Flow field analysis of fuel cells to determine temperature distribution and heat dissipation

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Introduction

The increasing demand for more efficient cooling options in the fields of fuel cell mobility and power electronics motivates for the development of novel cooling strategies with improved heat transfer. Forced convection of liquids is a common cooling method and allows high temperature gradients between the heat source and the coolant to be maintained, thus achieving a high heat transfer rate. By using a liquid with a low boiling point, additional thermal energy can be removed from a system by an intended phase transition. With the ambition to increase the lifetime and power density in fuel cell systems, cooling by evaporation is a suitable approach. In this context, the phase transition behaviour into the internal structure of bipolar plates as a central functional element for cooling in a fuel cell must be understood and designed.

In this paper, a model geometry for the study of fluid dynamics and temperature distribution in a section of a fuel cell concept, called bipolar plate, is described. Thereby, the paper pursues the approach to evaluate the temperature distribution and heat dissipation in the bipolar plate that is focused on simulating a sequence of 12 periodic cell elements in a row. The cell element is defined by the smallest geometric shape that can be mapped periodically in x-, z-direction to generate the full structure of a bipolar plate flow field. Phase transition of ethanol used as a cooling medium is considered with the aim to represent an evaporative cooling system. The described approach uses the modules turbulent flow L-VEL (spf) and heat transfer in fluids (ht). The spf is solving for the flow field and the ht for the temperature distribution in the bipolar plate models.

The flow pattern and temperature distribution provide information about the potential of the regarded cooling strategy and about the layout of the bipolar plate system for effective cooling. The results of the simulations will help to design an efficient evaporative cooling system for high performance fuel cells.

Geometry

In this simulation, a small area of the fuel cell where the coolant flows through is investigated. The geometry of this small area is built from a step file out of CAD and is completed as a periodic cell element in COMSOL Multiphysics. This is done to prevent any thin geometric interfering at touching boundaries. The periodic element is shown in Figure 1.
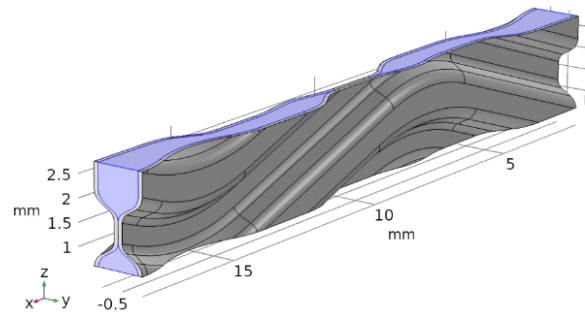

Figure 1. Example of the periodic cell element

The periodic element has a width of 16 mm, a height of 2.15 mm and a thickness of 1.2 mm. The solid part, the bipolar plate, is shown in grey colour with a material thickness of 0.1 mm and the fluid part in blue colour. The periodic element can be mapped in x- and z-direction to create the full-size flow field of a fuel cell. Mapping periodic elements allows quick changes in the size of the resulting geometry and thus helps to limit the required resources for the simulation. For the simulation of the temperature distribution and the heat dissipation in the flow field of the fuel cell, 12 periodic elements are mapped in a row in z-direction.

Material

The material of the bipolar plate is defined to be steel AISI 4340 and the fluid is defined as ethanol. Ethanol has its boiling point close to the desired fuel cell operating temperature of 353.15 K. To avoid convergence problems during the simulation of phase change of ethanol due to inconsistent material properties, a so-called pseudo fluid was created. [1] In this context, a pseudo fluid is a material that is continuously defined as a function of temperature in the liquid and gas area. The material properties change over the range of 1.5 K from liquid to gas with the help of separately created functions.

COMSOL Multiphysics provides various types of functions under the definition node to define the material parameters. The function types step, interpolation, piecewise and analytic are used in this simulation. For the material properties density $rho(T)$, dynamic viscosity $eta(T)$ and thermal conductivity $k(T)$, the characteristic curves of the properties before and after the phase transition are interpolated. The values are given by the material library in COMSOL Multiphysics for the single-phase material of ethanol. A step function is used to couple the functions which define the material properties for the gaseous

as well as the fluid area. The smoothing factor enables a smooth transition between the material functions and the step function which leads to a good convergence of the results.

