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VOF modelling of gas–liquid flow in PEM water electrolysis cell micro-channels

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ABSTRACT

In this study, the gas–liquid flow through an interdigitated anode flow field of a PEM water electrolysis cell (PEMEC) is analysed using a three-dimensional, transient, computational fluid dynamics (CFD) model. To account for two-phase flow, the volume of fluid (VOF) method in ANSYS Fluent 17.2 is used. The modelled geometry consists of the anode channels and the anode transport layer (ATL). To reduce the complexity of the phenomena governing PEMEC operation, the dependence upon electro-chemistry is disregarded. Instead, a fixed source of the gas is applied at the interface between the ATL and the catalyst layer. An important phenomenon that the model is able to capture is the gas–liquid contact angle on both the channel wall and ATL-channel interface. Particularly, the latter interface is crucial in capturing bubble entrainment into the channel. To validate the numerical simulation, photos taken of the gas–liquid flow in a transparent micro-channel, are qualitative compared against the simulation results. The experimental observations confirm the models prediction of long Taylor bubbles with small bubbles in between. From the simulation results, further intriguing details of the flow are revealed. From the bottom to the top of the outgoing channel, the film thickness gradually increases from zero to 200 μm. This increase in the film thickness is due to the particular superficial velocity field that develops in an interdigitated flow. Here both the superficial velocities change along the length of the channel. The model is capable of revealing effect of different bubble shapes/lengths in the outgoing channel. Shape and the sequence of the bubbles affect the water flow distribution in the ATL. The model presented in this work is the first step in the development of a comprehensive CFD model that comprises multiphase flow in porous media and micro-channel, electro-chemistry in catalyst layers, ion transport in membrane, hydrogen evolution, etc. The model can aid in the study of gas–liquid flow and its impact on the performance of a PEMEC.

Introduction

It is highly agreed that the emission of greenhouse gases (GHG) is the greatest cause of global warming. A large fraction of the emitted GHG originates from the use of fossil fuels in energy production and transportation [1]. Denmark has started using different methods for the green transition. An energy agreement was signed by Danish government in 2012 with the target of supplying at least 50% of the electricity consumption using wind power by 2020. Moreover, the target claims that 35% of the total consumption of energy should be

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supplied from renewable energy sources. To achieve these targets, a full reorganisation of the energy matrix with renewable sources is required [2]. Such a transition needs a high degree of energy availability and storage capacity of secondary fuels produced from electricity. Here, electrolysers play a vital role as a means of converting and storing energy. By converting water and electricity into hydrogen, an efficient energy carrier is produced. As a chemical compound, hydrogen is furthermore useful in various applications; from production of chemicals to fuel cell based vehicles [3–5].

Water electrolysis will play a key role in the future renewable energy system to facilitate storage of intermittent renewable energy from wind and sun. The key challenge facing the hydrogen based energy production is sustainable production of hydrogen, without dependence on fossil fuels, in large quantities at lower costs than existing technologies [6].

Unlike Alkaline water electrolysers, proton exchange membrane electrolysis cells (PEMEC), offer significantly higher current densities, and in turn a more compact design. Even with the expensive noble metals as an electro-catalyst that the technology uses at the current time, its capabilities such as large load range (10–200%), rapid dynamic response and high operating pressure are supposed to overcome its drawbacks [7].

Han et al. [8] one-dimensionally modelled gas–liquid flow inside ATL. They captured the limiting value of current density by increasing voltage. They depicted that the ATL contact angle, porosity and thickness has a great impact on ATL. They concluded that high ATL porosity and low surface contact angle improves PEMEC performance at high current densities. Yigit et al. [9] have done dynamic simulation of a PEMEC system using Simulink in MATLAB. Their study showed stack has the highest loss than other components like water pump, cooling fan and etc, especially at high current density. Tijani et al. [10] studied effect of different temperatures, pressures and membrane thicknesses on the performance of a PEM electrolyser. They found that by increasing current density, Faraday efficiency increases but by decrease in membrane thickness, Faraday efficiency decreases.

