Determination of water saturation dependent gas transport properties of PEFC gas diffusion layers via the Lattice Boltzmann method

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Abstract

The development of polymer electrolyte fuel cell (PEFC) technology is increasing rapidly and scientists are continuously working on optimization strategies to further improve PEFC performance. One crucial aspect of PEFC optimization is the subject of water management inside the cell. X-ray tomographic microscopy (XTM) has been proven to be an important tool to characterize in situ water behaviour. This report focuses on investigating how liquid water saturation influences gas transport properties inside the porous gas diffusion layer (GDL) during PEFC operation. First, XTM scans were quantified using a specially developed segmentation method based on thresholding. The gas transport through the structure was simulated using an in-house single phase Lattice Boltzmann model (LBM), which was modified and verified for porous media flows. Furthermore a parameter analysis was done to see the influence from the segmentation thresholds. It was seen that saturation does have a large influence on permeability and diffusivity in the GDL. However, the current implementation of the LB model was shown to give results of permeability which have a significant dependency on the chosen lattice viscosity and this parameter must be carefully chosen in order to obtain correct results.
Acknowledgements

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Chapter 1

Introduction

Day after day we hear numerous reports about extreme weather causing floods and hurricanes, leaving millions of people without homes, supply of food or clean water. Scientists are now convinced that the increase in this type of natural disasters is a consequence of global warming due to increased amount of carbon dioxide emissions. This, in turn, is caused by our constant burning of fossil fuels in order to meet our ever increasing energy demand. Furthermore, the supply of fossil fuels is projected to run out during the next century. We are facing a serious energy crisis and measures have to be taken now in order to leave a habitable planet for our future generations.

Even though measures have been taken to reduce global CO$_2$ emissions, the problem still remains in one area: Transportation.

Every day millions of people depend on their gasoline cars to take them to work, emitting a considerable amount of CO$_2$ directly to the atmosphere. With this in perspective, new automotive solutions are constantly investigated and one attractive technique is to use fuel cell systems. The electrochemical reaction of hydrogen and oxygen in the Polymer Electrolyte Fuel Cell (PEFC) provides electrical power and heat whilst just emitting water. Besides the insights gained since the early developments of PEFC technology, there are still some open questions in the research remaining. Cost, life time and power density still needs to be improved in order to be a serious competitor to the standard combustion engines.

One of the limits on power density in the PEFC is due to the presence and removal of liquid water inside the cell. This report focuses on improving the understanding of water transport through porous structures in PEFCs.
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1.1 The Polymer Electrolyte Fuel Cell

The Polymer Electrolyte Fuel Cell (PEFC), also called Proton Exchange Membrane Fuel Cell (PEMFC), is an electrochemical device allowing the conversion of chemical energy of $\text{H}_2$ into thermal and electrical energy [1]. This whole process is illustrated in Figure 1.1. The reaction can be divided into two half cell reactions. At the anode, the hydrogen molecules are split up into protons and electrons.

$$\text{H}_2 \rightarrow 2\text{H}^+ + 2e^-$$

The membrane in the PEFC is an ion conductor for protons but an insulator for electrons. The protons thus travel through the polymer electrolyte membrane, whilst the electrons must go through an external electrical circuit to the cathode. At the cathode, protons, electrons and oxygen are combined into water. The PEFC can be operated using pure oxygen as well as regular air.

$$\frac{1}{2} \text{O}_2 + 2\text{H}^+ + 2e^- \rightarrow \text{H}_2\text{O}$$

The total cell reaction thus becomes:

$$\frac{1}{2} \text{O}_2 + \text{H}_2 \rightarrow \text{H}_2\text{O}$$

The theoretical electrochemical potential of the $\text{H}_2/\text{H}_2\text{O}$ reaction is 1.23 V, but generally the open current voltage of a PEFC is around 1 V. However if
several fuel cells are connected in series, electrical power can be provided at high enough voltage to, for example, be part of the power train in cars.

The PEFC is composed of three distinct components: Flow field plates, Gas Diffusion Layer (GDL) and the Membrane Electrode Assembly (MEA).

### 1.1.1 Membrane Electrode Assembly

The heart of the fuel cell and where all the reactions take place is in the so called Membrane Electrode Assembly (MEA). The MEA consists of two highly porous carbon electrodes separated by an electrolyte membrane.

The reactions, as described in the previous section, are slow and there is a strong need to catalyse them, especially the oxygen reduction reaction (which is slower than the hydrogen oxidation reaction). A catalyst used for both reactions is platinum and these particles are usually supported on the carbon electrodes and then fixed to the membrane allowing the three phase boundary between electrolyte, reactant gas and electrode catalyst. The configuration where electrodes are directly built onto the membrane is referred to as a catalyst coated membrane (CCM).

As previously mentioned, the most important function of the membrane is to conduct protons and to be an electrical insulator, disallowing the electrons at the anode to short circuit to the cathode. Equally important is that the membrane should separate the gases at the anode from the gases at the cathode. A material which is commonly used for this purpose is called Nafion™ and its chemical structure is shown in Figure 1.2. The backbone of the membrane structure is PTFE (known under the trade name Teflon).
CHAPTER 1. INTRODUCTION

Attached to this polymer, is a side chain which ends with a sulphonic acid group. This group is highly hydrophilic in contrast to PTFE, which we know is hydrophobic. The membrane can thus absorb considerable amounts of water and when hydrated, H\(^+\) dissociates from SO\(_3\)\(^-\) and the protons can move through the material.

1.1.2 Gas Diffusion Layer

The Gas Diffusion Layer is usually made of carbon, due to the need of electrical conductivity [3]. However, as the name indicates, the structure must be porous in order to allow the gases to diffuse to the catalyst layer. Usually the GDL also contains a certain amount of PTFE in order to improve liquid water transport from the catalyst layer to the gas channel. Research has also shown [4] that introducing a micro porous layer (MPL) close to the catalyst layer can further improve water management in the PEFC. For the experiments in this thesis a GDL from Toray TGP-H-060 with 20 \% PTFE (and no MPL) was used. This GDL is made from carbon fibres, with a diameter around 6-8 \(\mu\)m, which are mainly aligned in the in-plane direction and held together by a binder.

1.1.3 Flow field plates

The flow field plates are responsible for current transport, heat dissipation and the mechanical stabilization of the cell. The plates are made out of an electrical conducting material such as steel or graphite and each one contains a system of channels to help the distribution of gas to the whole active surface.

1.1.4 Water management in the PEFC

From the previous description of the membrane, it is obvious that certain amount of water is needed for the membrane to conduct protons. However, if the cell contains too much water, the pores in the GDL can be filled, thus blocking the reactant gases from reaching the catalyst. It is clear that the water content needs to be balanced, but improvements of water management are hard to achieve without having proper knowledge of the water behaviour inside the cell, and particularly in the GDL. This is a topic which there have been a lot of research done both through modelling and experiments [1,5–9].
1.2 Objective of the thesis

As described in Section 1.1.4, water management is critical and influences the overall PEFC performance, especially when operating at high current density. This is due to pores inside the GDL being partially or fully blocked by liquid water. Many methods have been realized to study liquid water distribution in the PEFC [10]. Most of them fail however to give insight on the processes on a pore scale level, and therefore also fail to describe water blocking effects in the GDL.

Recently, X-ray tomographic microscopy (XTM) has been proven to be a very promising method for visualizing liquid water on a pore scale level inside the GDL [6]. With a special single channel fuel cell, designed to have comparable hydrodynamic properties as technical cells, liquid water distribution and the GDL solid structure can be visualized with a pixel size around 2 µm. Using image processing, segmentation of gas, liquid and solid phases are possible in order to quantify and visualize the XTM data in three dimensions.

In order to analyse gas transport properties, the most common approach for computational fluid dynamics (CFD) is to use continuum methods based on the Navier-Stokes equations (NSE). However, using this approach has been a major challenge when handling complex geometries, like the ones obtained from XTM of GDLs. During the last twenty years, an alternative way has been developed based on kinetic gas theory and the Boltzmann equation, called the Lattice Boltzmann Method (LBM). LBM has been proven to have many advantages against NSE based methods including easy handling of complex geometries, easy parallelization and accurate micro-flow simulation. The LBM is using a regular Cartesian grid and therefore voxel-based images, like those obtained from segmenting the XTM-data, are easy to use as input for the flow simulation.

The objective of the thesis is to combine in-situ PEFC XTM and LBM to describe saturation dependent gas transport properties, namely permeability and effective relative diffusivity, of PEFC GDLs.
Chapter 2

Measurements at the Swiss Light Source

2.1 The Swiss Light Source

With its futuristic doughnut shaped architecture, the Swiss Light Source is definitely the most remarkable building at the PSI. It houses a 2.4 GeV synchrotron of the third generation and can produce photon beams with exceptional brightness and stability [11].

The storage ring, with a circumference of 288 m, contains accelerated electrons which are into the circular motion using a magnetic field. The electrons response to this force is to emit electromagnetic radiation spanning a spectrum from infra-red to X-ray radiation. Due to the extremely high velocity of the electrons, the radiation is emitted tangentially from the ring and is extracted at one of nineteen different beamlines at the facility.

The large difference between conventional X-rays produced in an X-ray tube and synchrotron light, is the brilliance of the beams. The high brilliance of the synchrotron light means that it emits a lot of photons per unit time from a small source area and the light is emitted within a very narrow angular cone. The sharply focused synchrotron light beams have more resemblance to laser beams.

These features of synchrotron light allow researchers to look closer at material structure, for example when determining the structure of proteins, analysing magnetic properties of surfaces or analysing catalytic surfaces etc.
CHAPTER 2. MEASUREMENTS AT THE SWISS LIGHT SOURCE

2.2 The TOMCAT beamline

The TOMographic Microscopy and Coherent rAdiology experiments beamline, or the TOMCAT beamline, has been in operation since 2006 [12]. It spans an energy range of 8 up to 45 keV, with the high energies made accessible thanks to a 2.9 T superbend magnet [13]. The desired energy can be chosen by adjusting the monochromator. As the name says, this beamline allows researchers to perform X-ray microscopic radiography and microscopy experiments. Making a series of X-ray radiography images of a sample, while it is rotating 180 degrees, a computer can then reconstruct the material distribution, giving the entire three-dimensional structure through tomographic images.

The sample which is investigated is mounted on a sample stage. The stage position can be adjusted in every Cartesian direction with micrometre precision. The stage can also rotate, allowing tomographic images to be made (Figure 2.1).

The microscope contains a scintillator, optics and the CCD camera. For the objective with the largest magnification in the standard setup, a pixel on the CCD will amount to 0.37 \( \mu \text{m} \). The CCD contains 2048 times 2048 pixels,
CHAPTER 2. MEASUREMENTS AT THE SWISS LIGHT SOURCE

<table>
<thead>
<tr>
<th>Objective</th>
<th>Field of view [mm]</th>
<th>Pixel size [$\mu$m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.25x</td>
<td>12.1 × 12.1</td>
<td>5.9</td>
</tr>
<tr>
<td>2x</td>
<td>7.5 × 7.5</td>
<td>3.7</td>
</tr>
<tr>
<td>4x</td>
<td>3.7 × 3.7</td>
<td>1.9</td>
</tr>
<tr>
<td>10x</td>
<td>1.5 × 1.5</td>
<td>0.74</td>
</tr>
<tr>
<td>20x</td>
<td>0.75 × 0.75</td>
<td>0.37</td>
</tr>
</tbody>
</table>

Table 2.1: Field of view and pixel size for the standard setup when using different objectives

leading to a field of view of 0.75×0.75 mm. Other objectives could also be chosen, leading to field of view and pixel size according to Table 2.1.

It should be said as a comment that the separation of each tomographic image also is the same distance as the pixel size. So the pixel size stays the same (and quadratic), regardless of looking at X-Y, X-Z, or Y-Z-slices of the sample. Consequently a voxel (a volumetric pixel) in the sample will be isotropic.

All the previously mentioned equipment are contained in an experimental hutch which must be properly closed and sealed before conducting any experiment to provide radiation shielding. However, everything can be controlled via remote in the Control Room.

As mentioned before, there are a lot of methods of visualizing liquid water inside PEFCs [10], but what makes XTM (X-ray Tomographic Microscopy) attractive is the fact that it is a non-destructive three-dimensional imaging method with little or no influence on the sample itself. It also provides the necessary spatial and temporal resolution needed for observing micrometre phenomena. This makes it perfect for the purpose of analysing the in-situ water distribution in PEFC GDL structures on the pore scale.

2.3 PEFC for in-situ XTM

Since the cross-section of the X-ray beam is limited and it is preferable to let the X-ray beam penetrate the same amount of material for each rotation angle to obtain optimal image quality, the fuel cell must be very small. The size is adapted in order for the full width to fit inside a 4x field of view which, as said before, is 3.7 × 3.7 mm. There are several designs proposed and re-
Figure 2.2: Schematics of the PEFC with an active area of 11.0 mm$^2$ with sub-gaskets (as shown). Flow fields are made of graphite composite and are clamped by small o-rings placed at the recesses of the thick flow field section.

Figure 2.3: Fuel cell at the rotating stage
alized for this purpose [6]. The design used in this thesis is a single channel fuel cell with vertically aligned MEA along the rotation axis perpendicular to the beam, see Figures 2.2 - 2.3. This design allows gas, supplied from the bottom, to flow parallel to the GDL and thus representing fluid dynamics in a real technical cell. This design also has advantages regarding the contrast between the phases which are easily distinguishable.

An experimental challenge is to get good cell sealing with this type of fuel cell. As seen in the figures, this cell is compressed with O-rings and a plastic girdle on the thin part.

Another issue has also to be taken into account for the fuel cell design. According to an article published by Schneider and Wieser in April 2010 [14], the fuel cell performance can be degraded due to synchrotron radiation. During the experiments, a Nafion sub-gasket is placed inside the cell between the flow field plates and the CCM. A window is cut into the sub-gasket with the intent of reducing the active surface to $2.2 \times 5$ mm. This is done in order to get the whole active surface of the cell inside the X-ray beam, allowing to detect influences and performance losses due to synchrotron radiation exposure, and further to avoid current density inhomogeneities between irradiated and non-irradiated domains. Nafion is used due to its ability to swell when moist, thus sealing the cell. The design of the used sub-gasket is shown in Figure 2.2.

### 2.3.1 Experimental setup

In order to run and study the performance of the PEFC, the following components in our experimental setup are needed. The components are shown in Figure 2.4.

- **Gas bottles** containing oxygen and hydrogen for supplying gases to the cell.
- **Mass Flow Controllers** (MFCs) in order to control the flow of gases to the cell.
- **Bubblers** in form of glass bottles containing water, where gases are humidified before supplied to the cell.
- **An External load** to control the current produced in the cell and to monitor the cell voltage.
CHAPTER 2. MEASUREMENTS AT THE SWISS LIGHT SOURCE

Figure 2.4: Components of the experimental setup

- A **Temperature control unit** to set and monitor the cell temperature using a heating foil and a PT100 resistance thermometer connected to the cell.

- An **AC Ohm meter** to measure the membrane resistance, and therefore also monitoring the water content.

- A **laptop** from which the MFCs and the external load could be controlled using a custom made program. This computer could also be operated by remote control through the institute network so that the operating conditions can be changed from the Control Room.

