Project Report
2008 MVK160 *Heat and Mass Transport*
May 02, 2008, Lund, Sweden

Transport in the porous electrodes in SOFC's

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ABSTRACT
Today the new energy sources become more important, one of these are the fuel cells. There is lots of research in fuel cell technology, how to make them more efficient is one big question**.** Simulation and modeling of the fuel cells are often used in the research. New and better models are made to make the results more accurate, both for commercial codes and for other applications.

This report shows how the transport in the porous media is simulated and what results can be found by that.

NOMENCLATURE
c_i	mass fraction of species *i*
C	total molar concentration
$D_{i,j}$	binary diffusivities
$D_{i,k}$	Knudsen diffusion coefficient for species *i*
$D_{i,\ mixture}$	diffusivity of species *i* in the mixture
e	gas internal energy
h_i	convective heat transfer coefficient of species *i*
$\vec{J}_i$	diffusive mass flux of species *i*
k_{eff}	effective thermal conductivity
$\vec{N}_i$	molar flux density of species *i*
N_j	molar fluxes of other species, from *j* to *n*
p	fluid pressure
S_{rad}	energy due to radiation term
$S_{i,j}$	additional species sources
S_e	energy due to source term
t	layer thickness
T	reaction temperature
V	velocity
$\boldsymbol{V}$	velocity vector
X_i	concentration of species *i*

Greek Symbols
ε	porosity
ρ	fluid density
ζ	shear stress tensor of the fluid
μ	fluid viscosity
κ	permeability

Subscripts
CH_4	methane
CO	carbon monoxide
CO_2	carbon dioxide
g	gas properties
H_2O	water
H_2	hydrogen
s	solid properties

INTRODUCTION
With the energy use today and the problems with carbon dioxide the world needs a new better way to produce energy. One way to do this is with fuel cells. There are different kinds of fuel cell, both high and low temperature. One kind is the high temperature solid oxide fuel cell, the SOFC.

PROBLEM STATEMENT
The most important part in producing energy trough an electrolytic process is the diffusive flow in the porous electrodes, see Figure 1.

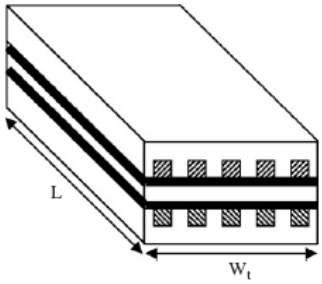

Figure 1: Schematic picture of a SOFC [2]

The transport in the porous electrodes can be described as a two phase flow with chemical reactions; this makes both the heat and the mass transfer solving a bit more complex. The heat transfer is quite the same as for gas flow channel problems, but there are some differences, due to the chemical reactions.[1]

For the transport there are some important things to take in to consideration. While there is a two phase flow the conservation law must be written for both phases. The governing equations for the transport are:[2]

The conservation of mass

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \nabla \cdot (\rho\varepsilon V) = 0$$

The conservation of momentum

$$\frac{\partial}{\partial t}(\rho \varepsilon \vec{V}) + \nabla \cdot (\rho \varepsilon \vec{V}\vec{V}) = -\varepsilon \nabla p + \nabla \cdot (\varepsilon \vec{\tau}) + \frac{\varepsilon^2 \mu \vec{V}}{\kappa}$$

The conservation of species

$$\frac{\partial}{\partial t}(\rho \varepsilon c_i) + \nabla \cdot (\rho \varepsilon \vec{V} c_i) = -\nabla \cdot \varepsilon \vec{J}_i + S_{g,i}$$

And the conservation energy

$$\frac{\partial}{\partial t}(\rho \varepsilon e) - \varepsilon \frac{\partial p}{\partial t} + \nabla \cdot \varepsilon \left(k_{eff} \nabla T - \sum_i h_i \vec{J}_i \right) + S_\varepsilon + S_{rad}$$

$$k_{eff} = \varepsilon k_g + (1 - \varepsilon) k_s$$

The different transports in the electrodes and in the electrolyte can be seen in Figure 2 below.

