A Numerical Study of the Gas-Liquid, Two-Phase Flow Maldistribution in the Anode of a High Pressure PEM Water Electrolysis Cell

Anders Christian Olesen ^{a1}, Carsten Rømer ^b and Søren Knudsen Kær ^a

^a Department of Energy Technology, Aalborg University, Pontoppidanstræde 101, 9220 Aalborg East, Denmark

^b IRD A/S, Odense, Denmark

Abstract:

In this work, the use of a circular-planar, interdigitated flow field for the anode of a high pressure (HP) proton exchange membrane (PEM) water electrolysis cell is investigated in a numerical study. While PEM fuel cells have separated flow fields for reactant transport and coolant, it is possible to operate a PEM electrolysis cell with the anode flow field serving as both. This allows for a simpler system and a thinner design, however sets new and more strict requirements for the flow field to distribute uniformly. For the conducted numerical study, two computational fluid dynamics models are developed; a single-phase flow model for establishing the effect of geometry and a two-phase flow model for studying the effect of dispersed gas bubbles. Both models account for turbulence and heat transport. In the literature, previous studies on square-planar, interdigitated flow fields for PEM fuel cells have demonstrated particular advantages in regard to increasing the limiting current density and achieving a uniform distribution of properties. In the present study, it is however found that the circular-planar shape of the interdigitated flow field causes maldistribution. Moreover, under nominal conditions and below a water stoichiometry of 350, flow and temperature maldistribution is adversely affected by the presence of the gas phase; particularly gas hold-up near outlet channels can cause excessive formation of hotspots. As the water stoichiometry increases above a water stoichiometry of 350, the flow maldistribution increases. Nonetheless, its impact on the temperature distribution is counterbalanced by the overall increase in heat capacity of the flow. Hence, a relative uniform temperature distribution is achieved at and above nominal flow conditions. Finally, in a parametric investigation it is underlined that the predicted formation of hotspots is sensitive to the employed particle diameter of the two-phase channel flow model. The larger the particle size, the more severe the maldistribution of temperature becomes. It is therefore concluded that further experimental validation and research into particle size modeling is necessary.

¹ Corresponding author

Email address: aco@et.aau.dk, telephone number.: +45 2136 9153

30 **Keywords:**

31 PEMEC; water electrolysis; modeling; two-phase flow; high pressure

32

33

34

35

36

37

38

39

40

41

42

43

44

45

1 Introduction

With the growing need for grid balancing as a result of the use of renewable energy sources, the long-term storage of electricity in the form of chemical compounds is becoming increasingly more attractive [1–3]. Here particular, the production of hydrogen through water electrolysis has received increasing attention [4,5]. This interest has further been sparked by the growing demand for a hydrogen infrastructure in relation to fuel cells, particular associated with automotive applications, and as a chemical building block for synthetic fuels and in upgrading of biofuels.

As a technology, water electrolysis has been commercially available for more than a century. These systems have typically been alkaline based, bulky and suffered from poor dynamic response to load changes [5]. With the recent developments in proton exchange membrane electrolysis cells (PEMEC), a technology has been developed that offers significantly higher current densities, and in turn a more compact design. Even though the technology at the present time utilizes expensive noble metals as an electro-catalyst, the potential benefits, which include good partial load range, good dynamic response and high pressure operation, are believed to outweigh its shortcomings. [4]

In the electrolysis of water using a PEMEC, the overall reaction is split into two half-cell reactions occurring at the anode and cathode, respectively:

While electricity is supplied to the PEMEC, the anode is fed with demineralized water. Throughout the anode, oxygen is produced and a gas-liquid, two-phase flow develops. Similarly in the cathode, hydrogen is produced along the channel length. Since water can permeate the polymer membrane, a gas-liquid, two-phase flow also develops at the cathode. In order to provide cooling to the PEMEC, an excess amount of demineralized water is supplied relative to the stoichiometric conditions required in the anode half-cell reaction.

Although PEMEC are competitive on many levels, price and particularly durability still need to be improved. One way is by optimizing the flow and heat distribution across the cell. Because the incoming liquid water both serves as a fuel and coolant, an even distribution not only ensures good mass transport characteristics, it also allows for a uniform heat removal. If either of these two issues cannot be ensured, hotspots and catalyst degradation may occur. Moreover, as developers try to increase the nominal current density of PEMEC beyond a mark of 1 A/cm^2 , the importance of a uniform heat removal becomes ever more acute.

A factor that both directly and indirectly affects the flow distribution is the operation pressure. On a system level, it has been shown favorable to apply some degree of pre-compression internally in the PEMEC. Although it increases the hydrogen crossover and the open circuit voltage, the total energy consumption decreases because of a reduction in the mechanical work associated with the subsequent compression [6,7]. The system topology and operation which has shown the highest efficiency is the so-called asymmetric configuration, where primarily the cathode is pressurized [7]. A disadvantage of the asymmetric configuration is that it

imposes a large differential pressure across the PEM, which creates a large force on the gas diffusion layer (GDL) of the anode, and the bipolar layer (BP). If the GDL is not properly selected, it may collapse, and similarly for the BP, it may break due to its often brittle nature.

