution

- Non-linear shooting scheme
- Multidimensional Newton algorithm
- Constant-step mesh
- The resulting nonlinear system of ordinary differential equations was solved by using the 4th order Runge-Kutta method.

Integration by our own FORTRAN code

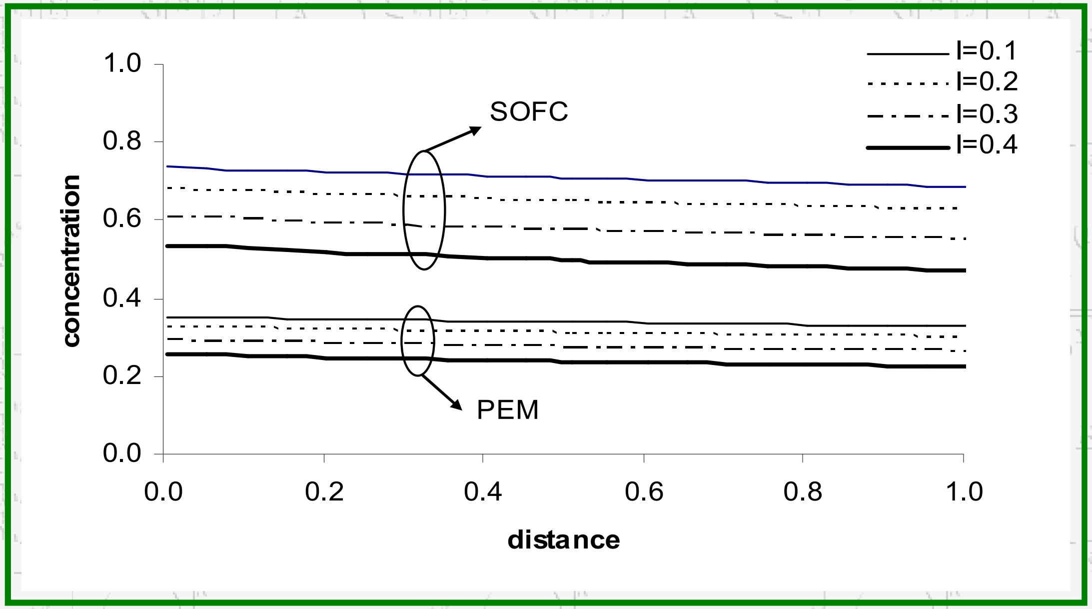
One-dimensional model:

Parameter values

Tafel constant for anode, a_a	0.7
Cell temperature, T (K)	1073 (SOFC) / 373(PEM)
Electro-osmotic drag coefficient of water, λ_W^d	3.16
Order of reaction, γ	0.25
Feed hydrogen concentration, C_f^{ref} (kg)	$3.069X10^{-7}$
Effective diffusivity of hydrogen in catalyst layer, D_f^{eff} (cm^2/s)	$1.9X10^{-6}$
Universal gas constant, R (J/mol K)	8.314
Faraday's constant, F (J/mol V)	96484
Effective ionic resistance in catalyst layer, R_m (Ω/cm)	312.5
Effective resistance of solid phase in catalyst layer, R_s (Ω/cm)	264550.3

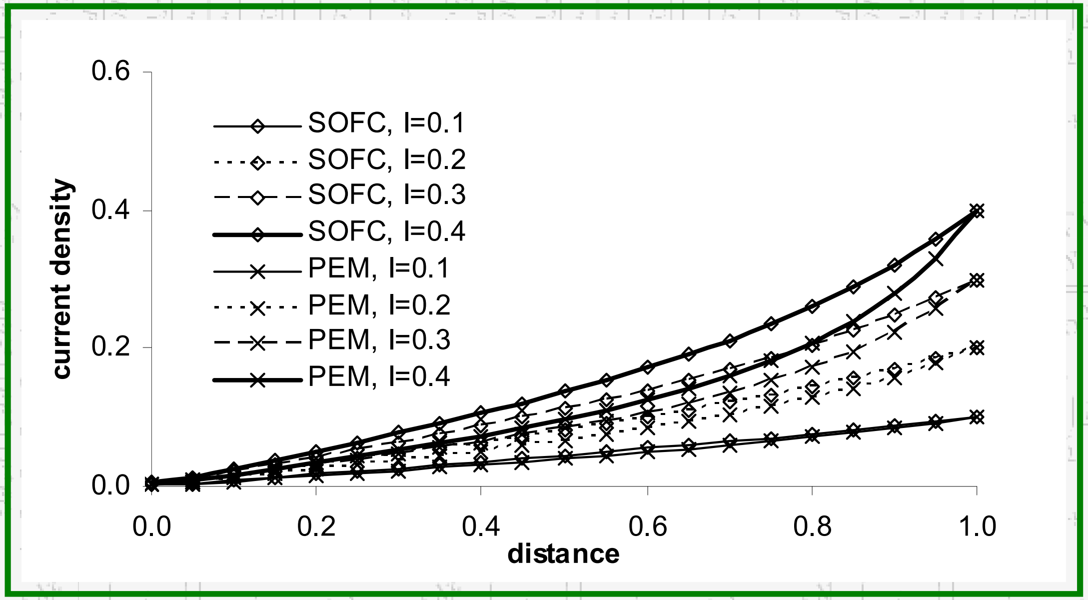
Results:

Hydrogen concentration



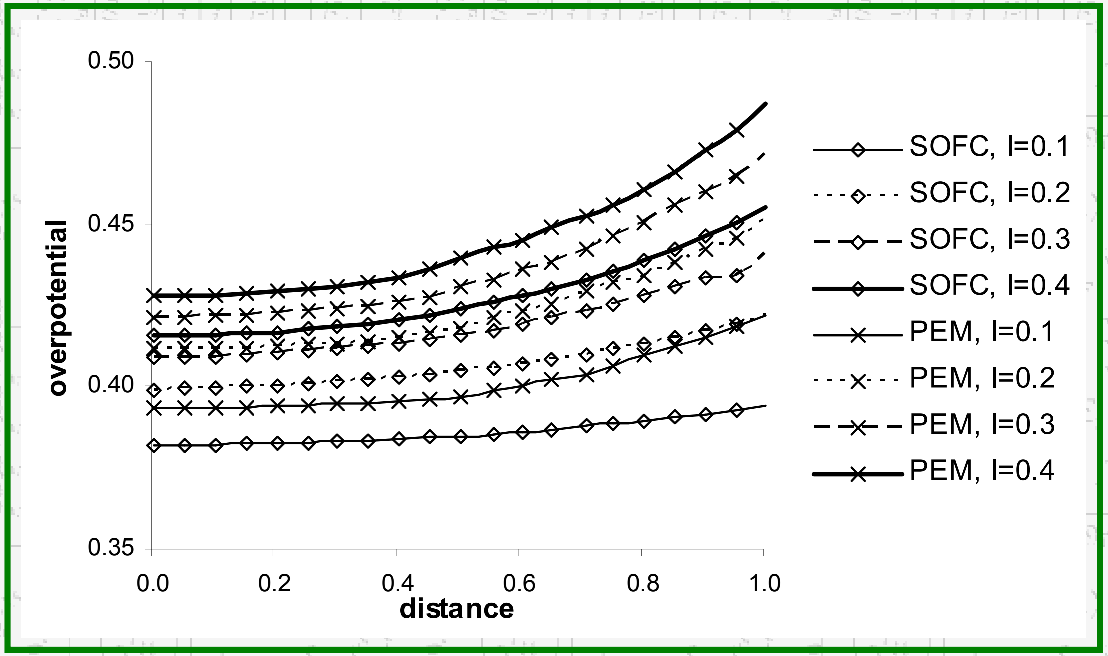
Results:

Ionic current density



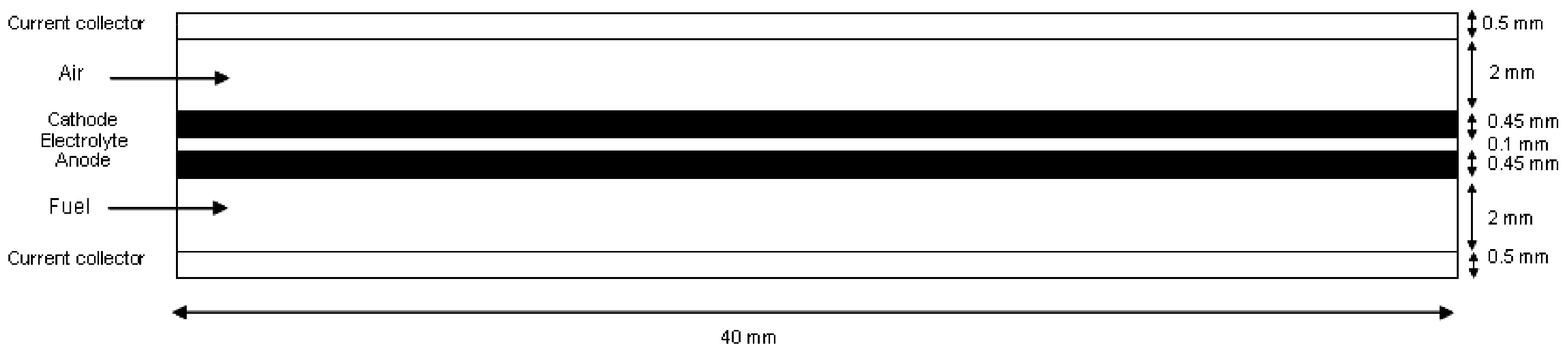
Results:

Overpotential



Two-dimensional model:

Area of interest



Two-dimensional model:
Differential equations

$$\left(\rho \underline{u}\right)\cdot\nabla\underline{u} = -\nabla p + \mu\nabla^2\underline{u}$$ Flow

$$\nabla\cdot\left[\left(\rho c_p T\right)\underline{u}\right] = \dot{Q} + \nabla\cdot a\nabla\left(\rho c_p T\right)$$ Heat

$$\underline{u}\cdot\nabla C_i - \nabla\cdot\left(D_{i,mix}\nabla C_i\right) = 0$$ Mass

$$i = i_0\left[\exp\left(\frac{a_a F}{RT}\eta\right) - \exp\left(-\frac{a_c F}{RT}\eta\right)\right]$$ Charge

Two-dimensional model:

Boundary conditions

- Constant mass flow rates at anode & cathode
- Fixed pressure (1 atm)
- Fixed temperature
- Voltage (0.73 V)
- Wall BCs

Two-dimensional model:
Numerical solution

- Finite volume method
- The four problems are solved as coupled

Integration by commercial software package CFD-RC©

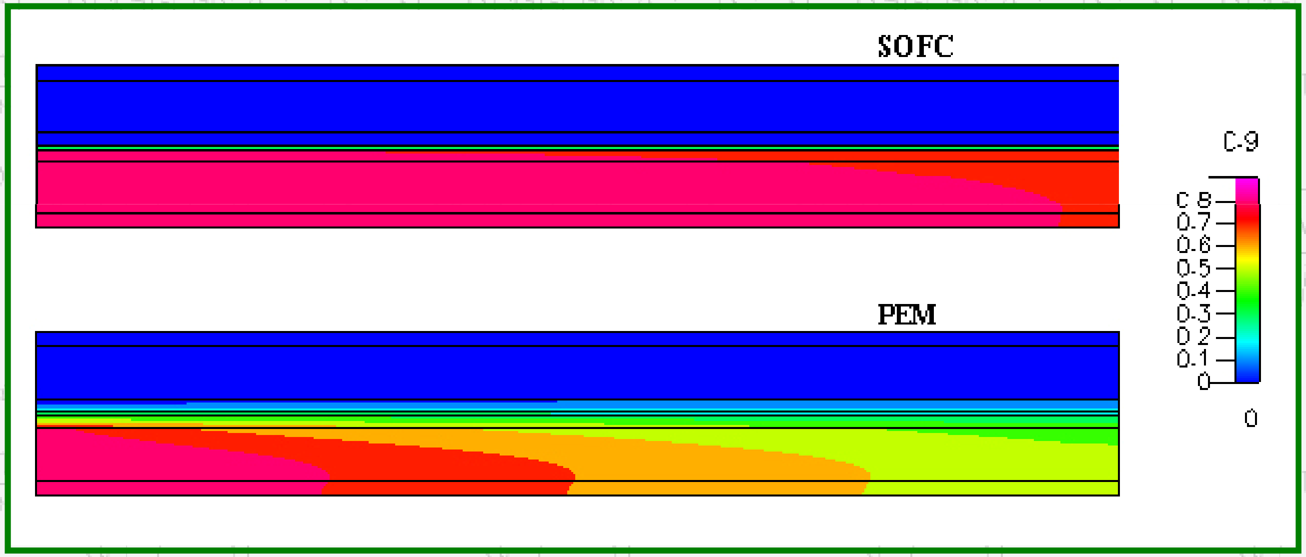
Two-dimensional model:

Parameter values

Density, ρ (kg/cm^3)	Calculated by CFD-RC© using Ideal Gas Law
Kinematic viscosity, ν (kg/cm s)	Calculated by CFD-RC© using Mix Kinetic Theory
Specific heat, c_p (J/kg K)	Calculated by CFD-RC© using JANNAF model
Diffusion coefficient, $D_{i,mix}$ (cm^2/s)	Calculated by CFD-RC© using Schmidt number (=0.7 for each species)
Exchange current density, i_0 (A/cm^3)	1X10^8
anodic charge transfer coefficient, a_a	0.7
cathodic charge transfer coefficient, a_c	0.7