The fuel cell is connected to the equipment and placed in a sample holder on the rotating stage. Important at this point is mainly to see that the gas tubes don’t get twisted during the rotation but also look so that no wires come in the way of the beam, thus disturbing the images. The tomograms used for the thesis are taken during a campaign in August 2010 (the author was participating in that campaign during an internship period in 2010) and were done using both the 2x and 4x objectives with 1001 projections during the 180 degree rotation with a beam energy of 13.5 keV. The whole scanning takes then about 4 minutes per tomogram when using the 4x objective and about 8 minutes with the 2x objective. This might seem as a long time, since the tomogram is only working if nothing is changing in the sample during the rotation. If water droplets are growing, then this will be visible.
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Table 2.2: Operating conditions for Sample A and Sample B

<table>
<thead>
<tr>
<th></th>
<th>Sample A</th>
<th>Sample B</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Objective used</strong></td>
<td>4x</td>
<td>2x</td>
</tr>
<tr>
<td><strong>Current density</strong></td>
<td>0.45 A/cm²</td>
<td>0.45 A/cm²</td>
</tr>
<tr>
<td><strong>Voltage</strong></td>
<td>502 mV</td>
<td>535 mV</td>
</tr>
<tr>
<td><strong>Operating temperature</strong></td>
<td>30 °C</td>
<td>30 °C</td>
</tr>
<tr>
<td><strong>Stoichiometries O₂/H₂</strong></td>
<td>&gt; 10</td>
<td>&gt; 10</td>
</tr>
<tr>
<td><strong>Room temperature</strong></td>
<td>24 °C</td>
<td>24 °C</td>
</tr>
<tr>
<td><strong>Scan time</strong></td>
<td>4 min</td>
<td>8 min</td>
</tr>
</tbody>
</table>

as disturbances in the image. The tomograms showed that the time is often short enough for things to remain fairly constant inside the fuel cell, especially for the 4x scans.

### 2.3.2 Operating conditions

During the XTM campaigns at the SLS, several operating conditions were realized to observe different saturation levels inside the fuel cell. The two samples, Sample A and Sample B, used in this thesis were carefully chosen and considered to show a valid saturation for the specific current density. There were mainly two factors leading to the decision of these samples:

1. Both samples have the same design and operated at the same conditions.
2. Both samples have not been exposed to any radiation prior to the XTM scan. Therefore any influence of radiation damage could be excluded.
3. Both samples have been running for at least 30 minutes before the scan at same operating conditions and can thus be assumed to be at steady state.

The operating conditions for these sample are presented in Table 2.2. The main difference between Sample A and Sample B is the type of objective used. Sample A had thus a smaller field of view, but the higher magnification allowed better contrast between phases. One other difference was the scan time. For the 4x scan, the CCD sensor was readout cropped, to achieve frame time close to exposure time of about 200 ms. On the other hand for the 2x scan, the full beam height of 5 mm and no sensor cropping was used, leading to a frame time of 459 ms per radiographic projection. This lead to
a scan time which differed from 4 minutes for the 4x scan to 8 minutes for the 2x scan.

The low cell temperature was necessary since so far no highly flexible and heated gas tubings were available to feed the XTM cells on the rotation stage. Therefore gases were humidified at room temperature (24 °C). A higher cell temperature would lead to a very low relative humidity which leads to loss of performance when the cell dries out.

In order to investigate the gas transport properties of chosen samples, the tomosgrams have to be segmented and quantified. But before further discussing the characteristics of the chosen samples the segmentation process must be understood.
Chapter 3

Segmentation of different phases in the PEFC

The experiments at the SLS result in a lot of data to evaluate. Each tomo-gram can contain over 1000 images adding up to several gigabytes. Example of the resulting tomographic images are shown in Figure 3.1. Note that further on in this thesis, the same Cartesian directions will be used.

- X is the direction parallel to flow field and membrane.
- Y is the direction perpendicular to flow field but parallel to membrane.
- Z is the direction perpendicular to the membrane.

In order to obtain any interesting quantities like porosity and saturation, a segmentation process is needed to label each voxel depending on the phases: Solid, water or void. A trained eye can easily see where the different phases are located, but it can be very time consuming to do a segmentation manually. Therefore it is very helpful to apply numerical methods for such analyses.

With this in perspective, a segmentation work-flow was developed in 2010. Some improvements have however been made for better accuracy during the span of this thesis and the final work-flow is also described in reference [6]. The description of the segmentation will just be shown for Sample A, but the same steps were done also when segmenting Sample B.
CHAPTER 3. SEGMENTATION OF DIFFERENT PHASES IN THE PEFC

Figure 3.1: (a) Y-Z cross section of Sample A cathode and the observed phases; (b) X-Y cross section of Sample A cathode
CHAPTER 3. SEGMENTATION OF DIFFERENT PHASES IN THE PEFC

Figure 3.2: Histogram showing the difficulty of setting global thresholds

Figure 3.3: Illustration of the impact of using a difference image. (a) original image of dry GDL; (b) original image of liquid water containing GDL (aligned to same position); (c) difference image
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PEFC

3.1 Description of the segmentation

The segmentation of the tomographic data set is based on grey scale thresholding. This means that a phase is determined by the grey scale value in the image, thus creating a binary mask representing the specific phase, i.e. voxels with grey scale values above the lower threshold get value 1 and the other get value 0. The biggest problem with this, is that water has a grey scale value which overlaps in the grey scale values of both void and solid phases (see Histogram in Figure 3.2). To go around this problem, water is segmented using a difference image. The difference image is just the subtraction of the dry data set from the wet data set. In this image, the sole presence of water can be observed (see Figure 3.3). Due to membrane swelling, both electrodes can’t be aligned at the same time, but must be treated separately. Since it is water transport inside the GDL that is of interest, it is sufficient to look on the cathode, where water is produced (and since the anode was dry at the chosen operating conditions). The following steps are included in the segmentation work-flow:

1. Cropping and precise alignment of both the dry image stack and wet image stack.

2. Subtraction of the dry data from the wet data, obtaining the difference image stack.

3. Median filtering (2D) of difference images.

4. Water segmentation by applying a global lower threshold to the difference images.

5. Void separation from solid phases using a lower threshold which is changing in the through-plane (Z) direction.

6. Catalyst layer segmentation using a lower threshold which is changing in the through-plane (Z) direction.

7. Membrane segmentation by binding together the catalyst layer and stating that the voxels underneath are membrane.

8. Graphite segmentation using spatial boundaries to the mask created in step 5.

9. GDL identification: all solid material which is neither graphite, membrane or catalyst layer.
CHAPTER 3. SEGMENTATION OF DIFFERENT PHASES IN THE PEFC

<table>
<thead>
<tr>
<th></th>
<th>Water</th>
<th>GDL</th>
<th>Catalyst Layer</th>
<th>Graphite</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D hole</td>
<td>250</td>
<td>50</td>
<td>25</td>
<td>250</td>
</tr>
<tr>
<td>2D island</td>
<td>25</td>
<td>5</td>
<td>5</td>
<td>25</td>
</tr>
<tr>
<td>3D hole</td>
<td>500'000</td>
<td>500'000</td>
<td>500'000</td>
<td>500'000</td>
</tr>
<tr>
<td>3D island</td>
<td>100</td>
<td>2'500</td>
<td>2'500</td>
<td>10'000</td>
</tr>
</tbody>
</table>

Table 3.1: Table specifying the minimum hole and island thresholds for each material respectively.

10. Merging the different segmentations together, where each voxel gets a specific value depending on material.

11. Correcting falsely segmented water by applying morphological processing.


Steps 4-6, 8 and 11-12 are finalized by removing small islands and holes in each Cartesian direction. An island is a group of connected voxels (pixels in the two-dimensional case) with value 1, which are entirely surrounded by voxels with value 0. A hole is basically the inverse case where a group of voxels with value 0 are surrounded by voxels with value 1. The minimum size of these are also controlled by thresholds, which were determined manually, see Table 3.1.

### 3.2 Choosing the thresholds

The determination of the grey scale thresholds is a manual task. By analysing the histogram of the image, it is often clear that we have two peaks of the phases that needs to be separated, and the threshold is set in-between the two peaks. To precisely choose the right threshold an observation of the binary mask has to be made, and then vary the threshold so that the size of the holes and islands are as small as possible. The small island and holes can thus be removed as previously described. How the threshold is determined, for both water and solid segmentation, is illustrated in Figures 3.4 and 3.5.
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Figure 3.4: Illustration of the determination of the grey scale threshold for water. a) difference image; b) histogram of the difference image showing in what region the grey scale threshold must be set; c) binary image using low threshold; d) binary image using middle threshold; e) binary image using high threshold.
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Figure 3.5: Illustration of the determination of the grey scale threshold for solid. a) original image of dry GDL; b) histogram of the difference image showing in what region the grey scale threshold must be set; c) binary image using low threshold; d) binary image using middle threshold; e) binary image using high threshold
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Z-dependent thresholding

It was found in the tomographic images that the grey scale of void is getting higher, closer to the catalyst layer. Setting a global threshold for solid that can separate the phases both close to the channel and catalyst layer is fairly impossible. The difficulty is clearly visible in Figure 3.6. The threshold is therefore set to be dependent on the Z-coordinate. By choosing thresholds for some characteristic X-Y images, and then linearly interpolate the threshold between these Z-locations, the result could be largely improved. The wavy form of the catalyst layer however, makes it difficult to set a threshold for void close to it since the void grey scale value is not homogeneous over the whole X-Y slice. This is a problem that persists and has to be taken into consideration when analysing quantities as porosity and saturation close to the catalyst layer.

3.3 Membrane and Catalyst Layer segmentation

It is hard to segment the membrane from the fibres since they have the same grey scale intensity. What is easier to segment is the catalyst layer which has, by far, the highest grey scale value in the original image. The whole membrane is covered with this layer, but at some points it is so thin that it can’t be seen, or it contains cracks and holes. However if the catalyst layer is bound together to form a continuous surface, it is easy to state that each pixel underneath should be interpreted as membrane.

For the catalyst layer segmentation there is also a need of Z-dependent thresholding, since the mean grey level intensity also changes with the Z-coordinate (See Figure 3.7). After thresholding, the segmentation is corrected with island and hole removal as before, leading to the result in Figure 3.8(a).

Creating Catalyst Layer boundary

When the catalyst layer is segmented, it is bound together to form a continuous surface. The boundary was created in the following way as illustrated in Figure 3.8:

1. An image is taken from the segmented catalyst layer data set as shown in Figure 3.8(a).
CHAPTER 3. SEGMENTATION OF DIFFERENT PHASES IN THE PEFC

Figure 3.6: Illustration of the need of a Z-dependent threshold. (a) original image of dry structure; (b) binary mask showing that the threshold is rather good close to the channel, but since void grey scale is increasing in Z-direction, the threshold is too low in the lower region close to the catalyst layer; (c) diagram showing the threshold dependence on the Z-coordinate for the solid segmentation; (d) binary mask after Z-dependent thresholding (and hole/island removal)
CHAPTER 3. SEGMENTATION OF DIFFERENT PHASES IN THE PEFC

Figure 3.7: Diagram showing the threshold dependence on the Z-coordinate for the catalyst layer segmentation

2. The layer is turned into a skeleton by just keeping the middle catalyst layer pixel for each Y as shown in Figure 3.8(b).

3. Holes in skeleton are filled by linearly interpolating pixels in between. Holes in the beginning and end of the image are just filled using the position of the first or last pixel in the skeleton. This is shown in Figure 3.8(c).

4. The thickness is added again to the skeleton. The thickness in the previous holes is also interpolated, leading to the resulting catalyst layer boundary in Figure 3.8(d).
CHAPTER 3. SEGMENTATION OF DIFFERENT PHASES IN THE PEFC

Figure 3.8: Illustrations of how the Catalyst Layer boundary is created

(a) Catalyst layer after thresholding and removal of holes and islands

(b) Skeleton of catalyst layer

(c) Skeleton of catalyst layer with filled holes

(d) Resulting catalyst layer boundary
3.4 Merging of the segmentations

When the different phases and materials are segmented they are combined together with a certain value depending on the material. The following voxel values are given:

<table>
<thead>
<tr>
<th>Material</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Void</td>
<td>0</td>
</tr>
<tr>
<td>Membrane</td>
<td>1</td>
</tr>
<tr>
<td>Water</td>
<td>2</td>
</tr>
<tr>
<td>Catalyst Layer</td>
<td>3</td>
</tr>
<tr>
<td>GDL</td>
<td>4</td>
</tr>
<tr>
<td>Graphite</td>
<td>5</td>
</tr>
</tbody>
</table>

If there still are some overlapping regions, the following rules applied:

- If a voxel is interpreted both as water and GDL, it should take the value of GDL. This, since we otherwise might loose fibres which are enclosed by fibres during the water segmentation.
- The catalyst layer and the membrane overwrites any overlapping interpretation of a voxel.
- If a voxel is segmented as both water and graphite, it takes the value of water.

Morphological processing of water

When merging the segmentations together, it was also seen that there were flat water clusters on top of the GDL surface. This was an artefact from slight misalignment when constructing the difference image. By doing a 2D morphological opening (erosion followed by dilation) with a structure element of a disc of radius 1 (i.e. a cross of five pixels), the most of these flat elements could be removed. This was also done for both islands and holes in each Cartesian direction. The result of the process can be illustrated in Figure 3.9.

3.5 Manual correction of segmentation

As mentioned in Section 1.1.2, the GDL is in our case made of carbon fibres which are held together by a binder. The problem with the segmentation process is that the inside of this binder has grey scale values which are as high
CHAPTER 3. SEGMENTATION OF DIFFERENT PHASES IN THE PEFC

Figure 3.9: Illustration of the need of morphological processing. (a) difference image; (b) segmented mask; (c) binary mask of water before the morphological processing; (d) binary mask of water after morphological processing.

Figure 3.10: Illustration of the need of manual correction of the solid segmentation. Water labels obtained as described in Section 3.2. Raw XTM data of wet sample is not shown here. (a) original dry image; (b) labelled mask before manual correction; (c) labelled mask after manual correction.
as the ones for void close to the catalyst layer. The resulting segmentation is therefore like the one illustrated in Figure 3.10. The edges of the binder are often well segmented, but the inside not. With the human eye this is easy to see where the binder should be, and since the problem is just occurring on the last 20-30 X-Y slices close to the catalyst layer, it can be manually corrected.

An example of the final result of the segmentation process is illustrated in Figure 3.11.
Chapter 4

Quantification of the segmented data and characterization of the samples

4.1 Sample domains

The resulting labelled mask of the segmentation process described in Section 3 defines which material each voxel represents. Therefore it is quite easy to make some quantification of the segmented data. The segmented images also allows to visualize the PEFC in three dimensions (Figure 4.1).

As discussed in Chapter 2, two different tomograms are used in this thesis, Sample A obtained through a 4x scan and Sample B through a 2x scan (See operating conditions in Table 2.2). The scan with the 2x objective made it possible to investigate the whole active area of the cell. However, the pixel size made it more difficult to observe the thin fibres inside the GDL (See Figure 4.4). By scaling up the sample in each Cartesian direction, the segmentation and quantification, with the same parameters regarding minimum hole and island size, could be made also for this cell.