To ensure mechanical stability at elevated pressures, as well as a uniform distribution of flow and heat, certain requirements apply to material strength and cell geometry. As opposed to PEMFC, circular-planar cells are used instead of square-planar cells. Evidently, this difference in geometry affects the channel design, and thus the distribution of temperature and flow. Another difference that affects channel design is the difference in two-phase morphology. In PEMFC the two-phase flow consists of a continuous gaseous phase and a dispersed liquid water droplets phase, however in PEMEC this is only true for the cathode. In the anode the continuous phase consists of liquid water and dispersed oxygen bubbles.

For square-planar cells three archetype channel configurations are traditionally preferred [8], i.e. parallel, serpentine and interdigitated channels, although many more exist [9], e.g. pin-type or integrated flow field. While parallel and serpentine channels distribute reactants over a porous GDL, through which species mainly diffuse, interdigitated channels force convective flow through the GDL. Although serpentine flow fields allow some extent of cross-convective transport, interdigitated flow fields offer significantly better mass transport characteristics. Even so, this enhanced mass transport comes at the expense of a substantial increase in pressure loss. For applications where a high flow and a low pressure loss are required, parallel channels are typically chosen. However, for systems subject to two-phase flow, parallel channels suffer from a high extent of maldistribution. This may occur because a single channel might become blocked by a gas bubble or a liquid droplet. To limit the extent of maldistribution, while keeping a low pressure loss, combinations of parallel and serpentine channels are by now the “industrial standard” [10]. These flow fields are in most cases the best compromise in partially flooded conditions.

In the literature, various experimental and modeling studies have been conducted with the aim of characterizing square-planar, interdigitated flow fields for PEMFC [11–20], however none are available for PEMEC. In the studies conducted on PEMFC, focus has often been on comparing interdigitated flow fields with parallel or serpentine, or analyzing the effect of various operation conditions.

In the first published study on interdigitated flow fields, Nguyen [11] made an experimental comparison between a straight and interdigitated channel structure. Their study showed that an enhanced performance could be obtained by moving the onset of the limiting current density, when mass transport was the limiting factor. This conclusion was further substantiated in the more comprehensive experimental work by Wood et al. [21]. Here, it was underlined that the observed mass transport improvement had two main causes. First of all, the main transport mechanism of species is altered from diffusion to convection dominated. Secondly, entrapped liquid water is removed from the GDL by a high shear force exerted by the gas flow.

In the modeling studies to follow [15,22–24], emphasis was on establishing the effect of gas flow rate, humidity, and GDL thickness on the performance and current density distribution. In these studies, it was shown that the observed performance improvement is a complex interplay between diffusion and convection phenomena as well as liquid water transport and evaporation. Wang et al. [14] further studied the significance

118 of pressure, temperature and humidity. Their work showed that performance is particularly sensitivity towards
119 humidity changes, even more pronounced than for serpentine flow fields.

120 Studies on water transport visualization in interdigitated flow fields have also been conducted. Owejan et al.
121 [25] used neutron radiography in both the GDL and channels. Their results showed that GDL flooding primarily
122 occurs near the outlet channels. Moreover, it was concluded that the effect of gas phase shear force cannot in
123 itself explain water removal, when evaporation is eliminated. It was hypothesized that capillary transport plays
124 a vital role. Su et al. [18] used a transparent bipolar plate for studying water flooding in the channels. In
125 addition to the previous observed water flooding near outlet channels, flooding was observed near channel
126 corners. The latter was attributed to a higher contact area and hence higher viscous resistance to water flow.

127 In the experimental work by W. M. Yan et al. [13,26], the effect of the land-to-channel area ratio in connection
128 with varying operating conditions was studied. The same focus was seen in the modeling studies by X.D. Wang
129 et al. [12,16]. In all these studies, a common conclusion emerged; using an interdigitated flow field,
130 performance is less sensitive to the number of channels and their geometry than straight channels for a
131 constant area ratio. In a later modeling study by Berning et al. [27], the effect of two-phase flow was studied in
132 much more detail. In their model, detailed phenomena associated with heat and liquid water removal were
133 taken into account. It was hereby underlined that an improved waste heat removal could be obtained with
134 interdigitated flow fields. Later, Berning et al. [28] further demonstrated that interdigitated flow fields enable
135 low stoichiometric operation which effectively reduces the required back pressure.

136 For PEMEC the available number of publications is scarce. A few studies have investigated the effect of gas-
137 liquid, two-phase flow in the anode using parallel and serpentine flow fields in PEMEC at atmospheric
138 pressures. Ito et al. 2010 [29] found in their experimental study that these flow fields are sensitive to the two-
139 phase flow regime. At high current densities when a large amount of oxygen is produced, slug or annular two-
140 phase flow develops and obstructs the liquid phase reactant flow towards the catalyst layer. In the numerical
141 modeling study by Nie and Chen [30] it was further shown that a high extent of flow maldistribution could
142 occur and even reversed flow in some channels.