For each of the three material properties mentioned before, two interpolation functions and one step function are merged by a piecewise function. This creates a continuous function that describes the material properties in the liquid, gaseous and transition areas at the constant pressure of 1 atm. The defined material functions of density, dynamic viscosity and thermal conductivity are shown in Figure 2 to Figure 4. Area I is the liquid phase, area II the transition area and area III the gas phase.
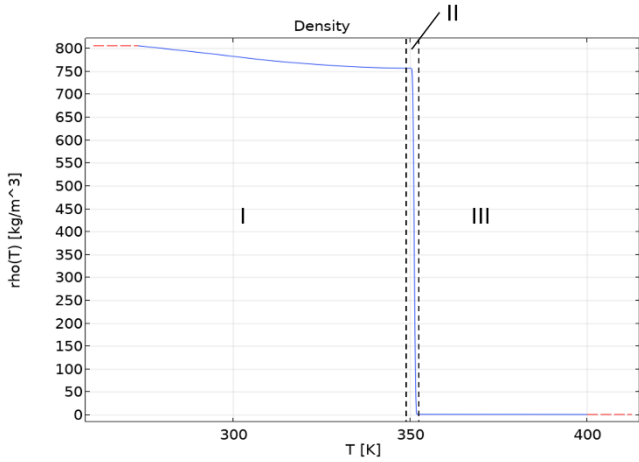

Figure 2. Density of ethanol as a function of temperature

With increasing temperature, the density of ethanol is slightly getting lower until 350.4 K. At this point the density drops in the range of 1.5 K from 756.4 kg/m³ to 1.65 kg/m³. This is the transition area from liquid to gas. From 351.9 K the density slightly decreases.
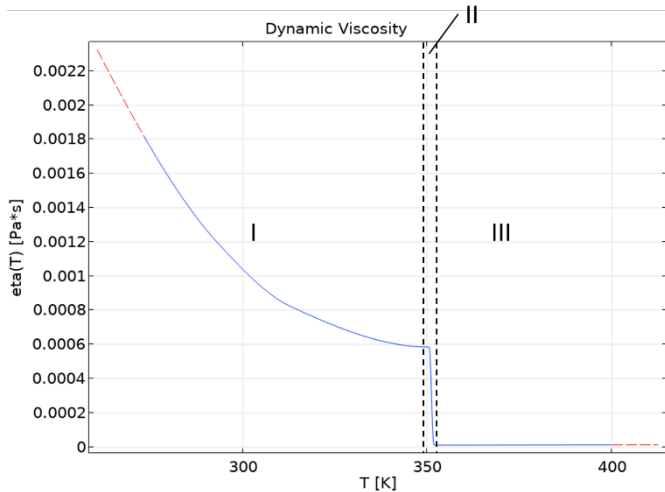

Figure 3. Dynamic viscosity of ethanol as a function of temperature

The dynamic viscosity of ethanol is lowering fast with increasing temperature until 350.4 K. At this point the dynamic viscosity drops in a range of 1.5 K from $5.8e^{-4}$ Pa·s to $1e^{-9}$ Pa·s. For the rest of the defined area it stays constant with increasing temperature.

The thermal conductivity is lowering slightly with increasing temperature until 350.4 K. At this point the thermal conductivity drops in a range of 1.5 K down to 0.02 W/(m·K).

From there it increases slightly with increasing temperature until the end of the defined temperature range.
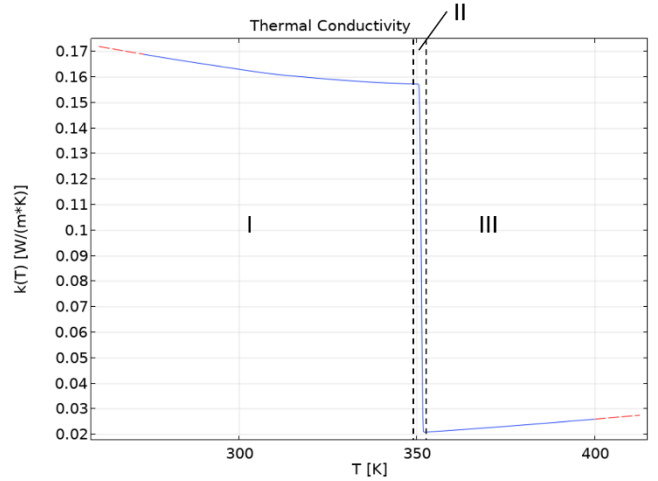