Before simulating the GDL gas transport properties, it is necessary to characterize the XTM GDL data sets in terms of porosity, liquid water saturation and local pore diameter distribution. Since these properties can’t be assumed to be the same under the gas channel and under the ribs, the GDL is divided into three regions: Channel, Left Rib and Right Rib.
Figure 4.1: Smoothed surface rendering of phase segmented images of Sample A. (a) Flow field, GDL, liquid water and CCM; (b) GDL and liquid water; (c) liquid water
Sample B was furthermore divided into three sub-samples, each having a comparable size as Sample A. They are as follows:

- Br1 = Outlet region
- Br2 = Middle region
- Br3 = Inlet region

How the division was made is shown in Figures 4.3 and 4.4. Note that the Left Rib is reduced, since the sub-gasket is partly covering the catalyst layer and stopping the activity in this region. The final dimensions of all domains used in this thesis are presented in Table 4.1.
CHAPTER 4. QUANTIFICATION OF THE SEGMENTED DATA AND CHARACTERIZATION OF THE SAMPLES

Figure 4.4: X-Y slice of Sample B divided into sub-samples: Br1, Br2 and Br3. These are then divided into the following coloured regions: Red = Left Rib, Black = Channel, Blue = Right Rib

<table>
<thead>
<tr>
<th></th>
<th>Left Rib</th>
<th>Channel</th>
<th>Right Rib</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>600 × 340 × 85</td>
<td>600 × 400 × 90</td>
<td>600 × 340 × 85</td>
</tr>
<tr>
<td>Br1</td>
<td>600 × 150 × 80</td>
<td>600 × 400 × 90</td>
<td>600 × 340 × 70</td>
</tr>
<tr>
<td>Br2</td>
<td>600 × 150 × 80</td>
<td>600 × 400 × 90</td>
<td>600 × 340 × 80</td>
</tr>
<tr>
<td>Br3</td>
<td>600 × 150 × 80</td>
<td>600 × 400 × 90</td>
<td>600 × 340 × 80</td>
</tr>
</tbody>
</table>

Table 4.1: Dimensions (expressed in amount of voxels in each direction) of the GDL samples in this thesis
4.2 Porosity

One of the most important characteristics of the GDL is the porosity. This quantity tells how much of the total volume is made up of empty space (pores), and therefore has a high influence on the gas transport properties of the material. The porosity $\epsilon$ is analysed in through-plane ($Z$) direction by using the simple formula:

$$\epsilon(Z) = \frac{N_{\text{void}}(Z) + N_{\text{water}}(Z)}{N_{\text{total}}(Z)} \quad (4.1)$$

$N_\alpha(Z)$ is the number of voxels of phase $\alpha$ in an X-Y plane at position $Z$. The Figure 4.5 show how the porosity changes for the different samples in through-plane direction in the GDL. To be able to compare the porosity of
Figure 4.6: Porosity in through-plane of the samples for different regions (The zero Z position is set at the uppermost Channel voxel for each sample respectively).
the particular regions (Channel, Left Rib and Right Rib) between the different samples, these were plotted in Figure 4.6.

These graphs clearly show that the porosity is lowest on the boundaries. This is due to the higher concentration of binder in these regions or can also be an artefact of the inhomogeneous PTFE treatment. There is also visible that the porosity is everywhere comparable between the samples and regions. At the boundaries, both close to flow field plates (FFP) and catalyst layer (CL), the porosity is \( \approx 0.6 \), whilst in the middle parts reaching \( 0.7 - 0.8 \).
CHAPTER 4. QUANTIFICATION OF THE SEGMENTED DATA AND CHARACTERIZATION OF THE SAMPLES

4.3 Saturation

In the investigated GDL, water is partially filling up the pore space. The amount of water in the GDL can be described by the liquid water saturation, $s$, and is also calculated in through-plane direction using the formula:

$$s(Z) = \frac{N_{\text{water}}(Z)}{N_{\text{void}}(Z) + N_{\text{water}}(Z)}$$

The Figures 4.7 and 4.8 show the saturation for the samples. What should be worthy of notice, is the fact that saturation is highest close to the catalyst layer where water production is taking place. It is found that the GDL has higher saturation under the ribs compared to the channel. Worth to note is also that a lot of water is filling up the void space in the graphite/GDL interface area due to condensation at the ribs (See regions marked with white rectangles in Figure 4.9). The GDL boundary was therefore excluded for the study in this thesis.
Figure 4.7: Saturation in through-plane of the samples for different samples (The zero Z position is set at the uppermost Channel voxel for each sample respectively).
CHAPTER 4. QUANTIFICATION OF THE SEGMENTED DATA AND CHARACTERIZATION OF THE SAMPLES

Figure 4.8: Saturation in through-plane of the samples for different regions (The zero Z position is set at the uppermost Channel voxel for each sample respectively).

Figure 4.9: Water volume fraction in X-direction. The white rectangles show regions where water is filling up the void space in the graphite/GDL interface area.
4.4 Local pore diameter analysis

Although the porosity and saturation gives an overview of the amount of pores and water inside the sample, it is hard to quantify characteristics which more in detail control gas transport inside the material. The size of the pores might also have an influence and can be obtained using local thickness analysis. The local thickness for a point inside a certain material is defined as the diameter of the largest sphere which [15]:

1. encloses the point
2. is bounded by the material surface

The local thickness is obtained using a plug-in in Fiji and applying it on the voxels representing void in the GDL. Through this, the local pore diameter is obtained. This is done for both the wet and the dry sample in order to better see how the pore distribution is changed due to water inside the GDL (For the wet sample, water was also considered solid). Further, the pore diameter maps are multiplied by the binary water mask to determine the diameter of the pores containing water. However, through this, it can’t be concluded if the pores are partially or completely filled.

The local pore diameter distribution for the samples is shown in Figures 4.10 - 4.13. The histograms show that the pore diameter distribution of the dry data seems to look similar, regardless of sample or sample region. As seen also in the histograms, the mean pore diameter is reduced due to water inside the GDL. For all samples, the water is mainly contained in the larger pores, since the mean value of the water occupied void is higher than for the dry data. As a comment on the histograms it should be said that some of the larger pores in the Channel region of each domain arrives from including parts of the actual gas channel in the local thickness analysis. This should be taken into account when evaluating the mean pore diameter of the Channel region.
CHAPTER 4. QUANTIFICATION OF THE SEGMENTED DATA AND CHARACTERIZATION OF THE SAMPLES

Figure 4.10: Pore size distribution in Sample A

Figure 4.11: Pore diameter distribution, Sample Br1
CHAPTER 4. QUANTIFICATION OF THE SEGMENTED DATA AND CHARACTERIZATION OF THE SAMPLES

Figure 4.12: Pore diameter distribution, Sample Br2

Figure 4.13: Pore diameter distribution, Sample Br3
4.5 Parameter sensitivity analysis

The segmentation described in Chapter 3 is controlled by several thresholds for the grey scale value but also thresholds determining minimum island and hole size, both in 2D and 3D. Changing these values slightly might have a significant influence on the segmentation result, and therefore a sensitivity analysis is made to quantify the influence from the segmentation parameters. The segmentation is furthermore done without any manual correction as described in Section 3.5. The analysis is then performed on Sample A, and the GDL is analysed as a whole and not divided into regions. Note that the zero Z position in the graphs in this section, is set to the uppermost part of the sample (See Figure 3.1(a)).

The values of the parameters were all varied with a certain percentage from the originally chosen ones and then porosity and saturation was determined for each set of values.

4.5.1 Sensitivity to water grey scale threshold

The values, between which the water grey scale threshold varies were shown before in the histogram in Figure 3.4. The values are hence chosen to all be in the region between the two peaks. The influence on porosity and saturation is shown in Figure 4.14. Porosity doesn’t change since it is only dependent on the solid segmentation. Saturation is as seen highly sensitive to changes in the grey scale threshold value for water. However, the difference image gives quite distinct peaks in the histogram, and therefore it is rather easy to
set this threshold so saturation variation can be well within ±2.5%.

### 4.5.2 Sensitivity to solid grey scale threshold

The values, between which the grey scale threshold varies were shown before in the histogram in Figure 3.5. Note that the histogram is just showed for one X-Y slice, and the values changed as shown in the Z-direction. However, each local threshold in the Z direction is changed using the same multiplier.

The influence on porosity and saturation is shown in Figure 4.15. Porosity is changing quite much under the influence of the solid threshold variation. The effect is furthermore a lot higher close to the catalyst layer. Porosity can vary as much as ±5% and this shows the importance of carefully choosing the solid thresholds.

Here, saturation is just barely affected by the variations of the solid threshold, except close to the catalyst layer, where the wavy form of the surface leads to areas where void is interpreted as solid or vice versa. The reason for this was already discussed in Section 3.5, and is due to void having same gray scale intensity as inside of the binder. Previously this was corrected manually, but such a step was not performed in the sensitivity analysis.

### 4.5.3 Sensitivity to hole and island thresholds

The hole and island thresholds that were used are shown in Table 3.1. The choice of these values was determined by observation and what the smallest
CHAPTER 4. QUANTIFICATION OF THE SEGMENTED DATA AND CHARACTERIZATION OF THE SAMPLES

Figure 4.16: Sensitivity to 2D water hole/island threshold of Sample A (a) Porosity; (b) Saturation

Figure 4.17: Sensitivity to 2D solid hole/island threshold of Sample A (a) Porosity; (b) Saturation
CHAPTER 4. QUANTIFICATION OF THE SEGMENTED DATA AND CHARACTERIZATION OF THE SAMPLES

objects, that can be separated from regular noise in the images, would be. The sensitivity to 2D hole and island thresholds for both solid and water is shown in Figures 4.16 and 4.17 respectively.

Although changing the values quite much, the porosity and saturation values are barely affected. If choosing a good threshold value for solid, the size of islands and holes are at a minimum, and well isolated, which means that they are easily eliminated in the hole and island removal process. The sensitivity to three-dimensional hole island threshold is not shown here, since it had no visible influence on porosity and saturation in the range $[-50\%, +50\%]$.

4.6 Summary

To summarize the quantification, the mean values of porosity, saturation and pore diameter are illustrated in Figure 4.18 for all sample regions used in this thesis.

Through all the characterizations done, it was shown that the dry sample regions do not have any significant difference in either porosity or mean size distribution. There is some tendency that the porosity is slightly lower in the ribs than in the channel, which can arrive from slight compression of the GDL. However, as was seen in 4.5.2, the exact value of the porosity should be evaluated carefully since the quantity is highly dependent on the chosen solid grey scale thresholds.

In spite of all the similarities in the dry structures, there are quite significant differences in local saturation which can’t really be explained so far. The only common trend regarding saturation for all regions is that water usually is concentrated to the ribs with a saturation of 20-40 % and that it is higher close to graphite and catalyst layer.

It was shown in the previous sections that the only predefined thresholds that had an significant influence on the segmentation are the ones for solid and water gray scale. One should also be careful in evaluating the saturation close to the catalyst layer where the segmentation contains a lot of errors. The regions chosen for the gas transport simulations were therefore cut off in such a way that the segmentation was considered valid. It is worth to note that this also was done close to the graphite under the ribs due to the same reason.
CHAPTER 4. QUANTIFICATION OF THE SEGMENTED DATA AND CHARACTERIZATION OF THE SAMPLES

Figure 4.18: (a) Total porosity in samples; (b) Total saturation in samples; (c) Mean pore diameter for the dry data sets; (d) Mean pore diameter for the wet data sets
CHAPTER 4. QUANTIFICATION OF THE SEGMENTED DATA AND CHARACTERIZATION OF THE SAMPLES

Since Sample A and Sample B were concluded to have comparable characteristics in terms of porosity, saturation and pore diameter distribution, they were considered valid parts to investigate. But in order to really conclude what the saturation at these operation conditions is, more research has to be made to get more statistics.
Chapter 5

Lattice Boltzmann Modelling: The method

Before going to describe the exact implementation of the particular Lattice Boltzmann (LB) model used for simulating gas flow through the GDL of the PEFC, some general concepts have to be clarified about the method. The reader which is already familiar with LB modelling can skip to Chapter 6.

5.1 Conventional CFD-methods

Computational Fluid Dynamics (CFD) has during a long time been based on continuum methods based on some of the most fundamental equations in fluid dynamics, the Navier-Stokes equations (NSE) [16]. These partial differential equations, describe that certain quantities have to be conserved within the flow. The most important conserved quantities for describing incompressible, isothermal fluid motion are mass (Equation 5.1) and momentum (Equation 5.2).

\[
\nabla \cdot \vec{u} = 0 \quad (5.1)
\]

\[
\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\vec{u} = -\frac{\nabla p}{\rho} + \nu \nabla^2 \vec{u} + \frac{\Psi}{\rho} \quad (5.2)
\]

Using these relations with given pressure gradient \( \nabla p \), other volumetric forces \( \vec{Ψ} \), kinematic viscosity \( \nu \), density \( \rho \) and boundary conditions, the velocity field \( \vec{u} \) can be obtained. Equation 5.2 includes the non-linear convective acceleration term \((\vec{u} \cdot \nabla)\vec{u}\), which makes the equation non-linear and therefore imposing difficulties when it comes to modelling. This term contains information about flow vortices arriving from inertial forces. These are constantly in battle with the viscous forces described in the \( \nu \nabla^2 \vec{u} \) term, which describes
the diffusion of momentum leading to the dissipation of vortices in the flow. The flow field behaviour is thus depending almost entirely on one dimensionless parameter, the Reynolds number, describing the ratio of the magnitude between these two forces.

\[
Re = \frac{\text{inertial forces}}{\text{viscous forces}} = \frac{U \cdot L}{\nu}
\] (5.3)

Here, \( U \) is the fluid velocity and \( L \) is a characteristic length of the flow. A high Reynolds number means that the inertial forces are significantly larger than the viscous forces, thus leading to an unstable turbulent flow.

Worth to mention is also the Mach number, which plays an important role in compressible flows.

\[
Ma = \frac{U}{c_s}
\] (5.4)

Here, \( c_s \) is the sound speed of the fluid. As long as this number is consequently kept \(< < 1\), the density is considered constant in space and the fluid can be considered incompressible thus meaning that Equations 5.1 and 5.2 apply.

5.2 Kinetic theory

Another way of describing fluid motion is through kinetic theory, pioneered by (amongst others) Daniel Bernoulli, James Clerk Maxwell and Ludwig Boltzmann [17]. The theory is describing matter as a system of many particles moving rapidly and only interacting through collisions. Each particle is described by its position in space \( \vec{r} \) and its momentum \( \vec{p} = m \vec{u} \). Although particles are translated at velocities exceeding maybe 1000 m/s, the macroscopic velocity of the fluid is a lot smaller and obtained by taking a statistical average. In Boltzmann’s statistical formulation, the probability to find a particle at position \( \vec{r} \) with the momentum \( \vec{p} \) at a certain time \( t \) is described by a distribution function:

\[
f = f(\vec{r}(t), \vec{p}(t), t)
\] (5.5)

5.2.1 The Boltzmann equation

One of Ludwig Boltzmann’s greatest achievements was when he 1872 described the evolution of the distribution function \( f \) with the famous Boltzmann equation.

\[
\frac{Df}{Dt} = \frac{\partial f}{\partial t} + \frac{\partial \vec{r}}{\partial t} \frac{\partial f}{\partial \vec{r}} + \frac{\partial \vec{p}}{\partial t} \frac{\partial f}{\partial \vec{p}} = C(f)
\] (5.6)
CHAPTER 5. LATTICE BOLTZMANN MODELLING: THE METHOD

The Equation 5.6 can be rewritten using the relations $\vec{u} = \frac{\partial \vec{r}}{\partial t}$ and $\vec{F} = m\vec{a} = \frac{\partial \vec{p}}{\partial t}$.

$$\frac{\partial f}{\partial t} + \vec{u} \frac{\partial f}{\partial \vec{r}} + \vec{F} \frac{\partial f}{\partial \vec{p}} = C(f) \quad (5.7)$$

The equation states that particles are streaming along trajectories due to a force field $\vec{F}$ (left-hand side of equation) as long as they are not colliding which then will take particles in or out of these trajectories (right-hand side of equation). The collision operator, $C(f)$, is hence describing change of the distribution function due to collisions between particles.