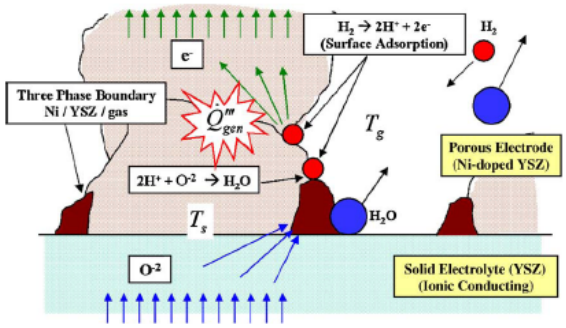

Figure 2: Schematic picture of the transports in the porous electrodes [5]

The channels in the porous media are very small and the velocity is small, laminar flow. This makes the transport dominated by diffusion. There are different ways to take this into the calculation; the most simple is with Fick's Law

$$\vec{N}_i = -C D_{i,j} \nabla X_i$$

$$\vec{N}_i = -C D_{i,mixture} \nabla X_i + \sum_{j=1}^{n} N_j$$

Two other ways to calculate the diffusion is with the Stefan-Maxwell model

$$-\nabla X_i = \sum_{j=1, j \neq i}^{n} \frac{X_j N_i - X_i N_j}{C D_{i,j}}$$

or The Dusty Gas Model

$$-\nabla X_i = \frac{N_i}{D_{i,k}} \sum_{j=1, j \neq i}^{n} \frac{X_j N_i - X_i N_j}{C D_{i,j}}$$

The last important thing to take into consideration is the chemical reactions. SOFC's are able to work with different fuels, one common fuel is methane. The chemical reactions will then be:[4]

$$CH_4 + H_2O \rightarrow 3H_2 + CO$$
$$H_2O \mid CO \rightarrow H_2 \mid CO_2$$

SOLVING TECHNIQUES

There are several ways to solve the governing equations, all numerical. There are three very often used; FDM (FDM = finite difference method), FVM (FVM = finite volyme method) and FEM (FEM = finite element method).[4]

These three are all alike, with some small differences. The main idea is to divide the computational domain into smaller ones for which the governing equations are solved numerically with, for example, TDMA.

MODELLING

When modelling the flow in the SOFC, it's possible to choose from 0- to 3-dimentional modelling. Depending on what result is needed.

0-D modelling

The modelling of a SOFC with zero dimensions is often used when not interested in the flow. This modelling gives the result for output power and cell voltages. It could also give the cell efficiency for different temperatures.

1-D modelling

One dimension modelling means taking two dimensions out of calculation. When doing this all properties of the fluids and the electricity must be considered uniform in these two dimensions. With this simple modelling the temperature, gas composition and density can be given.

2-D modelling

Two dimension modelling is the same as one modelling but just taking one dimension out of calculation. The same things as for the one dimensional modelling could be modelled.

3-D modelling

The three dimensional modelling is the most complete model. This gives a very detailed model of the SOFC. For the modelling commercial software is used, for example, FLUENT or STAR-CD. This model can calculate all the changes in gas composition, temperature changes, properties variation for both electricity and fluid.

LITERATURE SURVEY

Lots of research has been done on the SOFC, but with different points of view. This could be divided into three parts, the flow

and the temperature field modeling, electrochemical modeling and the modeling of chemical reactions.

The SOFC can also have different air and fuel flow systems, cross-flow, co-flow or counter-flow.

Haberman, B.A. and Young, J.B [3] have made a 3-dimensional numerical simulation on a cross-flow IP-SOFC (IP=inter planar), see Figure 2.

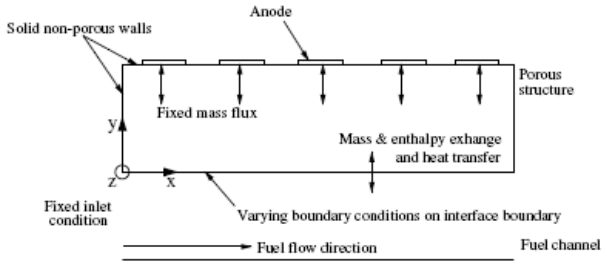

Figure 3: Transports in an IP-SOFC [3]

They got results for velocity-, temperature and pressure, but also for the reactions in the porous media. As can be seen in Figure 4 and Figure 5 the temperature distribution and the rate of hydrogen production in the porous electrodes quickly decrease after the first anode.