143 Although the use of an interdigitated, square-planar flow field in PEMFC has been shown to offer particular
144 benefits in avoiding mass transport limitations induced by gas-liquid, two-phase flow, no studies have been
145 published on interdigitated, circular-planar flow fields for PEMEC. In particular, the consequence of using
146 circular-planar, interdigitated flow fields for the anode is unknown. Moreover, studies on interdigitated flow
147 fields for PEMFC have only focused on mass transport in partially flooded conditions; hence conclusions are not
148 directly transferrable to PEMEC.

149 The main objective of this work is therefore the investigation of the flow and temperature maldistribution in an
150 interdigitated anode flow field using a macroscopic, three-dimensional model. While a single-phase model is
151 used for highlighting the effect of the geometry on maldistribution, a two-phase model is used for
152 understanding the effect of the gas-liquid flow interaction on maldistribution. Both models account for mass
153 and momentum transport in channels and the porous GDL. In order to avoid having to model the micro porous
154 layer (MPL), a mass flux boundary condition based on a uniform current density distribution is applied. The

155 devised models are studied under nominal conditions as well as by varying the water stoichiometry and
156 particle diameter size. The latter is done, to investigate the sensitivity of the two-phase model to applied
157 particle size.

158 The paper is organized as follows. Initially, a short description of the geometry, porous medium, heating, and
159 turbulence is given. Then the mathematical models, numerical solver and data treatment will be presented,
160 followed by a results and discussion section. Finally, the paper is ended with a conclusion.

161 2 Methodology

162 2.1 Geometry

163 In this work, the interdigitated, circular-planar anode flow field shown in Figure 2-1 is used. It consists of one
164 inlet, one outlet, an interdigitated channel structure and a porous medium. There are 8 incoming and 9
165 outgoing channels in the interdigitated channel structure. Each channel has a width of 1 mm and height of 0.5
166 mm. The inlet manifold has a height of 1 mm and width of 5 mm. The diameter of the circular GDL is 9.4 cm.

167
168 **Figure 2-1: Anode planar-circular flow field**

169 Because of the high operating pressure of the cathode, the channels are thin compared to the land width. This
170 prevents that the porous GDL intrudes into the channels and not to mention, improves the structural integrity
171 of the BP. Moreover, the channels are curved to achieve a more even flow distribution throughout the GDL
172 along the channel length.

173 2.2 Porous Medium

174 For the anode GDL to withstand the resulting forces, a material is required with a high tensile strength.
175 Typically, random organized titanium fibers are therefore used. These are untreated and are hence purely

176 hydrophilic by nature. In this work, the titanium felt (Ti-felt) from Bekaert Toko Metal Fiber Co. Ltc was used as
 177 a reference. It has a fiber diameter of 20 micrometer, a weight of 300 g/cm², a porosity of 81 % and a thickness
 178 of 0.35 mm. In Figure 2-1, the characteristic dependence of the Ti-felt as a function of compression pressure is
 179 shown. From left to right, the material strain, viscous permeability and volume porosity are depicted,
 180 respectively.

181 The strain of the Ti-felt was measured by initially compressing, relaxing and re-compressing. The re-
 182 compressing was repeated a couple of times to establish the extent of plastic deformation. From these test it is
 183 apparent that the Ti-felt permanently deforms after the first compression. The permanent deformation is more
 184 than 15 % of its initial thickness.

185

186 **Figure 2-2: Titanium felt deformation strain, viscous permeability and volume porosity as function of deformation pressure**

187 In order to determine the functional dependence of the volume porosity on compression pressure, the initial
 188 volume porosity without compression was measured and then using the following formula re-calculated as
 189 function of the measured strain [31]:

190
$$\varepsilon = 1 - \frac{1}{s} (1 - \varepsilon_0) \quad (1.3)$$

191 Here s denotes engineering strain as function of compression pressure and ε_0 the initial volume porosity.

192 From these calculations, a fairly linear dependence is visible on compression pressure. It should be noted that
 193 the material only shows a minor decrease in volume porosity even at 200 bars.

194 The in-plane, viscous permeability was found by compressing the fibrous Ti-felt and then measuring the
 195 pressure loss as function of volume flow. This was repeated for four different compression pressures. For each
 196 compression pressure, a Darcy-Forchheimer relation was fitted to the pressure-loss and volume flow data:

$$\Delta p = \frac{\mu}{K}u + \rho\beta u^2 \quad (1.4)$$

Here K denotes viscous permeability, μ viscosity, u superficial velocity, ρ density and β inertial Forchheimer coefficient. In Figure 2-2 the measured viscous permeabilities and 95 % confidence intervals are plotted. As a reference, the calculated volume porosity is correlated to the viscous permeability predicted using the relation by Tomadakis and Robertson [32] for 2D fibrous structures. Evidently, there is some discrepancy between the data and the estimated values from the volume porosity measurements. Nonetheless, both data sets are within the calculated 95 % confidence intervals. It should be noted that although the permeability decreases exponentially by approximately a factor of 4 from 0 to 200 bar compression, the fibrous Ti-felt remains relative permeable.

