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Dynamic simulation of molten carbonate fuel cell power plant in the FellowSHIP project

FC-tools conference,
Trondheim 2009

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Why model fuel cells?

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•Increase safety and reliability for ship owners by writing better rules
•Help manufacturers design for marine environment

The expertise DNV gains by creating and using models will help in making better rules for minimizing risk, increasing reliability and efficiency optimization.

RULES FOR
CLASSIFICATION OF

SHIPS

NEWBUILDINGS

SPECIAL EQUIPMENT AND SYSTEMS
ADDITIONAL CLASS

PART 6 CHAPTER 23

FUEL CELL INSTALLATIONS

JULY 2008

CONTENTS PAGE

9-2010

2008-2009

Ben
onsh
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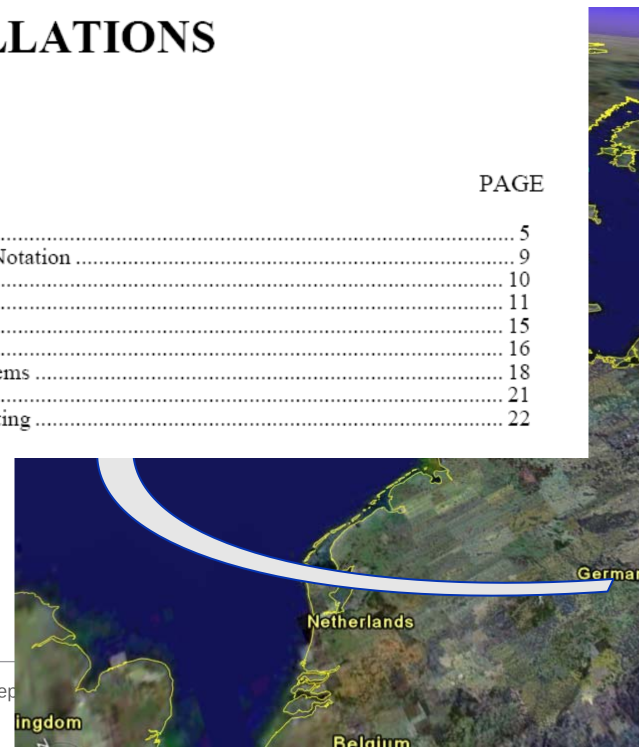
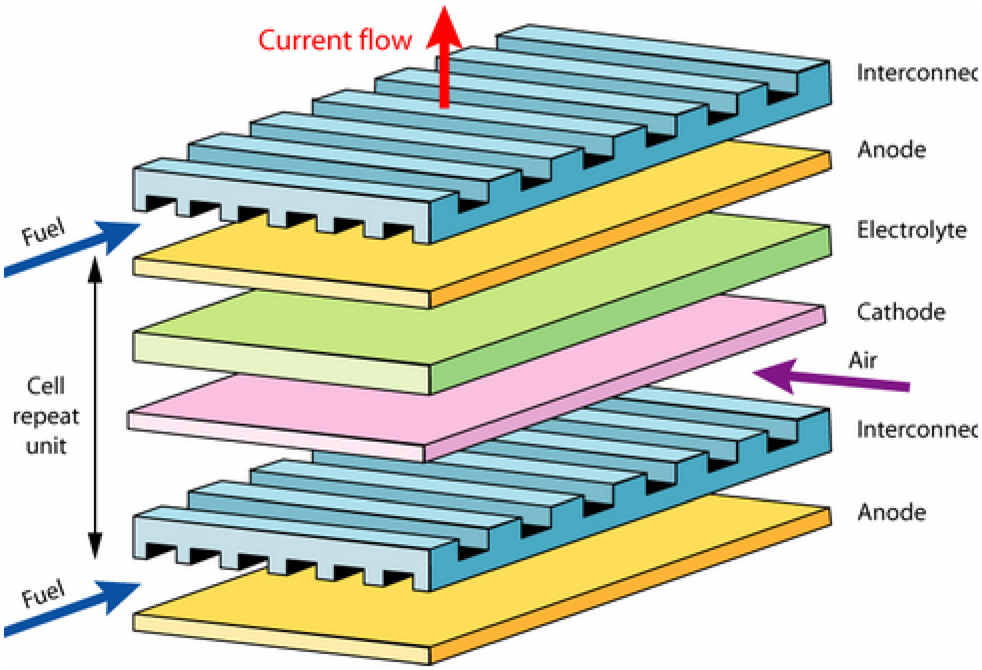


FC manufacture (2008)

The cell is a cross-flow molten carbonate fuel cell, which we model as consisting of three layers to achieve short enough solution times.