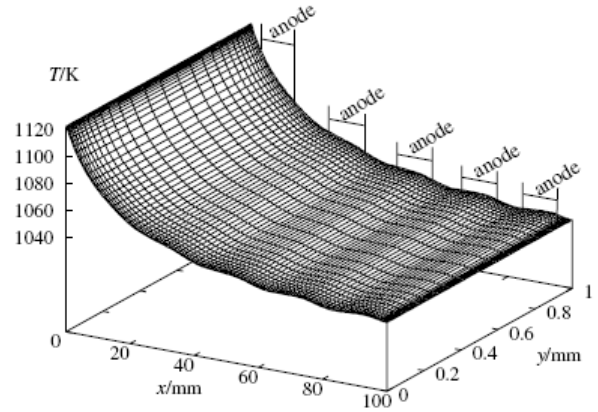

Figure 4: Temperature distribution [3]

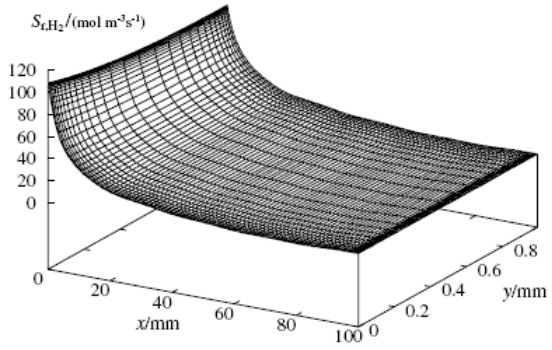

Figure 5: Rate of hydrogen production [3]

Tanaka, T., Inui, Y., Urata, A. and Kanno, T. [7] have made a numerical simulation of the influence of the thermal radiation from the outside of the co-flow SOFC in Figure 6. The boundary conditions and the other important facts for their study can be seen in [6].

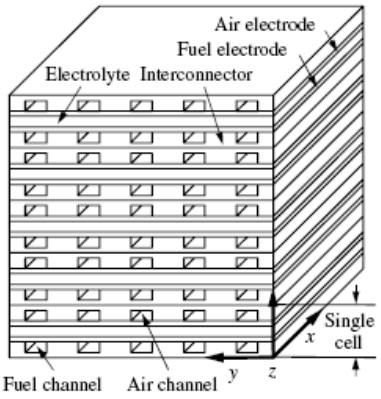

Figure 6: Schematic picture of the domain for Tanaka et al. [6]

Their result shows that the influence of thermal radiation is very big at the surfaces of the stack but much smaller in the middle; the temperature distribution for the y-z plane can be seen in Figure 7 below.

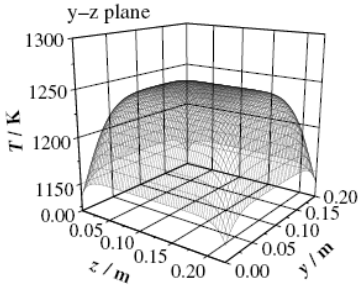

Figure 7: Temperature distribution in the y-z plane [6]

Tanaka et al. also compared the voltage output for the cell for two different ambient temperatures, 1123 K and 1223 K. The result is to be seen in Figure 8.

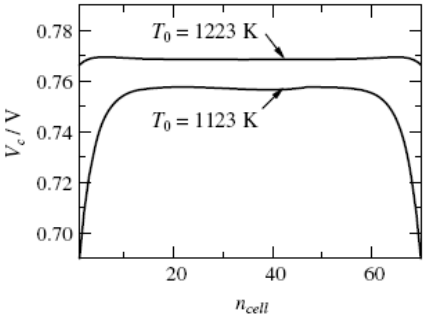

Figure 8: The voltage output for different ambient temperature [6]

CONCLUSIONS

A comparison of Figure 4 and Figure 5 it is seen that the temperature decrease with the decreasing production of hydrogen. The chemical process turning oxygen and methane into hydrogen and carbon dioxide releases lots of heat. When the fuel starts to run short, because of the process, the less hydrogen is produced and the less heat is produced.

In Figure 8 I can be seen that the ambient temperature has a strong influence on the fuel cells performance; a low ambient temperature affects the fuel cell more than a high.

The fuel cell is made of ceramic material with low thermal conductivity. The low thermal conductivity prevents the low outside temperature to force into the fuel cell. The thermal radiation of the ambient conditions could therefore be considered non influent.

REFERENCES

[1] Heat and Mass transfer, ch.13, Divison of Heat Transfer, LTH

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