2.3 Heat Generation

In order to evaluate the heat flux generated per cell during water electrolysis, the reversible and irreversible heat generation needs to be evaluated. Here the reversible heat is calculated as the difference between the usable work in terms of Gibbs free energy and the enthalpy of reaction, which constitutes the maximum available energy:

$$Q_{rev} = -T\Delta S = \Delta G^\circ - \Delta H^\circ = nFV_{rev} - \Delta H^\circ \quad (1.5)$$

Here Q denotes heat generation per mole, T absolute temperature, S entropy, G Gibbs free energy and H enthalpy. The irreversible heat is the heat generated from driving the electrochemical reactions and transporting ions and electrons. It is calculated as the difference between the reversible and irreversible cell potential:

$$Q_{irr} = (V_{cell} - V_{rev})nF \quad (1.6)$$

Here V is voltage, n is the number of electrons transferred during the electrochemical reactions and F is Faradays constant. The heat flux generated per cell q is then given as the sum of the reversible and irreversible heat generation multiplied by the number of moles reacting

$$q = (Q_{irr} + Q_{rev})\dot{N} = \left(V_{cell} - \frac{\Delta H^\circ}{nF} \right) I_{cell} \quad (1.7)$$

The cell current can be found by integrating current density:

$$I_{cell} = \int_{A_c} j dA \quad (1.8)$$

It should be noted that the point where the cell voltage is equal to the change in enthalpy over the number of electrons being transferred times Faradays constant, is defined as the thermo-neutral point:

225

$$V_{neutral} = \frac{\Delta H^{\circ}}{nF} \quad (1.9)$$

226

At the thermo-neutral point no heat is generated or required for the electrochemical reaction to take place.

227

Above heat is generated and below heat is consumed.

228

229

Figure 2-3: Polarization curve and heat generation of a PEMEC per unit area at 70 C, cathode pressure of 1.8 bar and different anode pressures.

230

231

In Figure 2-3, the resulting heat flux of a water electrolysis stack consisting of 33 cells is shown. The electrolysis cell is operated at three different cathode pressures for a fixed water stoichiometry of 350 and fixed outlet temperature of 70°C. The y-axis to the left depicts cell voltage, while the y-axis to the right shows the resulting heat flux per cell. The plotted heat flux is positive under the applied conditions and depicts a non-linear dependence on current density. This interplay illustrates that the requirement for cooling significantly increases with increasing current density. Furthermore, the higher the anode pressure, the higher the cell voltage and heat flux becomes. However, this effect is minor compared to the dependence on current density.

232

233

234

235

236

237

238

2.4 Turbulence

239

Because cooling is achieved through running water electrolysis at excess amounts of water, high flow rates are seen. In fact, under nominal conditions the flow may become turbulent. In Table 1 the superficial Reynolds number is depicted as function of water stoichiometry for two positions: the manifold inlet and one of the interdigitated channel inlets. In the latter case a uniform distribution among the channels is assumed. The superficial Reynolds number and water stoichiometry are defined as follows:

240

241

242

243

244

$$Re = \frac{\rho D_H u}{\mu} \quad (1.10)$$

245

$$\lambda_{\text{H}_2\text{O}} = \frac{\dot{m}_{in} 2F}{M_{w,\text{H}_2\text{O}} \int_{A_c} j dA} \quad (1.11)$$

246

Here $D_H = 2ab / (a + b)$ is the hydraulic diameter, $\dot{m}_{in}$ is the inlet mass flow rate and M is the molecular weight.

247

248

Table 1: Superficial Reynolds number as a function of water stoichiometry for a current density of 1 A/cm²

	Manifold		Interdigitated channels	
Water stoichiometry	200	500	200	500
Superficial Reynolds number	2044	5110	426	1065

249

250

While the flow in the inlet region moves from being transitional (i.e. Re = 2100-4000) to fully turbulent (i.e. Re > 4000) as a function of water stoichiometry, the flow in the interdigitated channels remains in the laminar regime (i.e. Re < 2100) for all water stoichiometries. Meanwhile, it should be noted that the superficial Reynolds number only accounts for shear induced turbulence. Hence, it does not reveal anything about the particle induced turbulence in the gas-liquid, two-phase flow, or the effect of fibers intruding into the interdigitated channel. Hence, it is to be expected that the onset of turbulence occurs at lower superficial Reynolds numbers.