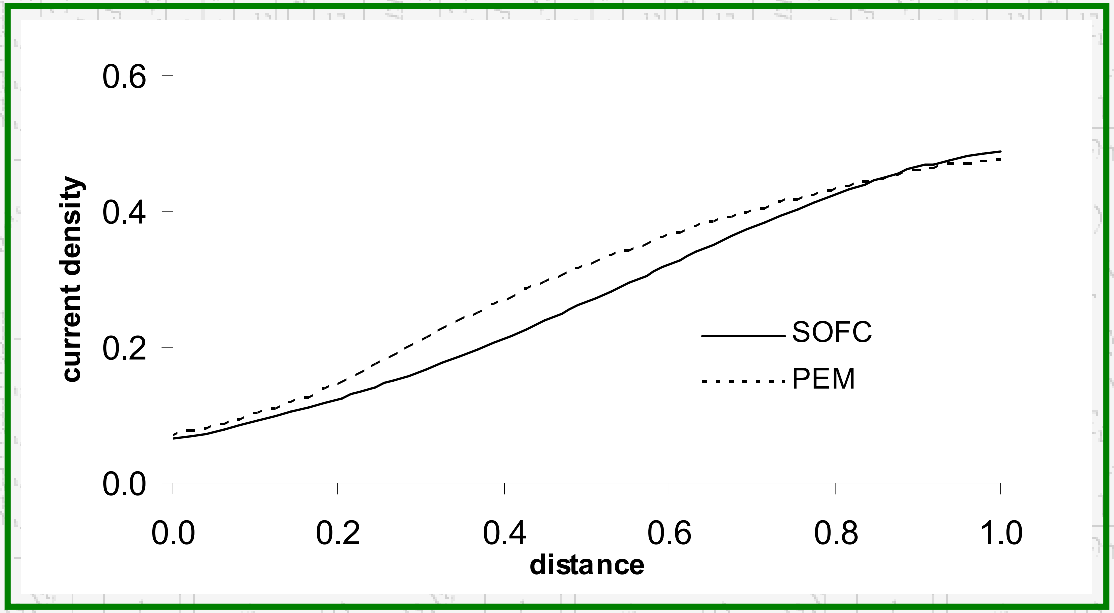
Results:

Hydrogen concentration



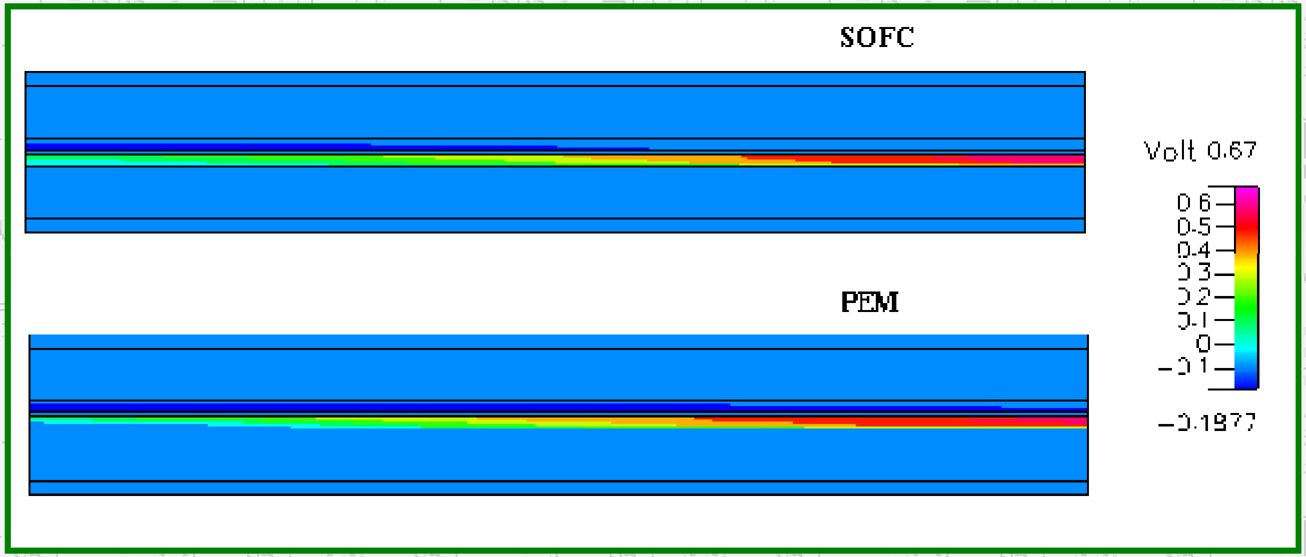
Results:

Ionic current density



Results:

- Overpotential



Summary:

- Two approaches (1-D and 2-D) and two types of fuel cell (SOFC and PEM) have been adopted
- Both models describe adequately the operation of a fuel cell in terms of feedstock concentration and overpotential produced
- A slight advantage of SOFC has been underlined compared with PEM

Conclusions:

- A slight advantage of SOFC has been underlined compared with PEM
- The 2-D model presented unexpected molar fraction profiles due to incomplete incorporation of physical properties of materials

We are working on a more detailed 3-D approach !!!

Thanks to …

- Mrs. Eleni Vakouftsi for her technical assistantship in CFD-RC© issues
- Mr. Dimitrios Sarantarides for some fruitful discussions on the topic

- **all of you for your attention**