Figure 4. Thermal conductivity of ethanol as a function of temperature

Because of the phase transition the latent heat has to be considered. The latent heat which is needed for phase transition makes an evaporative cooling very effective. Hereafter the method of defining the heat capacity varies in comparison to the other three defined material properties. In this example the heat capacity significantly increases to numerically consider the latent heat in the phase transition area. The specific heat capacity c_p^{ph} in the phase transition area is defined according to equation (1). This equation creates a Gaussian distribution, which takes the latent heat of phase transition into account. [2]

$$c_p^{ph} = c_p^f + L_u \cdot \frac{e^{-(\frac{(T-T_u)^2}{(T_f-T_g)^2})}}{\sqrt{\pi \cdot (T_g - T_f)^2}} \qquad (1)$$

Interpolation functions are also used for the liquid and gaseous areas. In the case of heat capacity, the three sub-functions are also combined into a continuous function with a piecewise function.

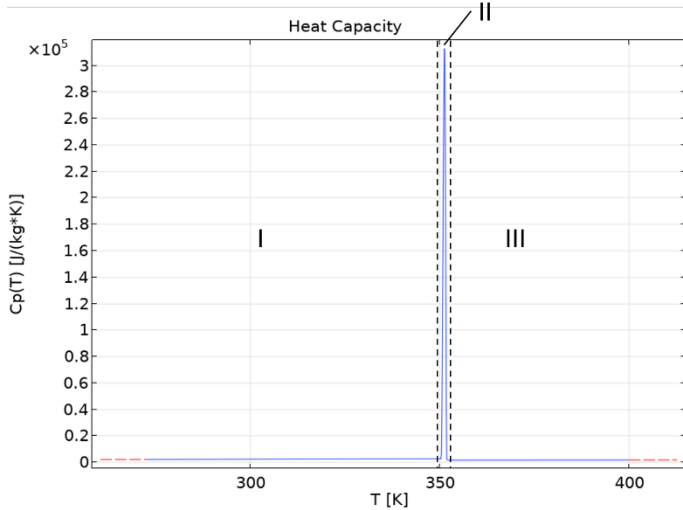The resulting material function of heat capacity can be seen in Figure 5.

Figure 5. Heat capacity of ethanol as a function of temperature

Until the temperature reaches 350.4 K the heat capacity remains almost constant before it strongly increases to a value of $3.13e^5$ J/(kg·K). Within the range of 1.5 K it drops back down and reaches $1.7e^3$ J/(kg·K). The strongly increasing heat capacity pictures the thermal energy which is used for the phase change of ethanol and the temperature is rising much slower. When the temperature is high enough the ethanol turned into gas with an even lower heat capacity than in liquid phase.

The combination of all specific material functions is the basis for the simulation of the thermodynamic behavior of the fuel cell.

Physics, domain and boundary conditions

For this simulation the physics modules turbulent flow, L-VEL and heat transfer in fluids are used. Both physics modules are coupled by the multiphysic node non-isothermal flow.

The turbulent flow is defined for the fluid area that can be liquid or gas, according to the material functions. The compressibility settings are set to compressible flow (Ma < 0.3) to accommodate density changes as a result of pressure changes. The Reynolds averaged Navier-Stokes model is used for the description of turbulence.

The defined boundary conditions of the 12 times mapped cell geometry are shown in Figure 6.