251

252

253

254

255

256

257

2.5 Assumptions

258

A number of assumptions are made in order to simplify the extent of the mathematical model:

259

- Current density and heat is produced uniformly across the active surface area.

260

- Due to a high anode pressure the molar fraction of water vapor is neglected, hence phase change and associated cooling or heating effects are likewise neglected.

261

262

- The crossover of water, hydrogen and oxygen is neglected.

263

- The effect of cooling due the bipolar plate redistributing heat is neglected.

264

2.6 Mathematical Model

265

In order to model single- and two-phase flow in the anode, two different models are required. Both models have to account for continuity and momentum conservation within channels and porous domain. At the applied range of mass flows, turbulent flow develops. To model turbulence, the Menter's Shear Stress Transport (SST) model is used. This type of turbulence model is a two-equation, eddy viscosity turbulence model [33].

266

267

268

269

270

2.6.1 Single-phase flow

271

2.6.1.1 Continuity and momentum conservation

272

The macroscopic, volume-averaged, steady-state continuity and momentum equations are modeled as follows:

$$\nabla \cdot (\varepsilon \rho \mathbf{U}) = \varepsilon S_c \quad (1.12)$$

$$\nabla \cdot (\varepsilon \rho \mathbf{U} \mathbf{U} - \varepsilon \boldsymbol{\tau}) = -\varepsilon \nabla p + \varepsilon \rho \mathbf{g} + \varepsilon \mathbf{M} \quad (1.13)$$

Here ε denotes volume porosity, ρ is density, $\mathbf{U}$ is the intrinsic or true velocity, S_c is a mass source term, $\boldsymbol{\tau}$ is the viscous stress term, p is pressure, $\mathbf{g}$ is the gravity force and $\mathbf{M}$ is the generalized momentum source term. The generalized momentum source term is equal to Darcy's law in the porous domain and zero elsewhere:

$$\mathbf{M} = \begin{cases} \mathbf{K}^{-1} \mu \varepsilon \mathbf{U}, & \Omega \in \text{GDL} \\ 0, & \Omega \in \text{Channel} \end{cases} \quad (1.14)$$

Here K denotes viscous permeability and μ is the viscosity. The viscous stress term can be modeled as follows:

$$\boldsymbol{\tau} = (\mu + \mu_T) \left(\nabla \mathbf{U} + (\nabla \mathbf{U})^T - \frac{2}{3} (\nabla \mathbf{U}) \mathbf{I} \right) \quad (1.15)$$

$$\mu_T = \rho \frac{k}{\omega} \quad (1.16)$$

Here μ_T is the turbulent eddy viscosity, k is the turbulent kinetic energy and ω is the turbulent eddy frequency.

2.6.1.2 Thermal energy conservation

The transport of energy at low velocities can be modeled using the thermal energy conservation equation:

$$\nabla \cdot \left(\varepsilon \rho \mathbf{U} h - \varepsilon \left(\lambda + C_p \frac{\mu_T}{\text{Pr}_T} \right) \nabla T \right) = \boldsymbol{\tau} : \nabla \mathbf{U} + \mathbf{S}_E \quad (1.17)$$

Here $h = e + \frac{P}{\rho}$ is the specific enthalpy, and $\mathbf{S}_E$ is the energy source term.

2.6.1.3 Turbulence

The effect of turbulence is modeled using the eddy viscosity hypothesis, where the effect of Reynolds shear stress is assumed proportional to the mean rates of deformation. In this work, the SST formulation by Menter et al. [33] is used for modeling the transport of the turbulent kinetic energy and turbulent eddy frequency:

$$\nabla \cdot \left(\varepsilon \rho \mathbf{U} k - \varepsilon \left(\mu + \frac{\mu_T}{\sigma_k} \right) \nabla k \right) = P_k - \beta' \rho k \omega + P_{kb} \quad (1.18)$$

$$\nabla \cdot \left(\varepsilon \rho \mathbf{U} \omega - \varepsilon \left(\mu + \frac{\mu_t}{\sigma_k} \right) \nabla \omega \right) = \alpha \frac{\omega}{k} P_k - \beta \rho k \omega^2 + P_{\omega b} \quad (1.19)$$

Here P_{kb} and $P_{\omega b}$ are the buoyancy turbulence production and dissipation terms, respectively, and P_k is the turbulence production due to viscous forces. Both terms are given as follows:

$$P_{kb} = - \frac{\mu_T}{\rho \sigma_\rho} \mathbf{g} \nabla \rho \quad (1.20)$$

$$P_{\omega b} = \frac{\omega}{k} \left[(\alpha + 1) C_3 \max(P_{kb}, 0) - P_{kb} \right] \quad (1.21)$$

$$P_k = \mu_T \left(\nabla \mathbf{U} + (\nabla \mathbf{U})^T - \frac{2}{3} (\nabla \mathbf{U}) \mathbf{I} (3 \mu_T \nabla \mathbf{U} + \rho k) \right) \quad (1.22)$$

Here $\alpha = 5/9$ and $C_3 = 1$ are model constants.