- Temperatures
- Gas flows
- Heat conduction
- Heat convection
- Chemical reactions
- Voltage and current

http://www.doitpoms.ac.uk/tlplib/fuel-cells/printall.php

The status of the modelling:

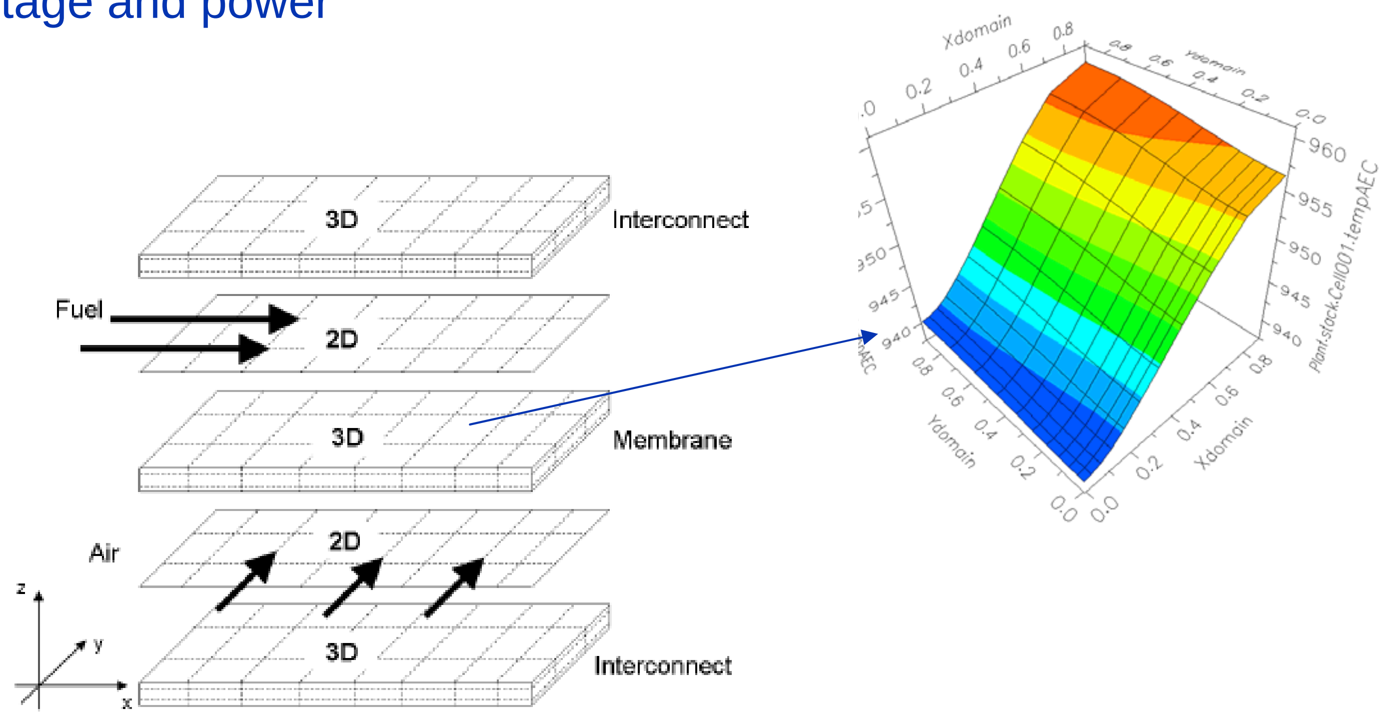
We have a model of the cell itself

i) With temperature distributions

ii) Fuel and air gas compositions

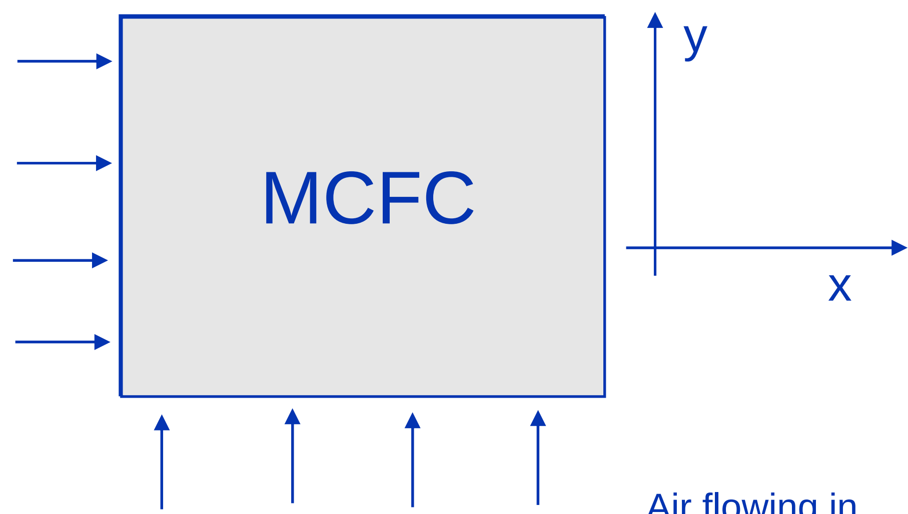
iii) Chemical reactions

iv) Electric current, voltage and power



We model the gasses as flowing in one direction in two-dimensional layers, neglecting both depth and the channel structure.