5.2.2 From kinetic theory to fluid dynamics

In order to get to fluid dynamics from kinetic theory, it is important to define the important macroscopic quantities mentioned in Section 5.1, density and momentum. These are easily obtained around any point in space and time by the following relations:

$$\rho(\vec{r}, t) = \int f d\vec{u} \quad (5.8)$$

$$\rho \vec{u}(\vec{r}, t) = \int f \vec{u} d\vec{u} \quad (5.9)$$

Higher order moments can furthermore be obtained in a similar way. Note that momentum is now defined in a volumetric sense, since a small control volume containing numerous particles is considered. The most important issue in describing fluid motion is to keep mass and momentum conserved in both the streaming and collision process. However to derive the full fluid dynamics equations 5.1 and 5.2 from Equation 5.7, the equilibrium values of higher order moments must have a specific form. The Navier-Stokes equations can then be derived using a first order Chapman-Enskog expansion. This procedure has been done by several people and will not be further discussed in this thesis [17]. However, it is important to mention that the derivation relies on the fact that there is a distinct separation of time scales between the microscopic events (time between particle collisions) and any relevant hydrodynamic time scale (convective, diffusive etc.). This is ensured by the smallness of the Knudsen number, defined as:

$$Kn = \frac{\lambda}{L} \ll 1 \quad (5.10)$$

where $\lambda$ is the mean free path (length between collisions) and $L$ is a relevant physical length scale.
5.2.3 The Bhatnagar-Gross-Krook model

Usually, the problem in solving the Boltzmann equation lies in the difficulty of getting a solution to the collision operator, which in Boltzmann’s formulation is a complicated non-linear integral. In 1954, Bhatnagar, Gross and Krook proposed a simplified form of $C(f)$:

$$C(f) = -\frac{f - f^{eq}}{\tau}$$ (5.11)

They claimed that the complicated collision process between particles can be treated as a relaxation process to a local equilibrium $f^{eq}$ which is defined by local quantities such as density and momentum. The time scale at which this process occurs is controlled by one single constant relaxation time, $\tau$. Although looking like this would be very drastic simplification, it was proven very useful in analysing problems using the Boltzmann equation.

5.3 The Lattice Boltzmann method

5.3.1 First LB-models

In 1988, McNamara and Zanetti [18] proposed the first Lattice Boltzmann (LB) model as a step to remove statistical noise from its predecessor, the Lattice Gas Cellular Automata (LGCA) model. The model was based on discrete particle distributions moving to neighbouring nodes in a square lattice. Space is hence discretized into integer positions $\vec{x} = (i, j, k)$ and the entire velocity space is reduced to a number of discrete velocities $\vec{c}_a$, such that $\vec{x} + \vec{c}_a$ is a neighbouring node in the lattice. The Lattice Boltzmann Equation thus becomes:

$$f_a(\vec{x} + \vec{c}_a, t + 1) - f_a(\vec{x}, t) = C_a(f)$$ (5.12)

The relevant macroscopic quantities are obtained in a similar way as before, with the following relations:

$$\rho(\vec{x}, t) = \sum_a f_a(\vec{x}, t)$$ (5.13)

$$\rho \vec{u}(\vec{x}, t) = \sum_a f_a(\vec{x}, t) \cdot \vec{c}_a$$ (5.14)
There are several different type of square lattices which can be used for Lattice Boltzmann modelling. The lattices are dependent on how many dimensions $n$ and how many discrete velocities $m$ are used. The notation $D^nQ^m$ then tells which lattice is used in the model. The easiest 2D lattice to illustrate is the D2Q9 (Figure 5.1). The nine velocities in this model are as follows (Note that particles can also be stagnant at the original position):

\[
\begin{align*}
\vec{c}_0 &= (0, 0) \\
\vec{c}_1 &= (1, 0) \\
\vec{c}_2 &= (0, 1) \\
\vec{c}_3 &= (-1, 0) \\
\vec{c}_4 &= (0, -1) \\
\vec{c}_5 &= (1, 1) \\
\vec{c}_6 &= (-1, 1) \\
\vec{c}_7 &= (-1, -1) \\
\vec{c}_8 &= (1, -1)
\end{align*}
\]

There are several types of lattices to choose also in three dimensions. These will be further discussed in the next chapter.
5.3.3 The Lattice BGK model

One year after McNamara and Zanetti published their work, Higuera and Jimenez [19] proposed a collision operator with the following form:

\[ C_a(f) = -A_{ab}(f_b - f_{eq}^b) + F_a \]  

(5.15)

where \( F_a \) denotes the external or internal forces and \( A_{ab} \) is a scattering matrix controlling the relaxation to a local equilibrium of the different modes. They furthermore showed that LB viscosity was just controlled by the leading non-zero eigenvalue of \( A_{ab} \). A few years later, several authors, almost at the same time, showed that fluid dynamics could very well be simulated by just using a one relaxation time scattering matrix of the form:

\[ A_{ab} = -\frac{1}{\tau}\delta_{ab} \]  

(5.16)

This leads to the following Lattice Boltzmann Equation:

\[ f_a(\vec{x} + \vec{c}_a, t + 1) - f_a(\vec{x}, t) = -\frac{1}{\tau}(f_a(\vec{x}, t) - f_{eq}^a(\vec{x}, t)) + F_a \]  

(5.17)

Due to its similarities to the BGK-model in Section 5.2.3, this particular LB-model is referred to as the Lattice BGK (LBGK) model.

The LBGK equilibrium function

The LBGK equilibrium function is basically a Gaussian function dependent on the density, momentum and lattice sound speed. The lattice sound speed, \( c_s \), is dependent on the type of lattice that is used and is due to the discretization of space. For all examples used in this thesis, \( c_s \) is a constant and equal to \( \sqrt{1/3} \) lattice units per time-step \( (lu \cdot ts^{-1}) \) [20]. One of the many ways to get the equilibrium function is by expanding a Maxwell-Boltzmann distribution around \( \vec{u} = \vec{0} \) (Low Mach). It must furthermore have same density and momentum as the real distribution function:

\[ \rho(\vec{x}, t) = \sum_a f_{eq}^a(\vec{x}, t) \]  

(5.18)

\[ \rho \vec{u}(\vec{x}, t) = \sum_a f_{eq}^a(\vec{x}, t) \cdot \vec{c}_a \]  

(5.19)

The most commonly used equilibrium function for simulating incompressible flow is [21]:

\[ f_{eq}^a = w_a \rho \left[ 1 + 3 \frac{(\vec{c}_a \cdot \vec{u})}{c_s^2} + \frac{9}{2} \frac{(\vec{c}_a \cdot \vec{u})^2}{c_s^4} - \frac{3}{2} \frac{\vec{u}^2}{c_s^2} \right] \]  

(5.20)
where Eq. 5.18 and 5.19 have to be fulfilled also for $\vec{u} = \vec{0}$, meaning that the lattice dependent weights, $w_a$, have to satisfy:

$$\sum_a w_a = 1$$  \hspace{1cm} (5.21)

$$\sum_a c_a w_a = 0$$  \hspace{1cm} (5.22)

Relations to fluid dynamics

The lattice fluid viscosity is related to $\tau$ through the following relation:

$$\nu_{LBM} = c_s^2 \left( \tau - \frac{1}{2} \right)$$  \hspace{1cm} (5.23)

The dimension of the lattice viscosity is lattice units squared per time-step ($lu^2 \cdot ts^{-1}$), with $1 lu$ being the distance between nearest neighbouring nodes in the lattice. With lattice velocity having the dimension of $lu \cdot ts^{-1}$, and length scales measured in $lu$, the Reynolds number of the flow can be computed:

$$Re = \frac{U_{LBM} \cdot L_{LBM}}{\nu_{LBM}}$$  \hspace{1cm} (5.24)

Furthermore, in this thesis, pressure is assumed to be related to density through the non-dimensional ideal gas law:

$$P = \rho T_{LB}$$  \hspace{1cm} (5.25)

The definition of sound speed is:

$$c_s^2 = \frac{\partial P}{\partial \rho} = T_{LB} = \frac{1}{3}$$  \hspace{1cm} (5.26)

which leads to the following definition of pressure:

$$P = \frac{\rho}{3}$$  \hspace{1cm} (5.27)

5.3.4 Obstacles

Due to the lattice base of LBM, any type of obstacles are very easy to implement and is done by labelling each node by the following boolean function:

$$h(i,j,k) = \begin{cases} 1 & \text{if } (i,j,k) \text{ is solid}, \\ 0 & \text{if } (i,j,k) \text{ is fluid}. \end{cases}$$  \hspace{1cm} (5.28)
This then leads to a staircase approximation of the boundaries, but compared to other CFD methods, the presence of corners does not implicate any significant problems, at least for flows with low \( Re \) (this will be further discussed in Section 5.4). Nodes that are labelled solid could be treated separately using different boundary schemes. This matter will be further investigated in the next chapter.

## 5.4 Advantages and limitations of LBM

### Parallelization

As mentioned before, the big problem when simulating the NSE, is the presence of the \( (\vec{u} \cdot \nabla)\vec{u} \) term. Evaluating the non-linearities this term, means information must constantly be taken from neighbouring fluid. The main advantage of using the Boltzmann equation instead is the fact that the streaming process is controlled by the \( \vec{u} \cdot \nabla f \) and is fully linear. The non-linearities are contained in the collision operator and are treated locally. This makes it optimal for parallelization of the code, since each node can be treated separately on one core each. Furthermore, since it’s compressible, there is no need of solving a Poisson equation which requires all information about the velocity field that is globally available.

### Microflows

Regular NSE based methods starts to break down when trying to describe flows where the Knudsen number becomes too high. In this regime, fluid can no longer be treated as a continuum and the NSE is no longer valid. In the same regime, with length scales around several micrometers, Molecular Dynamics simulations are too expensive to perform due to the large amount of particles. LBM however has successfully been proven to simulate microflows due to its kinetic theory origin. LBM can thus be used for a wide range of applications from macroscopic turbulence simulations to complex geometry microflows.

### Grids

Using conventional NSE based CFD-solvers, a lot of work usually have to be done constructing a well functioning grid. Different types of grids can also give different results. This also implies a strong limitation when coming to simulate flow through complex geometries. With LBM, the grid is always a square Cartesian grid, so the simplicity of introducing obstacles through
CHAPTER 5. LATTICE BOLTZMANN MODELLING: THE METHOD

Eq. 5.28, allows a lot of time to be saved on setting up the simulations. Also the Cartesian grid allow segmented tomographic voxel-based images to be directly used as the flow domain without further treatment. Even time-dependent boundaries are easily implemented by setting time constraints to Eq. 5.28. However, using a standard Cartesian grid also have drawbacks, for example when wanting to simulate flow including different length scales. The grid is uniform, so a too fine grid might implicate unnecessary long calculation time for catching both small scale and large scale phenomena. Today, multi-grid versions of LBM are used to overcome this problem and the coupling between fine and coarse grid is rather easy.

The biggest limitation of using a Cartesian grid, is the constraint of ”on the node boundary”. This leads to staircase representation of the boundary, and the natural question thus becomes: What resolution do you need in order to describe the real boundary of an object? This generally has no big influence on the general flow field, especially for low Re, but might impose difficulties concerning accuracy near walls. At higher Re, the staircase boundary might be insufficient in order to find where instabilities are triggered. Some interpolation schemes [17] has been proposed in order to get boundaries that are not constrained to go through the nodes, but they are a lot more complex and not very robust.

Another advantage of using simple grids, is the fact that moving geometries are easily implemented. Basically it is just to put a time dependency to the obstacle function in Eq. 5.28 and fluid behaviour around moving parts, such as wheels on a car or turbine blades, can be captured.

Multiphase/Complex fluid flows

The particle nature of LBM makes it accessible to manipulate particle forcing, and inter-particle interactions. By, for example, introducing a interaction potential function in the forcing term of Eq. 5.17, the existence of multiple phases of the fluid is allowed like Shan and Chen showed in [22]. The simplicity of the method of Shan and Chen shows how powerful LBE can be in describing different complex fluids. LBE is also easily extended into treating multicomponent flows.
CHAPTER 5. LATTICE BOLTZMANN MODELLING: THE METHOD

Thermal compressible flows

As previously mentioned, a low Mach number is a requirement for the LB-models discussed in this thesis. LB methods are never incompressible due the fact that density always propagating with the particle populations. But the compressibility is limited by the lattice sound speed and therefore, simulating flows with high compressibility ($Ma \gtrapprox 0.5$), both thermally and isothermally, is still is a problem which needs further research.
Chapter 6

Lattice Boltzmann Modelling: Implementation

This chapter will treat the actual methods used for simulating flow through the GDL of the PEFC. All the implementations are done in Fortran which is a programming language which is especially used for high performance computing due to quick array handling, easy optimization and easy parallelization. Therefore it is commonly used within computational physics. The model which is used is well tested in the doctoral thesis of N. Prasianakis [20]. The model was developed to be able to simulate thermal compressible flows as well as simpler flows. It had however not previously been tested for flows in porous media, so a larger portion of the work done for this thesis was to modify the code for this type of flow and to verify the model. Knowing that the model also works for transport in complex geometries, a very flexible LB-model can be obtained which can simulate a large number of fluid flow problems.

In order to avoid confusion of the directions mentioned in the thesis, the LB grid will be referring to a coordinate system of \((x, y, z)\), where the main flow direction is always in the \(x\)-direction. This in contrast to the coordinate system \((X, Y, Z)\) mentioned in Chapter 3 which is fixed to the sample. Simulating flows in different directions through the porous media, the sample itself is rotated in order to align the desired flow direction with the \(x\)-axis.

The model was hence set up on a calculation domain of size of \(N_x \times N_y \times N_z\), where the exact number depended on what part of the sample that was treated (Table 4.1).
CHAPTER 6. LATTICE BOLTZMANN MODELLING: IMPLEMENTATION

6.1 Assumptions

Before implementing the LB-model to treat the problem at hand, some assumptions have to be made:

Single phase, single component flow

Although water in liquid form is present inside the GDL, it is assumed to not be affected by the gas flow and the boundary is not deformed (a fact that is proven by having good contrast of the water boundary in the tomograms) at $Re << 1$. Therefore, liquid water is treated as constant solid material for the gas simulations.