2.6.2 Two-phase flow

2.6.2.1 Continuity and momentum conservation

As opposed to the single-phase model, the two-phase model solves for two sets of macroscopic volume-average, steady-state equations, rather than one set. For the continuity and momentum conservation this gives in total 8 equations, as opposed to 4 in the case of single phase flow:

$$\nabla \cdot (s_\alpha \varepsilon \rho_\alpha \mathbf{U}_\alpha) = s_\alpha \varepsilon S_{c,\alpha} \quad (1.23)$$

$$\nabla \cdot (\varepsilon s_\alpha \rho_\alpha \mathbf{U}_\alpha \mathbf{U}_\alpha - \varepsilon s_\alpha \boldsymbol{\tau}_\alpha) = -\varepsilon s_\alpha \nabla p_\alpha + \varepsilon s_\alpha \rho_\alpha \mathbf{g} + \varepsilon s_\alpha \mathbf{M}_\alpha \quad (1.24)$$

Here s denotes phase volume fraction, or what is called saturation, when dealing with porous media, and the subscript $\alpha \in [l, g]$ each thermodynamic phase; liquid and gas. This type of model is known as a two-fluid model and essentially assumes two interpenetrating continua. Coupling between each phase is achieved through the use of interfacial transport terms.

In the momentum equation interfacial transport is accounted for in the generalized momentum source term as follows:

$$\mathbf{M}_\alpha = \begin{cases} \mathbf{K}^{-1} \frac{\mu_\alpha s_\alpha \varepsilon}{k_{rel,\alpha}} \mathbf{U}_\alpha, & \Omega \in \text{GDL} \\ \pm (\mathbf{F}_D + \mathbf{F}_{TD}), & \Omega \in \text{Channel} \end{cases} \quad (1.25)$$

316 Here $k_{rel,\alpha}$ is the relative permeability of phase α , $\mathbf{F}_D$ is the interfacial drag force and $\mathbf{F}_{TD}$ is the turbulent
 317 dispersion force. Inside the GDL porous resistance dominates, drag can be neglected. The interfacial drag term
 318 is modeled as follows:

$$319 \quad \mathbf{F}_D = a_{cd} \rho_g C_D |\mathbf{U}_g - \mathbf{U}_l| (\mathbf{U}_g - \mathbf{U}_l) \quad (1.26)$$

320 Here a_{cd} is the interfacial area density and C_D is the drag coefficient. The drag coefficient is modeled using the
 321 Ishii Zuber drag law for densely distributed fluid particles. For the dense spherical particle regime, the model
 322 takes the following form:

$$323 \quad C_D = \frac{24}{Re_l} \left(1 + \frac{1}{6} Re_l^{\frac{2}{3}} \right) \quad (1.27)$$

$$324 \quad Re_l = \frac{d \rho_l |\mathbf{U}_l - \mathbf{U}_g|}{\mu_m} \quad (1.28)$$

$$325 \quad \frac{\mu_m}{\mu_l} = \left(1 - \frac{s_g}{s_{dm}} \right)^{-2.5 s_{dm} \mu_*} \quad (1.29)$$

$$326 \quad \mu_* = \frac{\mu_g + 0.4 \mu_l}{\mu_g + \mu_l} \quad (1.30)$$

327 Here $s_{dm} = 1$ is the maximum packing value.

328 Interphase turbulent dispersion force is modeled using a Favre averaged interphase drag model:

$$329 \quad \mathbf{F}_{l,TD} = -\mathbf{F}_{g,TD} = C_{TD} C_{cd} \frac{\mu_{tl}}{\rho_l \sigma_{tl}} \left(\frac{\nabla s_g}{s_g} - \frac{\nabla s_l}{s_l} \right) \quad (1.31)$$

330 Here $C_{cd} = 1$ is the momentum transfer coefficient for the interphase drag force.

331 In addition to the shear induced eddy viscosity given by the turbulence model, particle induced turbulence in
 332 the liquid phase is accounted for using the implementation by Sato [34]. The additional liquid phase eddy
 333 viscosity is now given by:

$$334 \quad \mu_{T,l} = \mu_{Ts} + \mu_{Tp} \quad (1.32)$$

$$335 \quad \mu_{Tp} = C_{\mu p} \rho_l s_g d_p |\mathbf{U}_g - \mathbf{U}_l| \quad (1.33)$$