Fuel flowing in
x-direction



Air flowing in
y-direction

The conservation of mass leads to the convective flow of molar density, c_i , for each chemical specie, below is the case with no chemical reactions for species *i* in the fuel flow with speed *u*

$$\frac{\partial c_i}{\partial t} + u \frac{\partial c_i}{\partial x} = 0$$

For the case of hydrogen in the fuel we have three different reactions leading to change in the concentration

$$\frac{\partial c_{H_2}}{\partial t} + u \frac{\partial c_{H_2}}{\partial x} = -r_{electrochemical} + 3r_{ref-CH_4} + r_{ref-CO}$$

The chemical reactions are described by empirical equations taken from literature.

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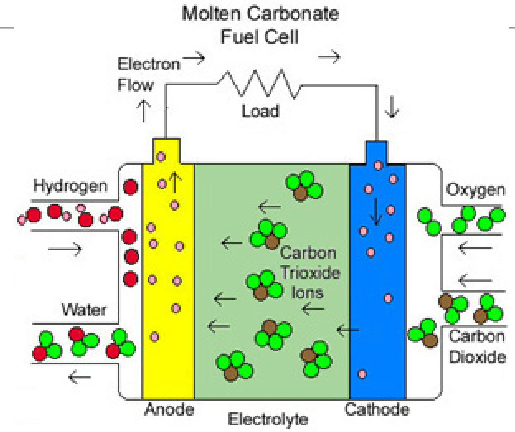
$$r_{electrochemical} = \frac{I}{2F}$$

current

Faraday constant



$$H_2 + CO_3^{2-} \rightarrow CO_2 + H_2O + 2e^-$$

$$\frac{1}{2}O_2 + CO_2 + 2e^- \rightarrow CO_3^{2-}$$

The current is proportional to the reaction rate of the electrochemical reaction.

$$r_{ref-CH_4}$$

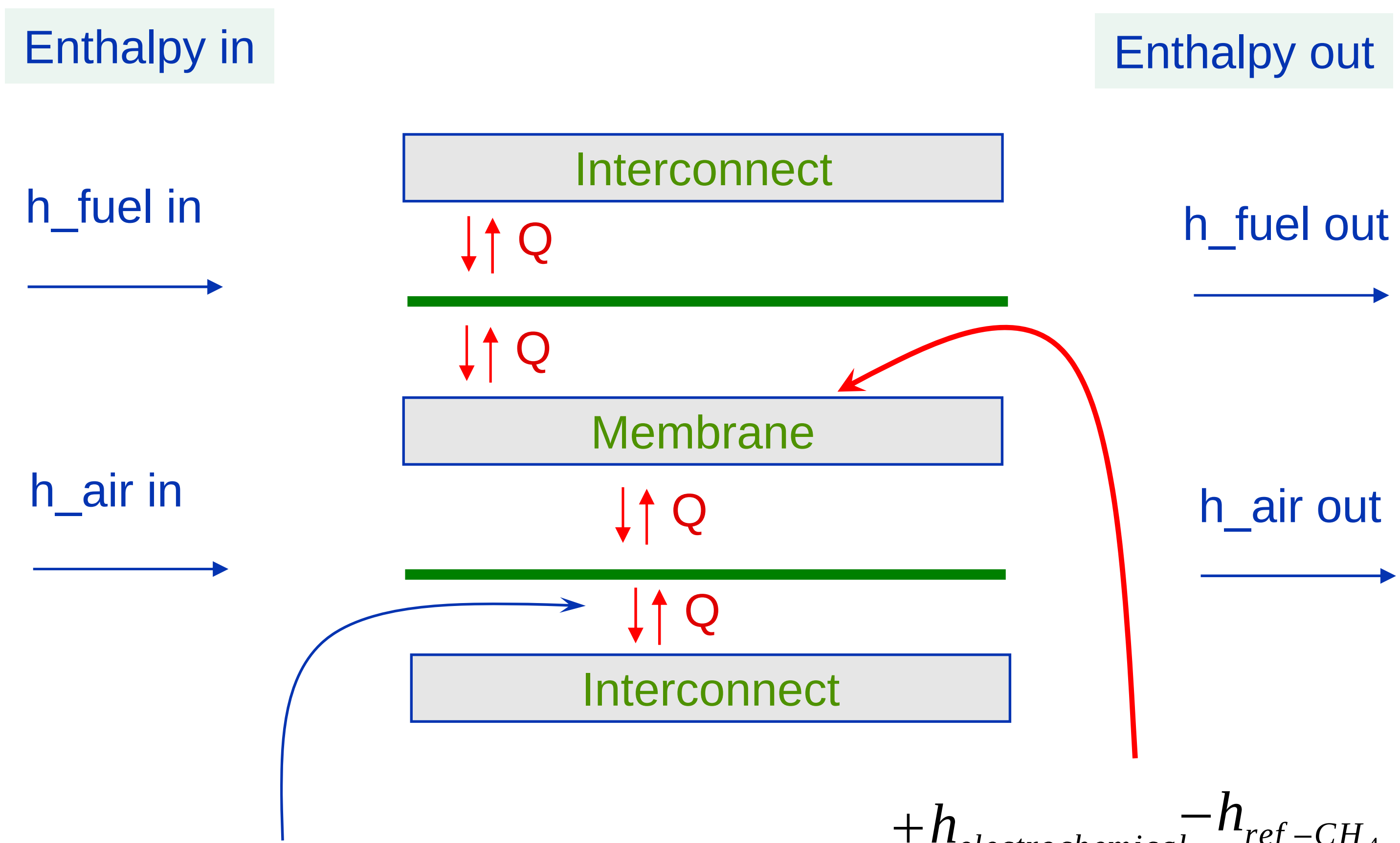
$$CH_4 + H_2O \Leftrightarrow 3H_2 + CO$$