At the bottom of the model the inlet is defined. The boundary is set to a temperature of 349.4 K. The pressure of the inlet is defined to 2 atm and the velocity of the ethanol is 1 cm/s. To the fluid, streaming upwards in z-direction, force of gravity is applied. In x-direction, on both sides of the geometry, periodic flow conditions are used. At the top of the wavy structure the boundary heat sources are defined with 3000 W/m². The thermal load will heat up the solid bipolar plate and will be transferred into the fluid. The fluid will pick up the thermal energy and will transport it towards the outlet. The outlet is defined with no back flow and a pressure of 0 Pa.
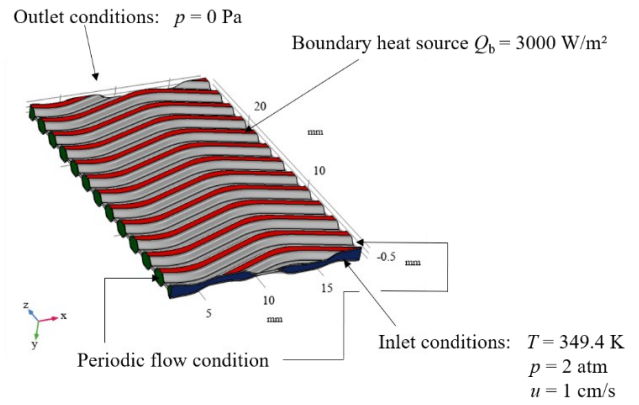

Figure 6. Illustration of different boundary conditions

Mesh

Figure 7 shows a detailed view of the mesh and the boundary layers in the fluid domain.

Boundary layers are defined where the fluid domain touches with the solid domain. This is important for the simulation of flow problems because it enables the development of the characteristic flow field and the viscous sublayer in the fluid domain. Each stack of boundary layers consists of 6 elements. The start thickness is set to automatic. The boundary layer stretching factor is set to 1.2. Free tetrahedral mesh elements are used for the meshing of the other domains. The mesh consists in total of about 4000000 mesh elements with an average quality of 0.65 due to a lot of narrow regions as a result of the complex geometry.
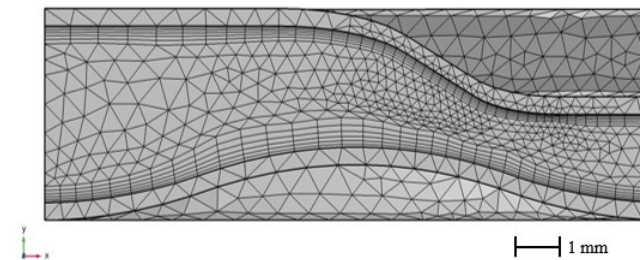

Figure 7. Detailed view of the boundary layer mesh

Results

The velocity field of the coolant ethanol is visualized in Figure 8.

It can be seen that there are two lateral flow chambers in the z-direction with a speed of about 4 cm/s at both sides of the chambers. The flow field is interrupted by the contact points of the bipolar plates Next to these areas the velocity of the ethanol is almost 0 cm/s, while the ethanol can flow unhindered in the middle parts. The highest speed is reached near the inlet. There, the maximum value is 6.34 cm/s. This can be explained by the first narrowing of the cross-section area at this point. Due to the fact that the volume flow is fixed, the velocity has to increase and reaches a maximum. Later on, the flow stabilizes and creates a desirable mixing flow pattern.
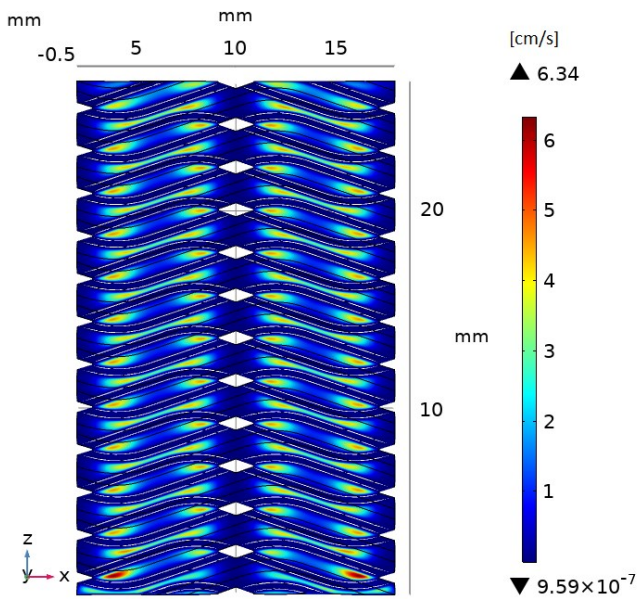
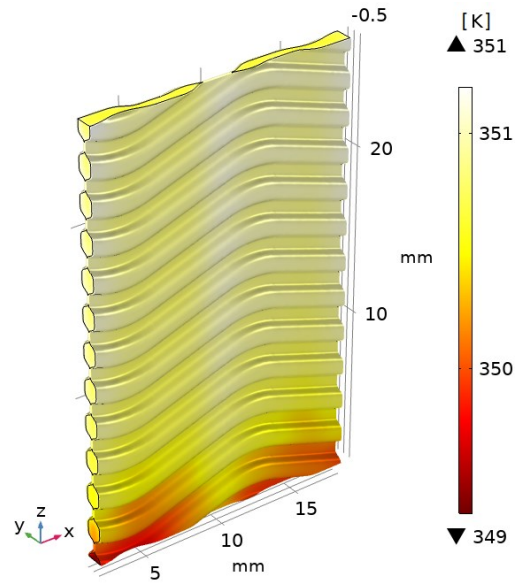**Figure 8.** Depiction of the resulting velocity field in the cell elements