336 Here $C_{\mu p} = 0.6$ is an empirical constant.

337 In two-fluid modeling it is customary to assume that all phases share the same pressure field. This assumption
338 is in most cases acceptable for free flow; however within the GDL the pores are so small that capillary pressure
339 effects need to be accounted for when two immiscible fluids are present. By definition, the capillary pressure is
340 given as the pressure difference between the non-wetting and wetting phase in the following manner:

$$341 \quad p_c = p_g - p_l \quad (1.34)$$

342 Here it is assumed that the liquid phase is the wetting phase and the gas the non-wetting phase. In order to
343 introduce this condition in the model, while only solving for one pressure field, an additional momentum
344 source term needs to be added to either phase. In this work it is assumed that we solve for the liquid phase
345 pressure, hence a momentum source term is added to the gas phase as follows:

$$346 \quad \mathbf{S}_{gM} = -\nabla p_c \quad (1.35)$$

347 Different types of models exist for relating the saturation and the capillary pressure of a porous medium; some
348 more mechanistic by nature than others. A popular one is the van Genuchten model [35]:

$$349 \quad p_c = p_{cb} \left(s_e^{-1/m} - 1 \right)^{1/n} \quad (1.36)$$

350 Here m and n are empirical constants, s_e is the effective saturation of the porous medium and p_{cb} is the
351 break through pressure. The effective saturation is related to the saturation as follows:

$$352 \quad s = s_e (1 - s_r) + s_r \quad (1.37)$$

353 Again, applying the van Genuchten model yields the following relations for the relative permeability of each
354 phase as a function of saturation [36]:

$$355 \quad k_{rwp} = s_e^{1/2} \left(1 - \left(1 - s_e^{1/m} \right)^m \right)^{1/2} \quad (1.38)$$

$$356 \quad k_{rnwp} = (1 - s_e)^{1/3} \left(1 - s_e^{1/m} \right)^{2m} \quad (1.39)$$

357 **2.6.2.2 Thermal energy conservation**

358 The transport of thermal energy is done using a homogeneous formulation. Although an equation is solved for
359 each phase, the interfacial heat transfer term in each equation is selected to be large enough relative to the
360 other transported processes in the equation. This effectively ensures the phasic temperatures are in
361 equilibrium:

$$\nabla \cdot \left(\varepsilon s_\alpha \rho_\alpha \mathbf{U}_\alpha e_\alpha - \varepsilon s_\alpha \left(\lambda_\alpha + C_p \frac{\mu_T}{Pr_T} \right) \nabla T_\alpha \right) = \varepsilon s_\alpha \boldsymbol{\tau}_\alpha : \nabla \mathbf{U}_\alpha + S_{E\alpha} + Q_\alpha \quad (1.40)$$

$$\nabla \cdot \left((1 - \varepsilon) \rho_s \mathbf{U}_s e_s - (1 - \varepsilon) \lambda_s \nabla T_s \right) = S_{Es} + Q_s \quad (1.41)$$

Here $S_{E\alpha}$ denotes external heat source and Q_α the interface heat transfer.

2.6.2.3 Turbulence

The modeling of the turbulence is done using a homogeneous formulation, where the same equation that is used for single phase flow is solved. The main difference lies in the use of phase volume averaged densities, viscosities and velocities.

2.6.3 Boundary conditions

In the modeling domain different types of boundary conditions are applied, in addition to the standard no-slip condition and wall-functions for turbulence.

2.6.3.1 Mass

At the manifold inlet, the mass flow of liquid water is specified as function of water stoichiometry and current density as follows:

$$\dot{m}_{in} = \frac{M_{w,H_2O} \lambda j_c A_c}{2F} \quad (1.42)$$

Here λ is the stoichiometric factor, and A_c is the cross-sectional area.

At the GDL-MPL interface a mass flux opening is specified. This opening reflects the flux of liquid and gas phase respectively being consumed and produced in the CL due to the electrochemical reactions:

$$\bar{m}_l = - \frac{M_{w,H_2O} j_c}{2F} \quad (1.43)$$

$$\bar{m}_g = \frac{M_{w,O_2} j_c}{4F} \quad (1.44)$$

Here $\bar{m}$ denotes mass flux.

2.6.3.2 Temperature

In this work, an adiabatic temperature conditions is specified at all walls except the GDL-MPL interface:

$$\nabla T \cdot \mathbf{n} = 0 \quad (1.45)$$

Here $\mathbf{n}$ is a normal vector. At the GDL-MPL interface, the following heat flux is specified:

386

$$q = \left(V_{cell} - \frac{\Delta H^{\circ}}{nF} \right) I_{cell} \quad (1.46)$$

387

388

389

390

At the outlet, the temperature is fixed. This means that the inlet temperature varies depending on the operating conditions. By setting up an energy balance and assuming that heat only is removed through the gas and liquid phases, the inlet temperature can be calculated as function of outlet temperature, the heat generated during water electrolysis and the inlet mass flow.

391

$$T_{in} = \left(1 - \underbrace{\frac{1}{\lambda}}_{\approx 0} + \frac{\bar{m}_{g,out} A c_{g,p}}{\underbrace{\dot{m}_{l,in} c_{l,p}}_{\approx 0}} \right) T_{out} - \frac{qA}{\dot{m}_{l,in} c_{l,p}} \quad (1.47)$$

392

Here A is the cross-sectional area and c_p is the specific heat capacity at constant pressure.