The models for the reforming reaction rates are taken from Sundmacher et al. ”Molten carbonate fuel cells – modeling, analysis, simulation, and control” 2007, p231

$$r_{ref-CO}$$

$$CO + H_2O \Leftrightarrow H_2 + CO_2$$

Energy conservation leads to the equations for the temperature of the two-dimensional gas layers, the three dimensional ”solids” and the heat flows.



$$+h_{electrochemical} - h_{ref-CH_4} + h_{ref-CO}$$

Heat flows between gas and solids through convective heat transfer

The heat from the chemical reactions is deposited or taken from the top of the membrane, the solid approximating the anode, electrolyte and cathode.

The heat transfer is modelled using convective heat transfer between gas and solid, convective heat transport in the gas and heat conductance in the solid.

Fuel gas with no external heat coming in or out, just the transport through the flow.

$$\rho c_P \left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} \right) = 0$$

Fuel gas with heat flowing into/from the membrane and the upper interconnect

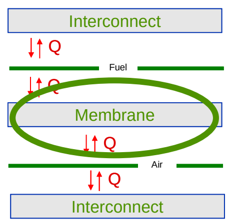
$$\rho c_P \left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} \right) = -h_m (T - T_m) - h_{IC} (T - T_{IC})$$

The convective heat transfer coefficients, *h*, are dependent on the geometry of the cell, and data on these will be important for a model to realistically depict a given cell.

- Gas channel width, height, number.
- Shape of channels.

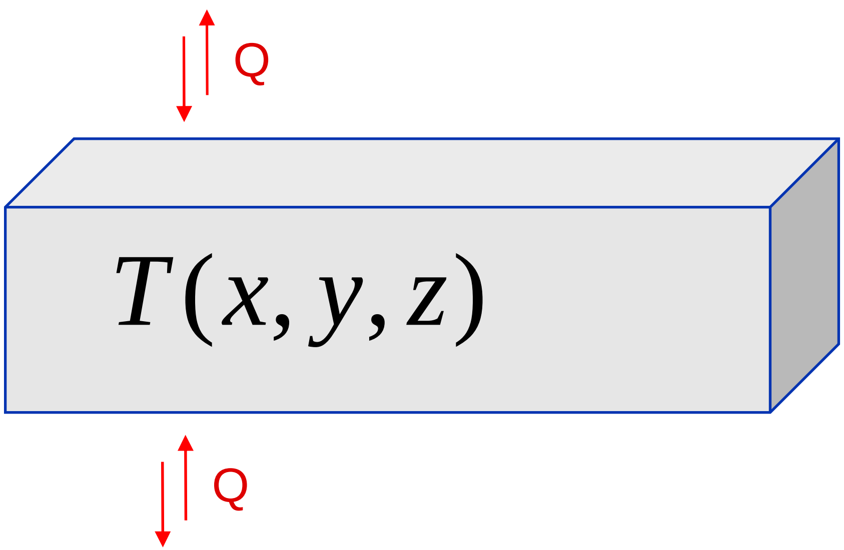
The fuel only flows in the x-direction, therefore we only include the derivative with regards to x. The air only flows in the y-direction, so for the air gas we use the derivative with regards to y.

We model the anode/electrolyte/cathode membrane as a solid, with the same thermal conductivity and heat capacity for all parts of the membrane.



The heat equation determines the heat flow within the solid

$$\rho c_P \frac{\partial T}{\partial t} = -k \nabla^2 T$$



Heat flowing in and out of the solid are governed by boundary conditions

The gPROMS tools combines an equation based solver with graphical connections between components.