Isothermal flow

Although the PEFC is known to produce heat, and activity might not be homogeneous along the catalytic surface, it is assumed that the sample is small enough for no significant temperature gradients to be present inside the cell. The difference between cell temperature and room temperature of 6 °C (From Table 2.2), is assumed to be eliminated as gases heat up at the entrance of the cell.

Incompressible flow

The interesting quantity to measure is gas permeability of the porous media, which can only be evaluated in the Darcy regime, where $Ma, Re << 1$. Therefore an incompressible assumption of the gas is allowed and the Mach number will always be sufficiently low such that the LB-model can be used without problem. The low $Re$ also allows for the use of staircase representation of the objects in the flow.

No proper microflow boundary conditions

As been described in Section 5.4, the Navier-Stokes equations start to break down when the Knudsen number is $O(1)$. Furthermore, no slip boundary conditions are not valid in this regime. Transport inside the GDL usually takes place at micrometer ($10^{-5}$ m) scales, while the mean free path of a gas molecule is of order $10^{-8}$ m. This means that the Knudsen number of this fluid problem is of $O(10^{-3})$ and well inside the continuum regime. Therefore no special microflow treatment must be implemented.
CHAPTER 6. LATTICE BOLTZMANN MODELLING: IMPLEMENTATION

Figure 6.1: Active elements of the D3Q27 lattice. The particle distributions can be propagated from the middle node to each of the other nodes in the figure. The particles can also be stagnant at the original position.

6.2 The D3Q27-Lattice

In this thesis a D3Q27 LB scheme was employed, which means that a 3D scheme is used where the velocity space is discretized to 27 different velocities, illustrated in Figure 6.1 and also presented in detail in Table 6.1:

Simulation of isothermal flows through complex geometries are usually done using simpler schemes like the D3Q15 and D3Q19 [17,23]. There are however stability and accuracy issues using these lattices including the presence of spurious hydrodynamic terms which can be active even for small velocities ($Ma << 1$) and that they deviate from the Navier-Stokes limit. The D3Q27 has been proven to be superior to the D3Q15 and D3Q19 [24] in these aspects and was therefore used (at the cost of extra computational effort).

6.3 Simulation steps

Every LB-model is based on the same algorithmic steps. At each time-step particle distribution first move to neighbouring nodes during the streaming process. They are then redistributed in a way such that they are approaching the local equilibrium during the collision process. The simulation steps are shown in Figure 6.2.
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Figure 6.2: Flow chart of the simulation steps in the LB-model.

6.3.1 Initialization

The LB-program is initialized by stating that all populations are at equilibrium with no fluid velocity. The following was set as initialization condition:

\[
\begin{align*}
\rho(i,j,k,t=0) &= 1 \\
\bar{u}(i,j,k,t=0) &= 0 \\
f_a(i,j,k,t=0) &= f_{a}^{eq}
\end{align*}
\]  

(6.1)

Since the LB-model is a transient code, it needs some time to build up a steady state velocity field. Starting from other initial conditions might therefore help reaching a solution faster. This was not investigated in this thesis and the described initialization conditions above were implemented in the model due to their simplicity.

6.3.2 Streaming

The streaming process is very straightforward. The populations \(f_a\) associated with the velocities \(c_a\) at node \(\vec{x} = (i,j,k)\), are translated to the node at position \(\vec{x} + \vec{c}_a\):

\[
f_a(i,j,k,t+1) = f_a(i - c_{ax}, j - c_{ay}, k - c_{az}, t)
\]  

(6.2)

6.3.3 Collision

At each node \(\vec{x} = (i,j,k)\) the following is done during the collision step:
CHAPTER 6. LATTICE BOLTZMANN MODELLING: IMPLEMENTATION

1. $\rho$ and $\vec{u}$ are calculated through Eqs. 5.13 and 5.14.

2. The equilibrium distribution function $f_{eq}^{a}$ is calculated using above mentioned quantities.

3. The new particle distributions are distributed using the following formula. Note that collision does not occur on nodes which are defined as obstacles (where $h(\vec{x}) = 1$).

$$f_{a}^{post}(\vec{x}, t+1) = f_{a}^{pre}(\vec{x}, t+1) - \left( \frac{f_{a}^{pre}(\vec{x}, t+1) - f_{a}^{pre,eq}(\vec{x}, t+1)}{\tau} + F_{a} \right) \cdot (1 - h(\vec{x}))$$

$F_{a}$ is a forcing term which is introduced when using body forcing discussed in Section 6.4.3 and the ”pre” and ”post” superscripts note the pre- and post-collision state respectively.

Equilibrium distribution function

As mentioned before, the equilibrium functions for this LB-model were derived for the particular reason to guide the particle distribution to a thermal equilibrium. This, in order to accurately simulate both thermal and isothermal flows. The equilibrium functions for the D3Q27 are as follows:

$$f_{a}^{eq} = -\rho w_{a} \cdot \left( T_{LB} - 1 + c_{ax}^{2} + c_{ax}u_{x} + u_{x}^{2} \right) \cdot \left( T_{LB} - 1 + c_{ay}^{2} + c_{ay}u_{y} + u_{y}^{2} \right) \cdot \left( T_{LB} - 1 + c_{az}^{2} + c_{az}u_{z} + u_{z}^{2} \right)$$

The velocities $\vec{c}_{a} = (c_{ax}, c_{ay}, c_{az})$ are taken from the definition of the D3Q27 scheme in Section 6.2. The weights, $w_{a}$ are taken from Table 6.1 at the end of this chapter. Note that this model is expanded to the sixth order of velocity $O(u^{6})$ compared to $O(u^{2})$ used model in Eq. 5.20. This solution is also an exact solution, and not an approximation.

6.3.4 Boundary conditions

LB-modelling usually is very dependent on how to treat the boundaries. The natural problem is the fact of defining obstacles on a square lattice, which leads to the previously mentioned staircase surface. At low $Re$, this
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Figure 6.3: Illustration of periodic boundary conditions implemented in $x$-direction

effect is however small compared to the overall flow and is further reduced by increasing resolution. In this section, the two most common boundary conditions, which also is used in this work, are treated: The periodic and the half-way bounce-back boundary conditions.

Periodic boundary conditions

The periodic boundary conditions are just used on the calculation domain boundaries and are particularly easy to introduce in a LB-model during the streaming step described in Section 6.3.3. Periodic boundaries imply that the populations that exit the domain on one side, enters the domain on the opposite side. The periodic boundaries, illustrated in Figure 6.3, was implemented on all walls parallel to the main flow direction (i.e. the $x$-direction):

\[
\begin{align*}
  f_a(i, 1, k, t + 1) &= f_a(i - c_{ax}, N_y, k - c_{az}, t) & \text{if } c_{ay} = 1 \\
  f_a(i, N_y, k, t + 1) &= f_a(i - c_{ax}, 1, k - c_{az}, t) & \text{if } c_{ay} = -1 \\
  f_a(i, j, 1, t + 1) &= f_a(i - c_{ax}, j - c_{ay}, N_z, t) & \text{if } c_{az} = 1 \\
  f_a(i, j, N_z, t + 1) &= f_a(i - c_{ax}, j - c_{ay}, 1, t) & \text{if } c_{az} = -1
\end{align*}
\] (6.5)

Half-way bounce-back boundary conditions

Fluid-solid boundaries are treated with no-slip condition. This means that fluid that lies directly at a solid surface has zero velocity. The easiest way to implement this is through half-way bounce-back (HBB) conditions and
is applied to every solid node (where $h(\vec{x}) = 1$). The boundary conditions works like this:

$$f_{\text{post}}(\vec{x}, t) = f_{\text{pre}}(i - c_{ax,\text{opp}}, j - c_{ay,\text{opp}}, k - c_{az,\text{opp}}, t) \cdot h(\vec{x}) + \frac{f_{\text{pre}}(\vec{x}, t) \cdot (1 - h(\vec{x}))}{2}$$

The ”pre” and ”post” superscripts note the pre- and post-bounce-back state respectively. $\vec{c}_{a,\text{opp}} = (c_{ax,\text{opp}}, c_{ay,\text{opp}}, c_{az,\text{opp}})$ is the velocity in the opposite direction of $\vec{c}_a$, i.e. $\vec{c}_{a,\text{opp}} = -\vec{c}_a$. $f_{a,\text{opp}}$ is the particle distribution function associated with this velocity (See Table 6.1). The incoming particle distributions are hence copied and reversed at each solid node. During the streaming step, the two distributions, the one from the solid and the one from the fluid, will meet at the half-way point between the nodes, thus simulating a no-slip boundary. Note that a particle distribution function is defined even inside obstacles. Due to the bounce-back condition inside the solid material, the ”fluid” inside the obstacles never interact with surrounding fluid. An illustration of the bounce-back principle is shown in Figure 6.4.
6.4 Driving forces

The previous section described how the LB-method is set up, but there will be no flow if there is no driving force implemented. There are several ways to introduce these, and the ones used in this thesis are described in this section. Advantages and disadvantages of the different driving force implementations was not known for this particular method prior to this work. These will be further discussed in Chapter 8 when verifying the method.

6.4.1 Velocity driven flow

The easiest way of getting the flow moving is to have predefined velocity at the inlet. The unknown microscopic populations (those coming from outside the domain) can be set to be set accordingly to fit the given velocity. This in turn leads to the inlet density and is described in a paper by Zou and He 1997 [25]. Outlet is usually treated by assuming a zero gradient for both velocity and density.

\[
\begin{align*}
\vec{u}(1,j,k) &= \vec{u}_0(1,j,k) \\
\vec{u}(N_x,j,k) &= (u_x(N_x - 1,j,k),0,0) \\
\rho(N_x,j,k) &= \rho(N_x - 1,j,k)
\end{align*}
\] (6.7)

Velocity driven flow can be tricky when simulating flow through a random porous media, since the pore size distribution is usually not known. The flow is then forced through a few small channels and the velocity can increase rapidly to maintain the mass flux. If the velocity gets close to the lattice sound speed \(c_s\), the calculation will blow up as in the 2D example in Figure 6.5. Due to this reason, this type of driving force was concluded not to be suitable and therefore not used in this work.

6.4.2 Pressure driven flow

To avoid the problems given in the previous section, a given density (related to pressure through Eq. 6.5) can be defined instead at the inlet (\(\rho_1\)) and outlet (\(\rho_0\)). However, if a definite pressure is set at the outlet, the fluid can bounce back to conserve the mass. This will cause unnecessary movement in the flow, leading to slow convergence. Therefore the outlet density is instead set as the mean value of the nodes at \(x = N_x - 1\) and \(\rho_0\). The flow will then gradually converge towards the real pressure gradient over the domain. Inlet
CHAPTER 6. LATTICE BOLTZMANN MODELLING: IMPLEMENTATION

Figure 6.5: Simulation blow-up with velocity driven flow. The flow is forced through a number of small holes, where the velocity is rapidly increasing in order to maintain mass balance

and outlet was thus treated the following way:

\[
\bar{u}(1, j, k) = (u_x(2, j, k), 0, 0)
\]

\[
\rho(1, j, k) = \rho_1
\]

\[
\rho(N_x, j, k) = \frac{\rho_0 + \rho(N_x - 1, j, k)}{2}
\]

The pressure driven flow works better for flows in porous media, since if there is high resistance in the flow due to small channels, the velocity will decrease. The velocity is related to the pressure gradient through the material’s permeability which will be more discussed in the next chapter. However, the pressure gradient must be kept low enough so that the velocity does not at any point exceed \(c_s\).

### 6.4.3 Force driven flow

Since the simulations are going to be performed in a region where fluid can be treated as being incompressible, the pressure driven flow can be treated as a body force which acts on each particle distribution. The body forcing is usually introduced when the flow is driven by a constant force field e.g. gravity, but in this work this force takes the magnitude of the pressure gradient.
CHAPTER 6. LATTICE BOLTZMANN MODELLING: IMPLEMENTATION

The following modifications are done to the code for the implementation for the body forcing:

1. The pressure gradient is replaced with a constant force with the same magnitude:

\[ \Psi = \frac{\Delta p}{N_x} = \frac{(\rho_{\text{in}} - \rho_{\text{out}})}{3 \cdot N_x} \]  

(6.8)

The magnitude of the forcing term in this thesis is chosen to ensure \( Re << 1 \). The reason for this will be further discussed in Chapter 7 and 8.

2. It is just assumed force in X-direction. In the collision step (Eq. 6.3), \( F_a \) is therefore set to:

\[ F_a = \left( \frac{\tau - \frac{1}{2}}{\tau} \right) \left( \Psi_{a,x}^* \cdot \Psi \right) \]  

(6.9)

Here, \( \Psi_{a,x}^* \) are weight factors described in Table 6.1.

3. The velocity, calculated from Eq. 5.14, is corrected in the following way at each node:

\[ \rho \vec{u}(\vec{x}, t) = \left( \frac{\Psi}{2}, 0, 0 \right) + \sum_a f_a(\vec{x}, t) \cdot \vec{c}_a \]  

(6.10)

4. Inlet and outlet are treated as periodic boundaries:

\[
\begin{align*}
    f_a(1, j, k, t + 1) &= f_a(N_x, j - c_{ay}, k - c_{az}, t) \quad \text{if} \ c_{ax} = 1 \\
    f_a(N_x, j, k, t + 1) &= f_a(1, j - c_{ay}, k - c_{az}, t) \quad \text{if} \ c_{ax} = -1
\end{align*}
\]  

(6.11)

6.5 Convergence criteria

The following is set as convergence criteria for the simulations:

\[ \Omega = \left| \frac{\sum_{i,j,k} u_x(\vec{x}, t + 100)(1 - h(\vec{x})) - \sum_{i,j,k} u_x(\vec{x}, t)(1 - h(\vec{x}))}{\sum_{i,j,k} u_x(\vec{x}, t)(1 - h(\vec{x}))} \right| < 10^{-5} \]  

(6.12)

When this criteria is fulfilled, the simulation is considered to have reached steady state. Note that the criteria is set quite high for this type of simulations. However, to reach \( \Omega < 10^{-6} \) requires almost the double amount of iterations. The error due to the low convergence criteria is considered several orders less than the one arriving from errors in the segmentation and therefore a compromise is done to reduce the calculation time.
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6.6 Performance and compiling options

Running one of the fluid simulation in one of the domains described in Table 4.1, requires a lot of computer capacity. A calculation of a domain of size $600 \times 400 \times 90 = 21'600'000$ nodes, takes up around 9 GB of RAM, where the most of the memory is taking up by storing the particle distribution functions at double precision at each node.

The calculation time was seen to be rather dependent on the compiler and compiling options. At the end, it seemed Intel’s ifort was the optimal for this LB code and it was used with the following optimization flags:

ifort -openmp -shared-intel -mcmodel=large

The openmp-flag allows the parallelization on multiple cores using a shared memory while the shared-intel- and mcmodel=large-flags are required for running programs with large arrays.

In order to reach convergence determined by Eq. 6.12, which required about 5000-15000 iterations, the calculation time was reduced to 10-20 hours per sample.