Figure 9 shows the density distribution of ethanol.
It can be seen that the density decreases significantly in the z-direction. However, with a minimum density of 359 kg/m³, the ethanol is not completely in the gaseous state, but in the wet steam area, as mentioned before. At 171 kg/m³ ethanol would be fully converted to gas, the fuel cell would run dry and this must be avoided.
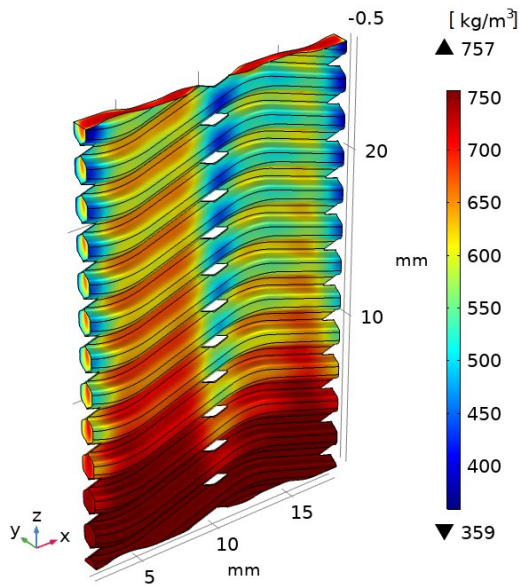

Figure 9. Depiction of the density distribution in the cell elements

The temperature distribution in the cell geometry is shown in Figure 10.
It can be seen that lowest temperatures are close to the inlet. There the boundary temperature is defined as a fixed value of 349 K. After the inlet, there is a rapid rise in temperature up to 350.4 K. This is the defined point of the increasing heat capacity and the phase change of ethanol.

Figure 10. Depiction of the temperature distribution in the cell elements

At the outlet, the maximum temperature of 351.2 K is reached. According to the defined material properties, this is the point of the maximum heat capacity of the fluid and ethanol is now in the wet steam area and half of the phase conversion area is passed through. These results can be justified by the material function of the heat capacity shown in Figure 5.
Comparative simulations with water as coolant and the same temperature of 349 K at the inlet showed a temperature difference of 5 K between the inlet and the outlet. Means the water heated up more than twice as much as the ethanol for the same boundary conditions. The benefit of the phase change in the fluid is well demonstrated by this result.

Conclusions

By implementing continuous material functions, a pseudo fluid was defined. The pseudo fluid helped to stabilize the computation and also reduced both the simulation time and the required random-access memory.
The results of the simulation show the great potential of the phase change cooling approach for fuel cells with metallic bipolar plates. It is possible to limit the temperature difference between inlet and outlet by taking advantage of the phase change.
By the use of ethanol as a liquid with low boiling point the fuel cell system can operate at a desired temperature of about 80 °C. The associated increase in heat capacity allows much more heat to be absorbed and used for the phase change of ethanol, resulting in more effective cooling, in comparison to a water-based cooling system.
As a next step 23 cell elements will be mapped to simulate the full length of the flow field of the new designed fuel cell. So far, the promising results led to the assumption that the phase change cooling approach is also feasible for bigger cell geometries. The new fuel cell system can be very efficient and reliable for stationary and mobile power sources.

References

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