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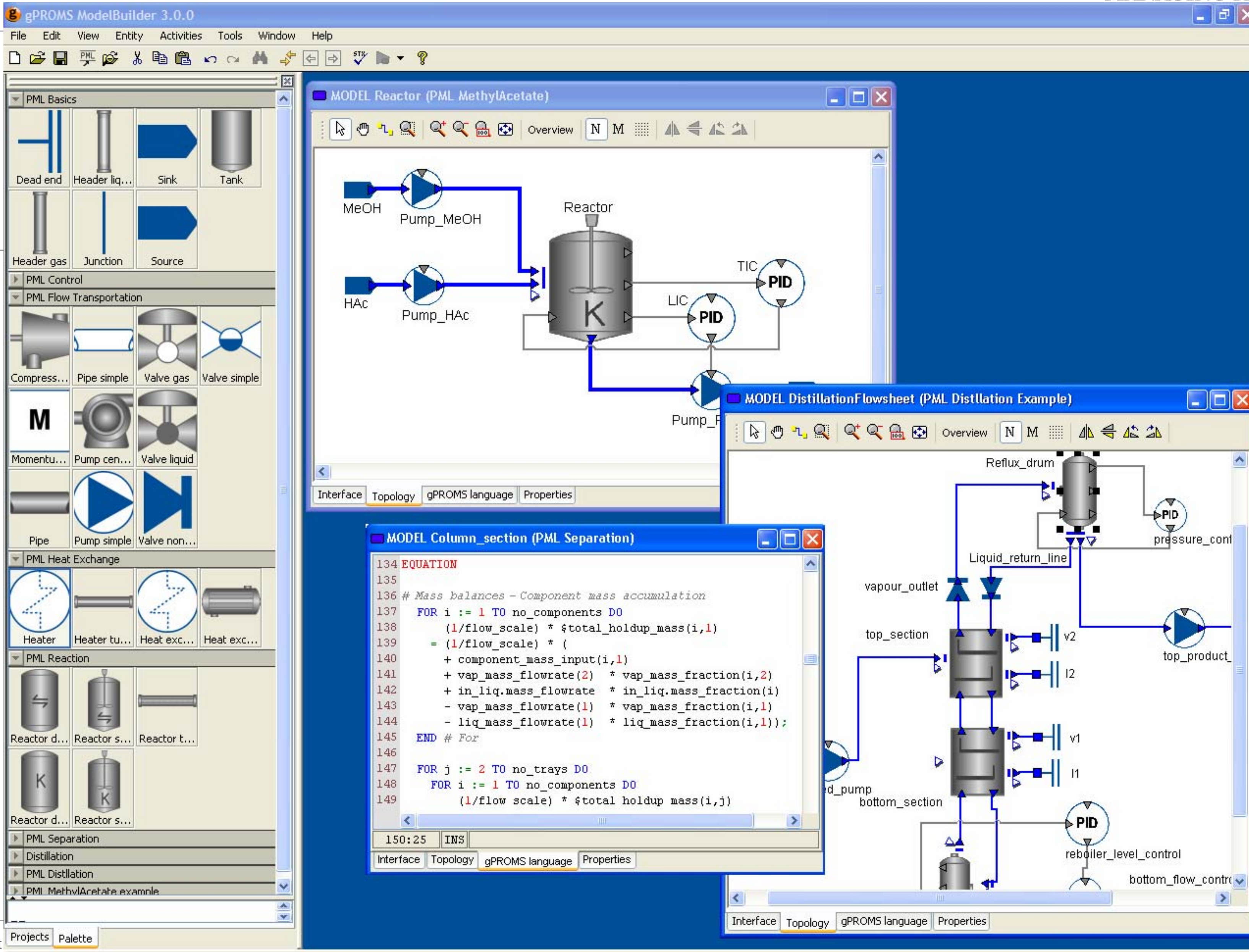