The calculations were mainly performed on four eight-core workstations with Intel Xeon E5450 3.00 GHz processors. However, the calculation time was also largely dependent on the amount of cores used and type of processors. Several workstations at PSI was tested and benchmarked for this LB-model,
with the results shown in Figure 6.6. As seen, the performance could be largely improved by running on better processors and more cores. However, the amount of cores resulted just in a speed-up up to 6-8 cores, then it stayed practically the same. This is probably due to parts in the code which are not optimally parallelized. These will limit the overall performance and not be affected by the amount of cores. For this work, not much time was spent in optimizing the parallelization of the code since the steady state of the needed simulations could be obtained after an acceptable period of time.
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</table>

Table 6.1: Properties of the D3Q27 model used in this thesis
Chapter 7

Lattice Boltzmann Modelling: Obtaining gas transport properties

The output from the fluid simulation described in the previous chapter is the complete steady state velocity vector field $\vec{u}(\vec{x})$ and density scalar field $\rho(\vec{x})$. Using these quantities a number of gas transport properties of the porous media can be obtained. For this thesis, the main focus will be on gas permeability, but some effort was also made in estimating the relative diffusivity of the material.

7.1 Permeability

The convective transport through a porous media at low Reynolds numbers is described through Darcy’s law \cite{23,26}:

$$\bar{u}_{\text{mean}} = -\frac{k}{\rho \nu} \nabla p$$

(7.1)

where $\nu$ is the kinematic viscosity, $k$ is the constant permeability matrix

Figure 7.1: Flow behind a cylinder at $Re > 1$
of the porous sample and $\bar{u}_{\text{mean}}$ is the volumetric mean velocity inside the sample. This relation shows how the mean velocity is related to the pressure gradient $\nabla p$, so permeability can hence be seen as a measure of the porous media’s resistance applied to the flow. Doing a dimensional analysis, it is seen that the unit of the permeability coefficient is $[m^2]$. Darcy’s law is just valid for $Re << 1$, in the “creeping” flow regime. As soon as $Re \approx 1$, vortices start to form behind obstacles (Figure 7.1), leading to a dramatic decrease in permeability, since the average velocity of the vortex region is almost zero. The permeability will thus not be an independent material constant.

Keeping $Re << 1$, the full matrix can be obtained by simulating the flow in each spatial direction, and for each simulation, calculating the volumetric mean velocity in each direction. In order to simulate flow through the same sample in another direction, the sample itself is, as mentioned before, rotated so that the same code could be applied with forcing in $x$-direction. The following steps are done to calculate the permeability in this thesis:

1. Simulate the flow with forcing $\Psi_a = \Delta p/N_x$ in direction $a$.

2. Calculate the volumetric mean velocity in each direction $b$ through [23]:

$$u_{b,\text{mean}} = \frac{\sum_{i,j,k} u_b(\vec{x})}{N_x N_y N_z} \quad (b = x, y, z)$$  \hspace{1cm} (7.2)

3. The permeability coefficients $k_{ab}$ are obtained through:

$$k_{ab} = \left| \frac{\rho \nu u_{b,\text{mean}}}{\Psi_a} \right| \quad (b = x, y, z)$$  \hspace{1cm} (7.3)

The density $\rho$ in the LB simulations is not deviating more than $\rho \approx 1 \pm 10^{-4}$ and is therefore set to be the same everywhere and equal to 1 in the permeability calculation.

4. The permeability is converted from lattice units to real units using the knowledge that the voxel size is known to be $\Delta x$ metres.

$$k_{ab,\text{real}} = (\Delta x)^2 \cdot k_{ab}$$  \hspace{1cm} (7.4)

5. Steps 1-4 are repeated for all directions $a = x, y, z$ in order to obtain the full permeability matrix.
CHAPTER 7. LATTICE BOLTZMANN MODELLING: OBTAINING GAS TRANSPORT PROPERTIES

7.2 Relative diffusivity

The diffusive transport inside a porous media can be described through Fick’s first law [26]:

$$ j = -D_{ab}^{eff} \nabla c $$

(7.5)

where $c$ is the concentration, $j$ is the molar flux and $D_{ab}^{eff}$ is the effective diffusion matrix and can in turn be divided into the bulk diffusivity $D_{ab}$ and a material constant $\epsilon/T$:

$$ D_{ab}^{eff} = \frac{\epsilon}{T} D_{ab} $$

(7.6)

The factor $\epsilon/T$ is usually referred to as the effective relative diffusivity, where $\epsilon$ is the porosity of the porous sample and $T$ is the tortuosity. Tortuosity is a measure of how pores are connected inside the sample, but there is no definite way of defining it. In two dimensions the tortuosity of a flow can be seen as the ratio between the Euclidean distance between two points in the

Figure 7.2: Difference between Euclidean $L_E$ and geodesic $L_G$ distance in (a) 2D; (b) 3D ($L_G$ is the streamline length)
flow and the actual flow distance between the same points, see Figure 7.2. In three dimensions this is a loosely defined quantity. Gommes (2009) [27] describes the tortuosity in a given direction \( x \), by looking at planes normal to this direction. If the perpendicular distance from starting plane \( (x = 0) \) to an arbitrary parallel plane in the porous media \( (x = i) \) is defined by \( L_E \), and the geodesic distance \( L_G \) is the mean nearest distance in pore space between points on the planes, the tortuosity can be defined by:

\[
T = \left\langle \frac{L_G}{L_E} \right\rangle
\]  

(7.7)

Since the output of the LB simulations gives us the velocity vector field, streamlines through the samples can be defined. It is then possible to approximate the geodesic distance with the streamline length. In this thesis the following procedure was performed to obtain the effective relative diffusivity:

1. The resulting velocity field \( \vec{u}(\vec{x}) \) from the LB simulation is used to to plot streamlines from the inlet using MATLAB’s streamline function with seeding from the inlet.

2. Each streamline with total length \( L_s \), start coordinates \( (i,j,k)_{s,start} \) and end coordinates \( (i,j,k)_{s,end} \) is evaluated and the streamline’s tortuosity is defined by:

\[
T_s = \frac{L_s}{i_{s,end} - i_{s,start}}
\]  

(7.8)

3. The sample’s tortuosity in the specific direction is regarded as the mean of all \( N_s \) streamlines:

\[
T = \frac{1}{N_s} \sum_{s=1}^{N_s} T_s
\]  

(7.9)

4. The total porosity of the sample is defined as:

\[
N_{coid} = \sum_{i,j,k} (1 - h(i,j,k))
\]

\[
N_{total} = \sum_{i,j,k} 1
\]  

(7.10)

\[
\epsilon = \frac{N_{coid}}{N_{total}}
\]

,where \( h(i,j,k) \) is the obstacle function defined in 5.28.

5. The effective relative diffusivity is calculated through \( \epsilon/T \)
Chapter 8

Lattice Boltzmann Modelling: Verification of the method and choice of parameters

In Chapter 6, the LB-model used in this thesis was discussed. As mentioned, this model has not previously been tested for flow in porous media. A lot of tests were therefore made to verify it, in order to trust the results from the calculations. The most important tests, which lead to conclusions about the model are presented in this chapter.

8.1 Investigating parameter dependence

Before setting up the simulations, there are two parameters that need to be determined. The first one is the viscosity $\nu$ which also in this model is related to the relaxation time through Eq. 5.23. Changing the viscosity, means also changing the model’s Knudsen number through the relation:

$$Kn = \frac{3\nu}{L}$$

(8.1)

The second parameter is the pressure gradient $\Delta p$, which controls the Reynolds for a constant viscosity. The different tests in this section are conducted in order to observe the behaviour of the model when changing $\nu$ and $\Delta p$. Since both $Re$ and $Kn$ are not constant in the sample, a characteristic point is chosen inside the sample to estimate the magnitude of these non-dimensional numbers. As characteristic length $L$, the local pore diameter of this point is chosen.
CHAPTER 8. LATTICE BOLTZMANN MODELLING: VERIFICATION OF THE METHOD AND CHOICE OF PARAMETERS

8.1.1 Flow through a small GDL sample

This test is made in order to see if permeability measurements are consistent when changing $Re$ and $\nu$ for the flow. Also interesting to see, is if these parameters have an influence on the amount of iterations needed to reach convergence. Here, both pressure driven and force driven flow are tested. As domain, a small GDL sample of $100 \times 50 \times 90$ nodes is used (See Figure 8.1). As discussed in the previous chapter, the expected behaviour is to get results of the permeability which does not depend on $Re$ and $\nu$ as long as $Kn, Re << 1$.

The important results are shown in Figure 8.2. As expected, the permeability stays constant as long as $Re << 1$. It is also clear that going above $Re \approx 1$ the permeability drops, just as expected from the theory described in the previous chapter. However, there is a dramatic change of the permeability results when changing viscosity, even for $Kn << 1$. This effect is seen both for pressure driven and force driven flow, even though the latter shows a smaller dependence. The figures furthermore show that the permeability is converging to a single value as $Kn \rightarrow 0$.

The amount of iterations needed for convergence is showed in Figure 8.3. It is clear that the Reynolds number has little influence on the convergence. More important is the viscosity, where a high value leads to much faster convergence. Generally, a reduction of the viscosity with a factor two leads to around two times slower convergence.

The Reynolds number has little or no influence on either the convergence...
CHAPTER 8. LATTICE BOLTZMANN MODELLING: VERIFICATION OF THE METHOD AND CHOICE OF PARAMETERS

Figure 8.2: Diagrams showing permeability as a function of Reynolds number for different viscosities (a) Pressure driven flow; (b) Force driven flow.
CHAPTER 8. LATTICE BOLTZMANN MODELLING: VERIFICATION OF THE METHOD AND CHOICE OF PARAMETERS

Figure 8.3: Diagrams showing number of iterations needed for convergence as a function of Reynolds number for different viscosities (a) Pressure driven flow; (b) Force driven flow
or permeability. Therefore the pressure gradient $\Delta p$ should be chosen such that $Re \ll 1$ is ensured everywhere in the domain.

Far more concerning is the viscosity dependence. The problem has been reported by several authors before. Some believe it to be a problem with all methods which use a single relaxation time for all modes. Ginzburg et al. said in 2009 that "the permeability dependency on the viscosity is unavoidable when using the BGK-model, whatever boundary scheme is involved" [28]. This is however not a general acceptable opinion and other propose it to be rather a problem of the boundary conditions [24]. Pan et al. also observed this problem in 2005 [29] and proposed a multi relaxation time (MRT) degenerated LB-model, which could remove the dependency. However, such a model is restricted to Darcy regime flows and there is no guarantee of rotational and Galilean invariance. Additionally it is doubted that the degenerated LB-model could give meaningful results in the case where $Re \geq 1$. Furthermore, the relaxation times needs to be tuned for the particular problem.

Nabovati et al. (2009) [30] referred to [29] and stated that "the effect of the relaxation parameter dependency is negligible for $\tau = 1$". This means that at each time, the populations are set to equilibrium directly since Eq. 5.17 reduces to:

$$f_a(\vec{x} + \vec{c}_a, t + 1) = f^{eq}_a(\vec{x}, t) + F_a$$  \hspace{1cm} (8.2)

With $\tau = 1$, viscosity is $\nu = 1/6$ and this could be regarded as a singular value or a "special" case. However, the $Kn$ which is the smallness parameter in the Chapman-Enskog analysis (which is used to derive the Navier-Stokes equations) is not any more small for this value of viscosity. However, the method is used by several authors, even though many do not present which $\tau$ was used for their permeability calculations using the BGK-model [23,31,32]. Still, using this "magic" viscosity seems to work for any type of porous media and it is possible to obtain the correct permeability. Of course this leads to low flexibility of the method also since viscosity then will be a fixed constant.
8.1.2 Plane Poiseuille flow

During the time of this thesis, the particular guided equilibrium LB-model in 2D applied on a D2Q9-lattice was tested by co-worker Jinfen Kang. The scheme was tested for the plane Poiseuille flow, illustrated in Figure 8.4. The incompressible plane Poiseuille flow is one of the simplest types of flows and the analytical solution of the velocity profile can be directly derived from the Navier-Stokes equations. The permeability of the plane Poiseuille flow can be calculated by inserting the mean velocity of the profile in to Darcy’s law.
CHAPTER 8. LATTICE BOLTZMANN MODELLING: VERIFICATION OF THE METHOD AND CHOICE OF PARAMETERS

Figure 8.5: Deviation from the Navier-Stokes solution of the 2D Poiseuille flow as calculated with the analytical solution of the guided equilibrium LB-model with HBB boundary conditions compared to other LB-models and boundary conditions
in Eq. 7.1 and will then be \( k_{xx,\text{analytical}} = H/12 \).

\[
\begin{align*}
    u_x(y) &= -\frac{1}{2\rho\nu} \frac{\partial p}{\partial x} \left( y^2 - \left( \frac{H}{2} \right)^2 \right) \\
    u_y &= 0 \\
    u_z &= 0
\end{align*}
\]

Due to the simplicity of this flow, the LB-model’s actual analytical solution for the plane Poiseuille flow could be derived from the equations used. Figure 8.6 shows the different LB solutions’ deviation from the Navier-Stokes solution expressed with a percentage. Here the solution of the current implementation of the LB-model is compared with the analytical results of the same flow problem using the LB-model of He [33] with half-way bounce-back (HBB) and regular bounce-back (BB) boundary conditions. It was shown that the equilibrium state will always imply a small deviation from the analytical solution except for one optimal viscosity. This is precisely in line with the investigations performed in the previous section. The error also stays constant when decreasing the viscosity below \( \approx 0.01 \), which is consistent with the behaviour observed in Figure 8.2(b). The optimal viscosity seems to be dependent on the boundary scheme involved. Due to this and the fact that the error is reduced when increasing the amount of nodes furthermore indicates that this behaviour is due to the bounce-back boundary conditions at the wall. This had to be verified also for the D3Q27 model, but due to the increased level of complexity, the behaviour is easier to investigate using simulations.

Even though the plane Poiseuille flow is a 2D problem, the flow can be simulated with the 3D model using the periodic boundaries, which implies that the plates are assumed to have infinite width.

The comparison between analytical and numerical solution for the current LB-model is performed in order to observe the influence of two parameters: The amount of nodes in the channel \( (H) \) and the dependence of viscosity \( (\nu) \). Also for this test, pressure driven and force driven flow are compared. The Figure 8.6 shows the velocity profiles for the different \( H \) and \( \nu \) and comparing them with the analytical ones as calculated from the Navier-Stokes equations. By normalizing the velocities with the maximum analytical velocity, and doing a least square, second order polynomial fitting of the simulated points, the profiles in Figure 8.7 are obtained.

The ratio between \( k_{xx,\text{analytical}} \) and \( k_{xx,\text{LBM}} \) is just dependent on the ratio
CHAPTER 8. LATTICE BOLTZMANN MODELLING: VERIFICATION OF THE METHOD AND CHOICE OF PARAMETERS

Figure 8.6: Velocity profiles for plane Poiseuille flow. (a) Pressure driven, \( H=5 \); (b) Force driven, \( H=5 \); (c) Pressure driven, \( H=19 \); (d) Force driven, \( H=19 \)
Figure 8.7: Normalized velocity profiles for plane Poiseuille flow. (a) Pressure driven, H=5; (b) Force driven, H=5; (c) Pressure driven, H=19; (d) Force driven, H=19
between the analytical mean velocity and the simulated one. This means, that in order to observe the deviation from the analytical permeability, it is sufficient to look at how well the velocity profile fits to the analytical one.