Regular PEM water electrolysers are commonly operated at a current density of about 1 A/cm^2. One means of increasing the hydrogen to cost ratio of the technology, is to increase the operating current density. This statement holds true, since the major cost of the system is the fixed cost associated with building the electrolyser. Thus, by simply increasing the production yield, the hydrogen to cost ratio has to decrease. Therefore, heat and mass transfer management in the anode transport layer (ATL) and flow plates at high current densities becomes essential.

These conditions may cause maldistribution of heat and water. By improving the cell performance for high current density condition, the technology will be matured for hydrogen production in large scales with a high efficiency. This necessitates that more understanding of the gas–liquid flow in both the ATL and the micro-channel from both numerical and experimental methods are crucial. Therefore, knowledge of the flow pattern forming under a given inlet and operational condition is essential for predicting the behaviour of gas–liquid flow in micro-channels.

Six major flow regimes can be distinguished in microchannels [11]: bubbly and Taylor flows that are dominated by surface tension, the churn and Taylor-annular flows that are transitional, and the dispersed and annular flows that are inertia dominated. According to the literature, channel size, phase superficial velocities, liquid phase surface tension, wall wettability and inlet conditions affect flow pattern. Meanwhile, the channel cross sectional geometry, liquid viscosity and flow orientation respecting the gravity has a lower degree of importance. The flow regime map is highly dependent on the inlets used in the various studies as well as different wall properties, such as wettability, contamination and roughness. Fig. 1 shows five different flow regimes encounters in microchannels [11].

Fig. 4 shows the gas–liquid (i.e. water–nitrogen) flow regime map of a vertical triangular channel with a hydraulic diameter of 0.55 mm. The flow map is used for selecting an appropriate operating condition for this study. The blue continuous line shows a roughly estimated gas and liquid superficial velocity from bottom to top of the channel. The estimation assumes a uniform flow of gas and liquid from ATL to the channel. The channel is vertical with a hydraulic diameter close to that of this study, i.e. 0.66 mm. As Fig. 10 shows, most of the gas–liquid flow in the PEMEC microchannels should be Taylor. Therefore, from hereon, a literature review of the methods of modelling Taylor flow is presented.

Shao et al. [11] depicted in their review paper, that the flow regimes map slightly differs between vertical and horizontal channels. There is a larger interest for gas–liquid flow to stay in Taylor flow regime in a horizontal channel than a vertical one. Furthermore, it is highly dependent on the channel diameter. The area in the flow regime map for Taylor flow in a channel increases by reducing the channel diameter and the flow gets into the bubbly flow regime at higher liquid velocities in a smaller channel than a large one. Also the flow gets into dispersed flow regime at higher velocities for both gas and liquid. It is also mentioned that the shape of the channel and contact angle has a very small impact on the flow regime map. Liquid surface tension has a high impact on the flow regime, as it shows a higher interest to the Taylor flow at higher liquid surface tensions. They also reported that a $U_{LS} - U_{GS}$ as coordinates, better represents the transition between flow regime maps than $ReWe_{LS} - ReWe_{GS}$.

Even though it is possible to map the borders between the different flow regimes of a specific gas–liquid flow and channel configuration, it is very difficult to create a

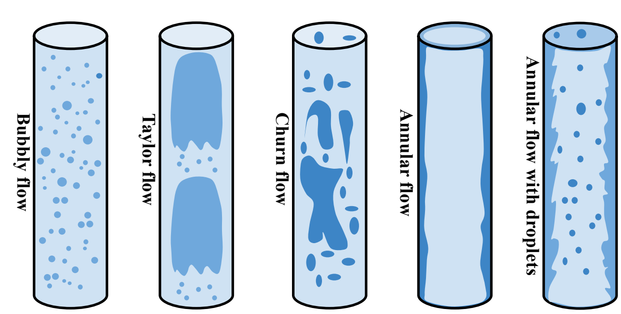

Fig. 1 – Gas–liquid flow regimes in micro-channels.