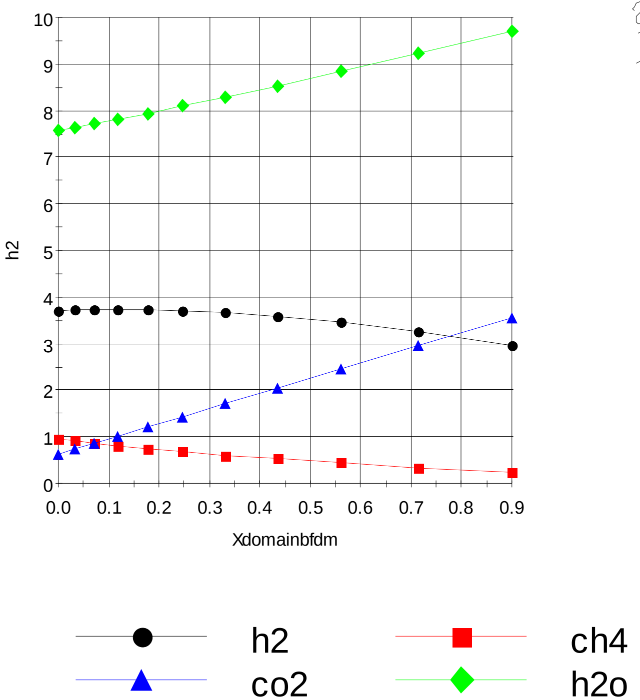
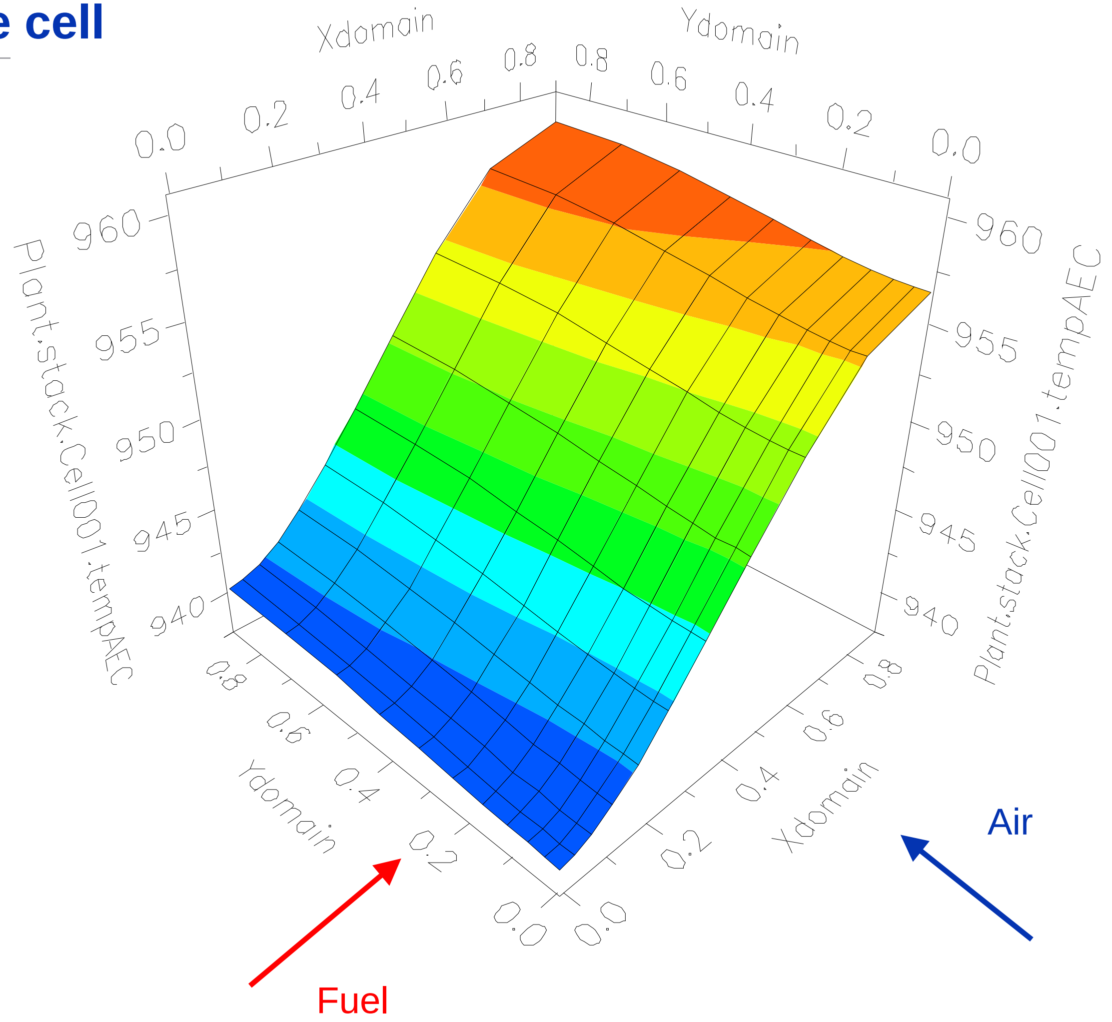