For pressure driven flow it seems like velocity in the small channels are always underestimated regardless of which viscosity is chosen, while at larger channels, the velocity profile is only correct when using $\nu = 1/6$, i.e. $\tau = 1$. The reason for this might be that there are more density changes in the flow, meaning the analytical solution of this flow can no longer be treated incompressibly, and Eq. 8.3 doesn’t apply. However, the case of pressure driven flow is not further investigated due to the preferred properties of the force driven flow.

For force driven flow the profiles seems to fit the analytical results quite well. There are still errors for the small channel, but they are practically eliminated when going to channels containing more nodes. Looking at the normalized curves, they appear to just be shifted due to a slight slip velocity at the wall. This of course leads to a false result of the permeability calculation, since the mean velocity is used for this. This slip velocity can be approximated using the value at the wall for the fitted curves and then plotted against viscosity for different channel heights. This is done in Figure 8.8.

Obviously, there seems to be a certain viscosity where slip velocity is at minimum for all channel heights, just like for the 2D case. For the current
CHAPTER 8. LATTICE BOLTZMANN MODELLING: VERIFICATION OF THE METHOD AND CHOICE OF PARAMETERS

Figure 8.9: Normalized permeability as a function of viscosity for different channel heights

implementation, this is not the reported value of $\nu = 1/6$ ($\tau = 1$), but rather $\nu \approx 1/30$ ($\tau \approx 0.6$). Another way of looking at slip velocity is to instead consider wall movement. It seems that the point of zero velocity, which should be the wall, is moving between the two outermost nodes under the influence of viscosity. When looking close to the wall in Figure 8.7(b) it seems that this point is actually half-way in-between these nodes only when $\nu \approx 1/30$. Since the exact wall position between the two nodes is just important for a channel with few nodes, the slip velocity goes to zero with increased resolution. This is a strong indication that the problem actually arrives from the boundary.

The slip velocity however does not seem to be the only source of error in small channels. For $1/30 \lesssim \nu \lesssim 1/10$, it seems that the velocity close to the centreline is underestimated, even though there is a positive slip velocity. The mean velocity, and thus also the permeability, in the channel will then be correctly obtained by using a viscosity value in this regime. This is shown in Figure 8.9.

Another fact that must be mentioned is the error arriving from the discrete description of the channel. The discretization error of the permeability is easy to estimate using the real mean velocity, compared to the mean analytical velocity at the discrete points. This error is significant in really small channels but goes away when increasing the number of nodes, see Figure 8.10. The discretization error is calculated by dividing the discrete analytical mean
with the continuous analytical mean:

$$DE = \frac{1}{H} \left[ \sum_{i=1}^{H} \left( y_i^2 - \left( \frac{H}{2} \right)^2 \right) - \frac{1}{H} \int_{-H/2}^{H/2} \left( y^2 - \left( \frac{H}{2} \right)^2 \right) dy \right] \left( \frac{1}{H} \int_{-H/2}^{H/2} \left( y^2 - \left( \frac{H}{2} \right)^2 \right) dy \right)^{-1}$$  \hspace{1cm} (8.4)

Since the simulated values are discrete, the comparison in Figure 8.9 use the discrete analytical solution as reference.

The remaining conclusion is that force driven flow at $\nu \approx 1/30$ is applicable for a permeability estimation of a porous sample containing different pore sizes, since the slip velocity at the boundary is at minimum. Even though these tests show that there is still a slight deviation from the centreline velocity when minimizing slip, this is hard to control in a complex porous media. Therefore the conclusion is drawn to minimize the slip velocity anyway. Furthermore it seems that the dependence on viscosity is largely reduced by increased resolution. The transport in the GDL mainly is through pores of 10-20 nodes, so choosing a value of viscosity between $1/30 \lesssim \nu \lesssim 1/15$, will keep the error of permeability to below 5%, which then most probably is significantly smaller than errors arriving from segmentation.
CHAPTER 8. LATTICE BOLTZMANN MODELLING: VERIFICATION OF THE METHOD AND CHOICE OF PARAMETERS

8.1.3 Effect from upscaling and downscaling

The results in Section 8.1.2 show the fact that the viscosity dependence seem to vanish as the flow is described with more nodes. This leads to the obvious question: By increasing the amount of nodes in the porous media, will the permeability dependency be smaller?

For this investigation, the same GDL sample is used as in Section 8.1.1 for force driven flow, but the amount of nodes is changed once by upscaling and once by downscaling the sample. For the upscaling each voxel is duplicated in each spatial direction. The amount of nodes are then eight times as many in a domain of size $200 \times 100 \times 180$. Note that the geometry is thus not changed from the sample in Section 8.1.1.

For the downscaling, the number of nodes is reduced by turning a cube of eight voxels into one voxel. The resulting sample then gets the dimensions $50 \times 25 \times 45$ nodes. The merging then follows the following rules, which also is illustrated in Figure 8.11:

Figure 8.11: Illustration of the effect of upscaling and downscaling the porous media
Figure 8.12: Diagram showing permeability dependence of scale for different viscosities, Force driven flow

1. If the sum of the eight original voxels are $< 4$, then the new voxel gets value 0.

2. If the sum of the eight original voxels are $> 4$, then the new voxel gets value 1.

3. If the sum of the eight original voxels are $= 4$, then the new voxel gets either value 1 or 0 and is determined by random.

The results from upscaling and downscaling the GDL sample are shown in Figure 8.12. Just as expected, the viscosity dependency is reduced and the permeabilities seem to converge into one point at around $2.5 \cdot 10^{-5}$ mm$^2$. The permeability for viscosities equal to 0.02-0.04, stays fairly constant regardless of how many nodes are used to describe the geometry. These results are in line with the results of the plane Poiseuille flow results in Section 8.1.2, where it could be seen that the velocity profiles all seem to come closer to the analytical one, when increasing the amount of nodes. Having a complex geometry, increasing the amount of nodes sufficiently much will lead to more and more viscosity independent permeability results. This will however in turn dramatically increase the calculation time, since it grows linearly with the amount of nodes.
What is also noticeable is that for $\nu \approx 1/30$ the permeability stays almost the same, even when downscaling. This in spite of the fact that the geometry has been slightly coarse-grained for this case. The porosity stays however somewhat constant. This indicates that a small downscaled sample could be used as first approximate results, or as initial conditions for the upscaled geometries.
CHAPTER 8. LATTICE BOLTZMANN MODELLING: VERIFICATION OF THE METHOD AND CHOICE OF PARAMETERS

8.2 Comparison with known data

In Section 8.1.2, the plane Poiseuille flow was investigated to compare how well the simulations fit the analytical results. It was shown that for force driven flow with $\nu \approx 1/30$, the compliance to the analytical solution was very good. The problem is that it can’t be verified against analytical solutions of random complex geometries since such does not exist.

In 2009, Becker et al. [26] showed the influences of GDL compression on material properties by combining XTM and numerical simulations. In their work, XTM tomograms of a small GDL sample was obtained at three different compression rates. The compression in turn affected the porosity inside the sample. Flow simulations were then performed on the segmented XTM data using the FFF-Stokes solver [34]. Values on the permeability of these samples could thus be obtained. Also effective relative diffusivity was obtained by simulating diffusive transport using the explicit jump solver by Wiegmann and Zemitis [35].

In this thesis, the same segmented structures as used by Becker et al. are used for verifying the LB-model. These GDL samples had higher resolution then the ones previously tested in Section 8.1. The voxel size is of 0.74 $\mu$m, and the uncompressed sample consisted of $600 \times 600 \times 224$ nodes. For this test, the force driven LB-model with $\nu = 1/30$ is used for simulating the flow through the samples. Afterwards, the values of permeability and effective relative diffusivity are calculated and compared with the ones of Becker et al.

Although solving different equations, the permeability calculated from the LB simulations show very good agreement with the results from the FFF-Stokes solver, as shown in Figure 8.13. This together with the results from Section 8.1 gives a good validation of the method for calculating permeability of complex porous structures. The values of the effective relative diffusivity however show a significant deviation from the ones calculated using the explicit jump solver (see Figure 8.14). The values behave similarly when increasing the porosity and are in the same order of magnitude. The remaining conclusion is that the method presented in Section 7.2 should probably not be considered anything else as an estimate of the in-plane effective relative diffusivity. For the through-plane case, the diffusivity deviates quite a lot from both measurements and the results from the explicit jump solver. The probable reason for this is the fact that the streamlines are too short, i.e. the GDL is too thin, to estimate a valid tortuosity through the material.
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Figure 8.13: Permeability comparison with the FFF-Stokes solver

Figure 8.14: Effective relative diffusivity comparison with the explicit jump solver
Chapter 9
Lattice Boltzmann Modelling: Results

After implementing (Chapter 6) and carefully testing (Chapter 8) the LB-model, it can be applied to the task at hand, which is to investigate the influence of liquid water saturation on the gas transport in the GDL of a running PEFC.

Sample A and Sample B are divided into the twelve regions as described in Section 4.1. The LB simulations are performed in three directions:

- IP-X = In-plane direction through the GDL parallel to flow field direction.
- IP-Y = In-plane direction through the GDL perpendicular to flow field direction.
- TP-Z = Through-plane direction through the GDL.

and are done both for the saturated and non-saturated samples, thus amounting to 72 different simulations. Afterwards, permeability and diffusivity are evaluated using the methods described in Chapter 7.

Figure 9.1 illustrates how the flow field changes under the influence of saturation in case of the Channel domain of Sample A. The velocity scale is the same for all sub-figures, so the fact that colour of the streamlines in the wet domain are more shifted to blue, means that the flow is generally slower. This in turn means that the material’s permeability is reduced due to the liquid water since the forcing term was identical for all the cases.
CHAPTER 9. LATTICE BOLTZMANN MODELLING: RESULTS

Figure 9.1: Figure of flow through the Channel domain of Sample A in IP-X direction. (a) dry domain; (b) wet domain; (c) streamlines of dry domain; (d) streamlines of wet domain

The other regions of Sample A and different flow directions are illustrated in Appendix A.

9.1 Permeability

The results from calculating the permeability from each flow simulation are displayed in Figure 9.2. As is seen, the permeability is usually higher in in-plane direction, and the Channel domain seems to always be more permeable than the Ribs. Furthermore, the dry permeability varies a lot between the same region (Channel, Left Rib and Right Rib) for the different samples. This shows that the sample sizes are smaller than the representative elementary volume (REV) of Toray TGP-H-060 GDL paper, i.e. they might be too small to be able to evaluate the behaviour in a specific region. The figure also shows that the permeability drops as the GDL gets saturated.

9.1.1 Permeability dependence on saturation

To investigate the permeability dependence on saturation, the relative permeability is evaluated. The reference value is the permeability of the dry
Figure 9.2: Scatter plots of real permeability vs region. (a) IP-X direction; (b) IP-Y direction (c) TP-Z direction
structure for each simulation respectively. Using the relative measure, it is possible to reduce the viscosity dependence of permeability which was presented in Chapter 8. This is shown in Figure 9.3, where the flow through the dry and wet sample is simulated using different viscosities. Even though the viscosity lies within a range where the slip velocity effects are anything but constant (compare also with Figure 8.6), the relative permeability change between dry and wet stays practically the same.

The relative permeability is plotted against saturation for all test samples in Figure 9.4. In the scatter plots, the relation commonly used in GDL modelling, \( k_{\text{rel}} = (1 - s)^3 \) [9,36], is also displayed as a reference. In Figure 9.4, it’s hard to determine if there is any directional dependence on the permeability drop due to saturation. By plotting the difference of the relative permeabilities, there is the possibility to investigate if the water inside the GDL is blocking more in any of the given directions, but in Figure 9.5 such an anisotropy can’t be detected.

The Figures 9.4 and 9.5 show that the relationship of \( k_{\text{rel}} = (1 - s)^3 \) could be nicely reproduced by the XTM/LBM results and it seems this relation is a good estimate when evaluating relative permeability in the GDL during operation. Furthermore, no distinct difference in the relative permeability drop with respect to the direction could be observed.
Figure 9.4: Scatter plots of relative permeability vs saturation. The mentioned power law of $k_{rel} = (1 - s)^3$ is drawn in black. (a) IP-X direction; (b) IP-Y direction (c) TP-Z direction
CHAPTER 9. LATTICE BOLTZMANN MODELLING: RESULTS

9.1.2 Permeability dependence on void fraction

The water inside the GDL is filling up the pores and therefore reducing the void fraction of the samples. How this affects the permeability is shown in Figure 9.6. From the figures, there seems to be a strong correlation between void fraction and permeability in the GDL. For the through-plane case, the permeability is not increasing quite as fast as the in-plane cases when increasing the void fraction. As was seen in Figures 4.5 and 4.6, the porosity was lower on the GDL boundaries due to presence of binder. For the through-plane case, this region is what is limiting the permeability, whilst for in-plane, the main flow goes through the porous middle region of the GDL, and is rather unaffected by the binder.

9.1.3 Permeability dependence on mean pore diameter

The void fraction does, as discussed before, not tell the whole story about the structure of the GDL. If, for example, just small pores are filled with water, then the flow might be rather unaffected even though void fraction is reduced, since it’s mainly concentrated to the larger pores.

To try and explain this a little bit clearer, consider a porous media with the cross section like in Figure 9.7. In the dry structure, the relevant flow is through the large pore, since the boundary surface area is relatively small compared to the volume, and hence flow resistance is smaller in this pore. If
CHAPTER 9. LATTICE BOLTZMANN MODELLING: RESULTS

Figure 9.6: Scatter plots of real permeability vs void fraction. Dry case is plotted with thicker lines on the symbols. (a) IP-X direction; (b) IP-Y direction; (c) TP-Z direction
CHAPTER 9. LATTICE BOLTZMANN MODELLING: RESULTS

Figure 9.7: Example of how mean pore diameter can affect the permeability

the smaller pores are filled up, the void fraction goes down, but almost the same flow is pushed through the large pore. If the large pored is filled up with water, the flow is forced through the smaller channels with more resistance, and thus also the permeability change will be more dramatical even though the void fraction reduction was the same. What is a better measure to compare the two cases? One answer can be the mean pore diameter. For case 1 the mean pore diameter is increasing, while for case 2 it is decreasing. If both large and small pores are affected by the water, the mean pore diameter goes down with about the same rate as the void fraction.

How the permeability changes for all test samples is illustrated in Figure 9.8. From this figure, it seems the mean pore diameter does indeed follow the trend of the void fraction, and thus showing a similar correlation to the permeability. This shows that water primarily is filling up medium and larger sized pores rather than the small pores, which is in line with the histograms showed in Figures 4.10 - 4.13.

9.2 Effective relative diffusivity dependence on saturation

The effective relative diffusivity, $\epsilon/T$, is, as discussed in Section 7.2 not dependent on anything else than the geometry. Therefore these results do not depend on the chosen lattice viscosity and the steady state flow field looks
Figure 9.8: Scatter plots of real permeability vs mean pore diameter. Dry case is plotted with thicker lines on the symbols. (a) IP-X direction; (b) IP-Y direction (c) TP-Z direction
Figure 9.9: Scatter plots of effective relative diffusivity vs saturation. Dry case is plotted with thicker lines on the symbols. (a) IP-X direction; (b) IP-Y direction (c) TP-Z direction

Just as for permeability, the effective relative diffusivity seem to decrease with increased saturation in the GDL, see Figure 9.9. The results show that the correlation furthermore is higher for the in-plane directions than for the through-plane. This is probably due to the issues discussed in Section 8.2, that the tortuosity is not correctly evaluated in through-plane, due to the short streamline length.

the same as long as $Re << 1$.
9.3 Permeability dependence on effective relative diffusivity

The previous results show that both permeability and effective relative diffusivity decrease with increased saturation. To see how these two quantities are correlated, the scatter plots in Figure 9.10 are made. It seems from these plots that permeability and effective relative diffusivity are highly correlated, at least in the in-plane direction. For through-plane, the results are more spread out, and this is probably due to the previously mentioned issues of the through-plane tortuosity.