We can use the model to look at the gas composition and temperature distribution inside the cell





A steady-state performance map can be generated to illustrate system performance for different control parameters.

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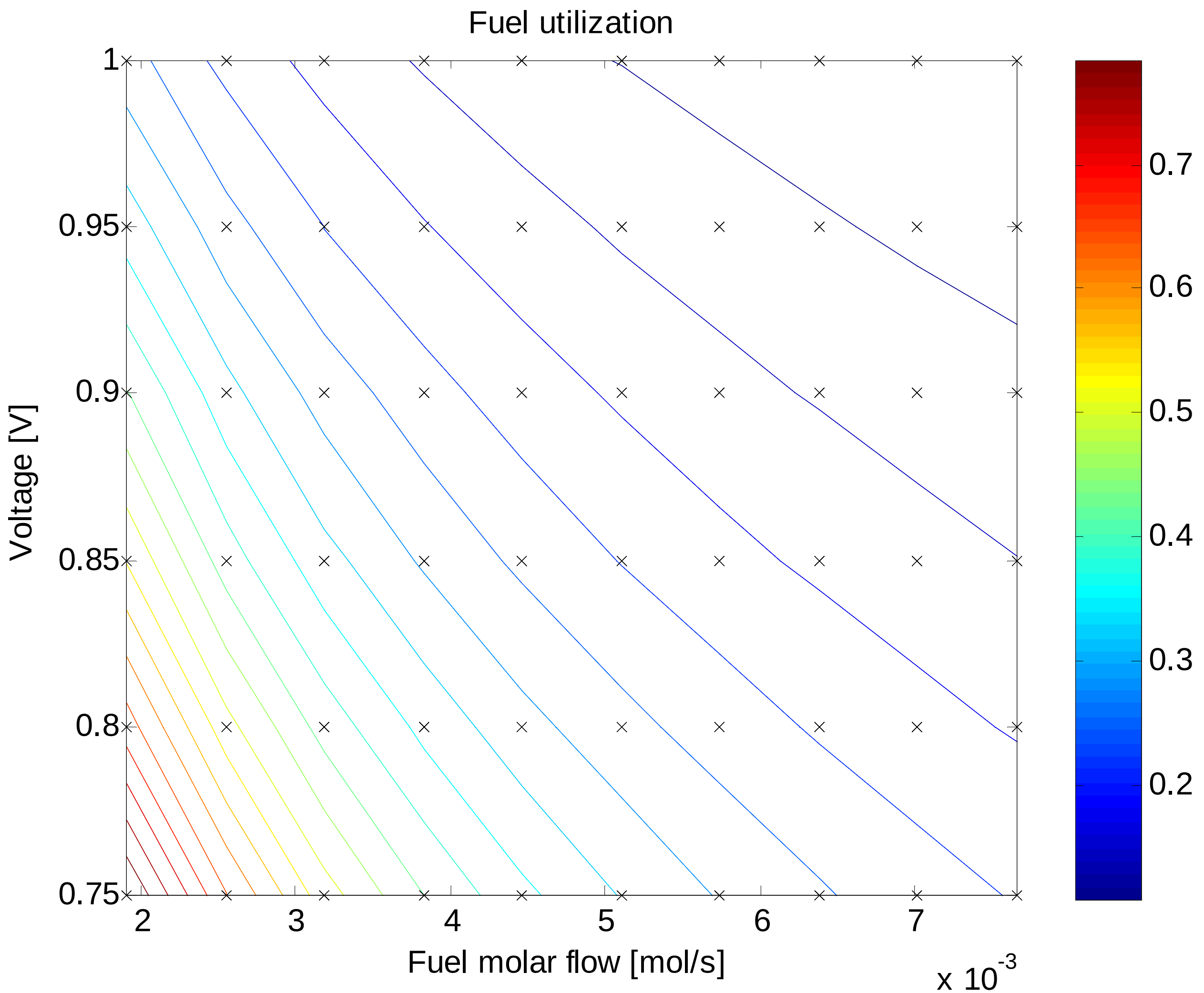

Transient simulations between different steady-state running points can be used to find the optimal ways of changing load.

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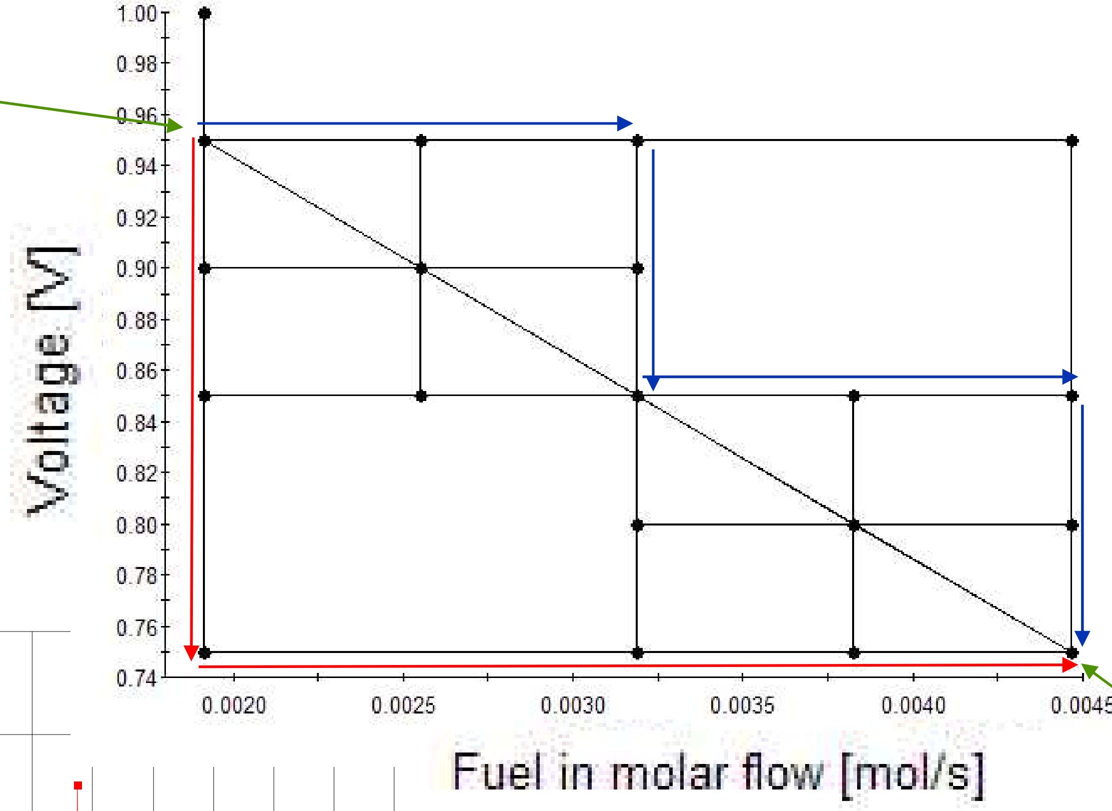
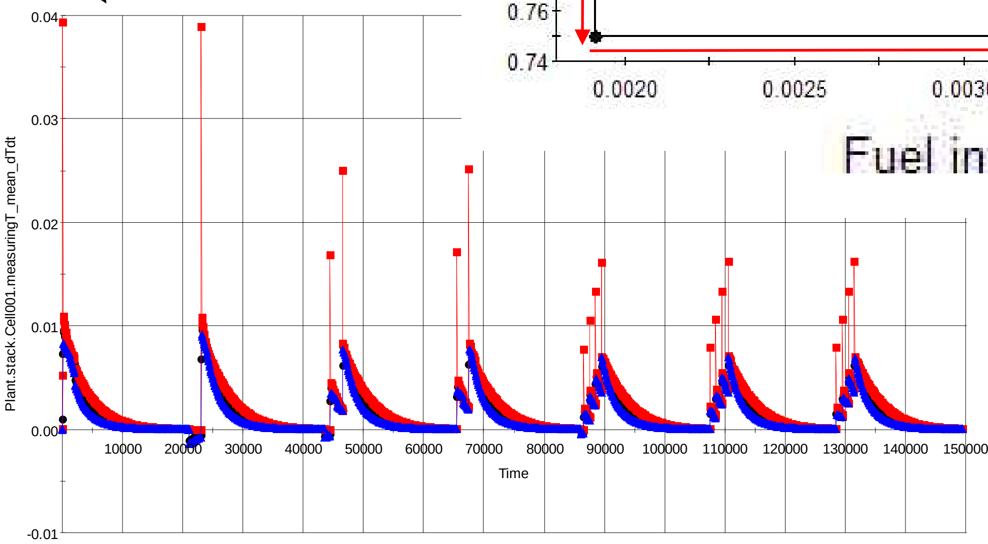


Starting state

End state

$$\frac{\partial T}{\partial t}$$



7 different paths from start state to end state

Simulations can be used to help introduce more environmentally friendly power generation systems

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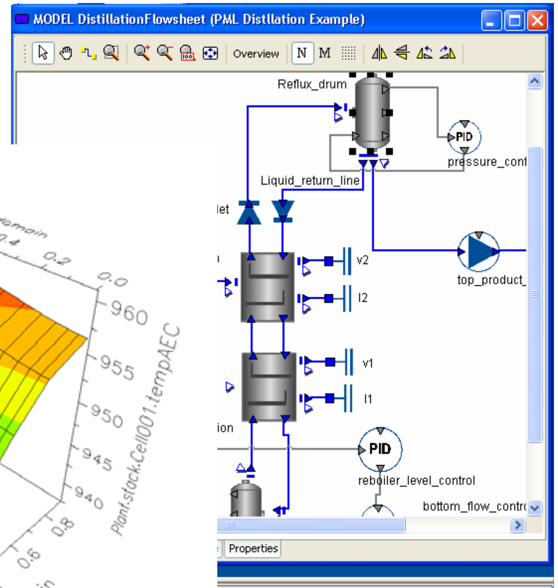

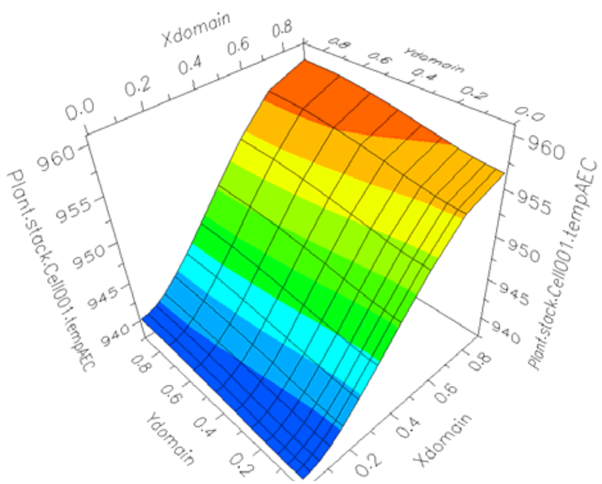

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C.Y. Yuh and J.R. Selman. Polarization of molten carbonate fuel cell electrodes ii. characterization by ac impedance and response to current interruption. *Journal of the Electrochemical Society*, 138(12):3649 – 365, 1991.