As a comment, permeability of porous media can be described with the so...
Figure 9.11: Permeability of Channel region of Sample A in IP-X direction depending on segmentation thresholds. (a) Dry structure, changing solid threshold; (b) Wet structure, changing water threshold

called Kozeny-Carman equation [37], with a dependency of

\[ k \propto \frac{\epsilon}{S^2(1 - \epsilon)^2 \left( \frac{\epsilon}{T} \right)^2}. \]

(9.1)

where \( S \) is the specific surface of the solid volume. It seems therefore that effective relative diffusivity should be correlated to the permeability. As a future perspective it might be interesting to investigate the properties in this equation further to be able to compare with the results.

### 9.4 Permeability dependence on segmentation thresholds

In Section 4.5, it was seen that the segmentation thresholds could have a significant influence on porosity and saturation inside the sample. Since these quantities influences the gas transport, it is considered valuable to see how the permeability and diffusivity changes due to changed threshold values. For this test the segmentation is performed without any manual correction of the domains as described in Section 3.5.

This test is done by simulating flow in IP-X direction through the Channel region of Sample A. This is divided into two parts:
1. Changing solid threshold of the dry data set with +4, +2, 0, -2 and -4 % change from originally chosen values and simulate flow through the dry structure.

2. Changing water threshold of the difference data set with +1, +0.5, 0, -0.5 and -1 % change from originally chosen values while keeping solid threshold at fixed level of 0 % change and simulate flow through the wet structure.

The results are shown in Figures 9.11 and 9.12. For permeability, the thresholds have high influence on the obtained results and the result for this case varies in the region of $1.4 \cdot 10^{-5} \pm 10^{-6}$ mm$^2$. This is due to the same fact that was observed in Section 4.5.2, i.e. that porosity is also changing significantly when varying the solid threshold. For the water threshold, it was also previously seen in Section 4.5.1, that the porosity and saturation were just marginally affected, hence leading to a small difference in permeability as well. However, taking the worst case scenarios when choosing the thresholds, the relative permeability can vary in the region of $0.60 \pm 0.06$ which is significant and shows once more the importance of choosing correct thresholds. By having experience, observing carefully when choosing the thresholds and also using manual correction, the error can probably be narrowed to lie within $\pm 0.02$. 

Figure 9.12: Diffusivity of Channel region of Sample A in IP-X direction depending on segmentation thresholds. (a) Dry structure, changing solid threshold; (b) Wet structure, changing water threshold
9.5 Comparing results with other software

In order to once more verify the obtained results, a software called GeoDict developed by Fraunhofer ITWM is used. This program is used to calculate permeability and diffusivity of the Channel region of Sample A, both with and without water. The results are illustrated in Figure 9.13.

The results show quite good agreement between the methods. If seeing the GeoDict results as the benchmark, the LB-model in the current implementation is slightly overestimating the permeability for the dry case and slightly underestimating for the wet case. For diffusivity, the streamline seems to only give fair results in the dry in-plane case.

![Figure 9.13: Comparison with the GeoDict software. (a) Permeability of wet and dry channel domain comparing LBM and the GeoDict software; (b) Effective relative diffusivity of wet and dry channel domain comparing LBM and the GeoDict software](image)
Chapter 10

Conclusions

10.1 Conclusions from the PEFC point of view

In this thesis it was proven that in-situ X-Ray Tomographic Microscopy, combined with Lattice Boltzmann Modelling, is a very powerful tool in order to obtain saturation dependent gas transport properties in PEFC Gas Diffusion Layers. Until present day, this has been an experimentally, very difficult task and previous simulations, like [38], have not used electrochemically produced water inside the GDL.

From the investigations in this thesis it was shown that permeability and diffusivity decreased with increased saturation. Relative permeability decreased with a very good correspondence to \( k = (1 - s)^3 \). Water seems furthermore to be arranged in the pore network of Toray TGP-H-060 GDL paper in such a way that the permeability drop is roughly the same in each Cartesian direction.

The permeability also seemed to be strongly correlated to both void fraction and mean pore diameter, which is reasonable since both quantities decrease with increased saturation. From analysing the mean pore diameter and void fraction of the GDL samples, a conclusion could not be drawn about where water usually accumulates in the GDL network. Since mean pore diameter is decreasing with about the same rate as the void fraction, the only conclusion from the pore diameter histogram analysis is that water is mainly filling up larger sized pores but smaller pores can also be affected.

Even though the scanned PEFCs were operating at the same current density of 0.45 A/cm\(^2\) and at high stoichiometry, the saturation levels of the
simulation domains differed from 0.1-0.4. This is probably due to the fact that the tested GDL samples are a lot smaller than the REV of the material. So, drawing any conclusions about how the water content behaves when changing the operation point, is too early from these results. As a future perspective, in order to achieve this, larger domains must be investigated and more statistics are needed.

It was shown that the segmentation process is very crucial for obtaining the correct permeability. The grey scale thresholds for determining which material is water and solid must be very carefully chosen. The segmentation process can also further be improved to increase the accuracy close to the catalyst layer.

10.2 Conclusions from the LBM point of view

A major part of the thesis was to further develop a Lattice Boltzmann Model for porous media simulations. The model was well tested for permeability calculations, where a big difficulty was to remove the dependency of lattice viscosity on the obtained results. The model shows that permeability values converge as $\nu$ goes to zero. Using the half way bounce back, the permeability will be underestimated at low viscosities due to slip velocity at the wall. Using the model presented in this thesis for a viscosity in the region $1/30 \lesssim \nu \lesssim 1/15$, the correct permeability of the porous media can be obtained. By implementing new boundary conditions, the problem of viscosity dependent permeability is believed to be removed.

The tests in the thesis proved that the method showed grid convergence, leading to exact values of permeability with increasing amount of nodes. Of course, this will lead to much longer calculation times. To decrease the calculation time, future development would include more effective parallelization and starting from a better initial condition using a solution from a downscaled flow field.

The method for analysing the effective relative diffusivity seemed not to be accurate enough, especially in through-plane direction. Using the streamline method as described in this thesis, the results can just be evaluated qualitatively. The method can probably be improved, but one would rather use other software, like GeoDict to obtain the quantity more accurately.

Both permeability and diffusivity are quantities which are obtained in the
Darcy regime where $Re << 1$. In this regime the advective term in the Navier-Stokes equations is negligible and the Stokes equations can be fully sufficient to describe the flow. Comparing the performance between the current LB model in comparison with Stokes based solvers, the LB simulations are very time-consuming even though the results are basically the same. The remaining conclusion is that the strength of the LB model is it’s flexibility, since it can be used to simulate flow, not just in the Darcy regime, but also when $Re \geq 1$. Therefore, simulating real gas behaviour in the PEFC, which is usually with a $Re > 1$, is best done with the LB-method. Due to the way the LB-method is implemented, this model can easily be extended to simulate the flow’s behaviour under the influence of thermal gradients. But if material constants like diffusivity and permeability needs to be obtained, this is best done with software like GeoDict.
Chapter 11

List of symbols and abbreviations

11.1 Symbols

\( \epsilon \) Porosity
\( s \) Liquid water saturation
\( N \) Amount of voxels or lattice nodes

\( \rho \) Fluid density
\( \vec{p} \) Fluid momentum
\( p \) Fluid pressure
\( \vec{u} \) Fluid velocity
\( U \) Absolute fluid velocity
\( \vec{u}_s, \vec{u}_{\text{slip}} \) Absolute slip velocity at wall
\( U_c \) Absolute centreline velocity
\( \nu \) Kinematic viscosity
\( \vec{\Psi} \) External volumetric force
\( Re \) Reynolds number
\( Kn \) Knudsen number

\( \vec{c}_a \) Discrete lattice velocity in direction \( a \)
\( \vec{c}_{a,\text{opp}} \) Discrete lattice velocity in opposite direction to \( a \)
CHAPTER 11. LIST OF SYMBOLS AND ABBREVIATIONS

\( f \) Particle probability distribution function

\( f_a \) Lattice Boltzmann distribution function of population moving in direction \( a \)

\( f_{eq} \) Equilibrium distribution function

\( f_{eq}^a \) Lattice Boltzmann equilibrium distribution function of population moving in direction \( a \)

\( c_s \) Lattice sound speed

\( \tau \) Lattice Boltzmann relaxation time

\( T_{LB} \) Lattice temperature

\( h \) Binary Lattice Boltzmann obstacle function

\( \Omega \) Convergence criteria

\( H \) Height of channel

\( k, k_{ab} \) Permeability matrix

\( k_{rel} \) Relative permeability

\( D_{ab}^{eff} \) Effective diffusion matrix

\( c \) Concentration

\( D_{ab} \) Bulk diffusivity

\( \epsilon/T \) Effective relative diffusivity

\( T \) Mean tortuosity

\( T_s \) Tortuosity of streamline \( s \)

\( L_G \) Geodesic distance

\( L_E \) Euclidean distance

\( N_s \) Amount of streamlines

\( \vec{r} \) Position vector (continuous)

\( \vec{x} = (i, j, k) \) Discrete position vector in lattice

\( X, Y, Z \) Directions in the tomographic data

\( x, y, z \) Directions in the Lattice Boltzmann model

\( \text{IP-X} \) In-plane direction through the GDL parallel to flow field direction.
CHAPTER 11. LIST OF SYMBOLS AND ABBREVIATIONS

IP-Y   In-plane direction through the GDL perpendicular to flow field direction.

TP-Z   Through-plane direction through the GDL.
### 11.2 Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>BGK</td>
<td>Bhatnagar-Gross-Krook model</td>
</tr>
<tr>
<td>CCD</td>
<td>Charge-Coupled Device</td>
</tr>
<tr>
<td>CCM</td>
<td>Catalyst coated membrane</td>
</tr>
<tr>
<td>CL</td>
<td>Catalyst layer</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational fluid dynamics</td>
</tr>
<tr>
<td>D\textsubscript{nQm}</td>
<td>Description of lattice with amount of dimensions $n$ and amount of discrete velocities $m$, for example D3Q27</td>
</tr>
<tr>
<td>DE</td>
<td>Discretization error</td>
</tr>
<tr>
<td>FFP</td>
<td>Flow field plates</td>
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<tr>
<td>GDL</td>
<td>Gas Diffusion Layer</td>
</tr>
<tr>
<td>HBB</td>
<td>Half-way bounce-back</td>
</tr>
<tr>
<td>KTH</td>
<td>Royal Institute of Technology, Stockholm</td>
</tr>
<tr>
<td>LB</td>
<td>Lattice Boltzmann</td>
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<tr>
<td>LBE</td>
<td>Lattice Boltzmann Equation</td>
</tr>
<tr>
<td>LBGK</td>
<td>Lattice Bhatnagar-Gross-Krook model (Single relaxation time model)</td>
</tr>
<tr>
<td>LBM</td>
<td>Lattice Boltzmann Modelling</td>
</tr>
<tr>
<td>lu</td>
<td>Lattice unit</td>
</tr>
<tr>
<td>MEA</td>
<td>Membrane Electrode Assembly</td>
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<tr>
<td>MFC</td>
<td>Mass flow controllers</td>
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<tr>
<td>MPD</td>
<td>Mean pore diameter</td>
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<tr>
<td>MRT</td>
<td>Multi-Relaxation time model</td>
</tr>
<tr>
<td>NSE</td>
<td>Navier-Stokes Equations</td>
</tr>
<tr>
<td>PEFC</td>
<td>Polymer Electrolyte Fuel Cell</td>
</tr>
<tr>
<td>PTFE</td>
<td>Polytetrafluoroethylene (commonly known as Teflon)</td>
</tr>
<tr>
<td>PSI</td>
<td>Paul Scherrer Institute</td>
</tr>
<tr>
<td>REV</td>
<td>Representative elementary volume</td>
</tr>
<tr>
<td>SLS</td>
<td>Swiss Light Source</td>
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<tr>
<td>ts</td>
<td>time-step</td>
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### Chapter 11. List of Symbols and Abbreviations

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOMCAT</td>
<td>Tomographic Microscopy and Coherent Radiology experiments beamline at the SLS</td>
</tr>
<tr>
<td>XTM</td>
<td>X-Ray tomographic microscopy</td>
</tr>
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</table>
Bibliography


BIBLIOGRAPHY


Appendix A

Sample A flow visualization
APPENDIX A. SAMPLE A FLOW VISUALIZATION

A.1 Channel

A.1.1 IP-X

Figure A.1: Figure of flow through the Channel domain of Sample A in IP-X direction. (a) dry domain; (b) wet domain; (c) dry domain with streamlines; (d) wet domain with streamlines; (e) streamlines of dry domain; (f) streamlines of wet domain
Figure A.2: Figure of flow through the Channel domain of Sample A in IP-Y direction. (a) dry domain; (b) wet domain; (c) dry domain with streamlines; (d) wet domain with streamlines; (e) streamlines of dry domain; (f) streamlines of wet domain
A.1.3 TP-Z

Figure A.3: Figure of flow through the Channel domain of Sample A in TP-Z direction. (a) dry domain; (b) wet domain; (c) dry domain with streamlines; (d) wet domain with streamlines; (e) streamlines of dry domain; (f) streamlines of wet domain
A.2 Left Rib

A.2.1 IP-X

Figure A.4: Figure of flow through the Left Rib domain of Sample A in IP-X direction. (a) dry domain; (b) wet domain; (c) dry domain with streamlines; (d) wet domain with streamlines; (e) streamlines of dry domain; (f) streamlines of wet domain
Figure A.5: Figure of flow through the Left Rib domain of Sample A in IP-Y direction. (a) dry domain; (b) wet domain; (c) dry domain with streamlines; (d) wet domain with streamlines; (e) streamlines of dry domain; (f) streamlines of wet domain
Figure A.6: Figure of flow through the Left Rib domain of Sample A in TP-Z direction. (a) dry domain; (b) wet domain; (c) dry domain with streamlines; (d) wet domain with streamlines; (e) streamlines of dry domain; (f) streamlines of wet domain
Figure A.7: Figure of flow through the Right Rib domain of Sample A in IP-X direction. (a) dry domain; (b) wet domain; (c) dry domain with streamlines; (d) wet domain with streamlines; (e) streamlines of dry domain; (f) streamlines of wet domain
A.3.2 IP-Y

Figure A.8: Figure of flow through the Right Rib domain of Sample A in IP-Y direction. (a) dry domain; (b) wet domain; (c) dry domain with streamlines; (d) wet domain with streamlines; (e) streamlines of dry domain; (f) streamlines of wet domain
Figure A.9: Figure of flow through the Right Rib domain of Sample A in TP-Z direction. (a) dry domain; (b) wet domain; (c) dry domain with streamlines; (d) wet domain with streamlines; (e) streamlines of dry domain; (f) streamlines of wet domain.