393

2.6.3.3 Pressure

394

At the outlet a static gauge pressure condition is specified:

395

$$p_{out} = 0 \quad (1.48)$$

396

At the GDL-channel interface the following boundary condition for the capillary pressure is implemented:

397

$$\nabla p_c = 0 \quad (1.49)$$

398

399

400

This condition is in good alignment with the fact that a constant particle diameter is assumed in the channel domain. According to the Young-Laplace equation, a constant diameter is equivalent to a constant capillary pressure assuming that the surface tension does not vary significantly with temperature:

401

$$p_c = \frac{4\sigma_{lg}}{d} = \text{Const.} \quad (1.50)$$

402

403

404

405

406

Consequently, the gradient of the capillary pressure within the channel domain has to be zero. It should be noted that the applied boundary condition for the capillary pressure is in contrary to the conventional applied condition of a fixed saturation or capillary pressure often found in literature. This condition is essentially neither mechanistic nor physically substantiated, and has therefore been subject to much debate in many modeling studies [37,38].

407

2.7 Numerical Model

408

409

410

The presented mathematical models are solved using the commercial CFD software, ANSYS CFX 15. In obtaining a solution, the coupled multiphase solver with a high resolution discretization scheme is used. The pressure-velocity coupling is modeled using a fourth order Rhie-Chow scheme. Moreover, a tri-linear pressure and

velocity interpolation is set. In order to capture steep gradients in the volume fraction, the compressive interface capturing scheme for arbitrary meshes is activated. Here, a default slope limiter of 2 is specified.

2.8 Data treatment

To be able to evaluate the extent of maldistribution in a systematic manner, a weighted arithmetic mean and standard deviation are calculated. Essentially, these quantities allow for a direct comparison between the individual simulation conditions for both single- and two-phase flow models:

$$\sigma_{\varphi} = \sqrt{\frac{1}{NW} \sum_{j=1}^N w_j (\varphi_j - \mu_{\varphi})^2} \quad (1.51)$$

$$\mu_{\varphi} = \frac{1}{NW} \sum_{j=1}^N \varphi_j w_j \quad (1.52)$$

$$W = \sum_{j=1}^N w_j \quad (1.53)$$

Here σ_{φ} is the weighted standard deviation, μ_{φ} is the weighted mean, φ is the distributed variable, N is the number of entities and w_j is the weight of entity j .

The standard deviations of three different variables are investigated:

$$\varphi \in \left\{ \frac{\dot{m}_{l,i}}{L_c}, T_l, s_g \right\} \quad (1.54)$$

Here $\dot{m}_{l,i}$ is the liquid mass flow rate of each channel, L_c is the channel length, $T_{l,i}$ is the liquid phase temperature and s_g is the gas volume fraction. The normalized mass flow is calculated on help-planes near the inlet and outlet as follows:

$$\dot{m}_i = \int_{A_i} \rho \mathbf{U} \cdot \mathbf{n} dA \quad (1.55)$$

Here $\mathbf{n}$ is the normal vector of the help plane and $\dot{m}_{in}$ is the mass flow at the inlet of the manifold. It should be noted that the channel mass flow is divided by channel length to account for the difference in cross-sectional surface area, and thus the amount of produced gas and heat. The active area each channel is in contact with is approximately proportional to the channel length.

While a mass flow has to be measured across a surface and hence discretely, the temperature and gas volume fraction are continuous field quantities that are locally defined for each control volume. Because each control volume may differ in size (i.e. volume or mass), a specific weight applies to each variable:

$$w \in \{1, m_l, V\} \quad (1.56)$$

Here m_l is the liquid mass in each control volume and V is the control volume.

3 Results and Discussion

The results section is split into two parts; a comparison between the single- and two-phase models under nominal conditions and a parameter variation relative to nominal conditions. The selected parameters under nominal conditions are depicted in Table 2. It should particularly be noted that the mean gas particle diameter, which is used in the applied two-phase flow model for calculating interfacial transport phenomena in the channel flow field, is somewhat unknown. In this study, the gas particle diameter is therefore specified to be equal to the characteristic pore diameter. This seems to be a reasonable starting point as it is the largest characteristic particle size exiting the pores. The actual size is difficult to predict because of interfacial forces, turbulent mixing as well as particle coalescence and break-up.

In the parametric study two factors are investigated; the effect of stoichiometry for both the single- and two-phase models, and the effect of particle diameter for two-phase flow model.

Table 2: Nominal operation conditions

Parameter	Symbol	Value	Unit
Temperature	T	343	K
Permeability	κ	2.25×10^{-11}	m^2
Porosity	ε	0.82	-
GDL thickness	L_T	300	μm
Water stoichiometry	λ	350	-
Cathode pressure	P_{cat}	6	Bar
Anode pressure	P_{an}	100	
Cell voltage	V_{cell}	1.9	V
Cell current density	j_{cell}	1.0	A
Average gas Reynolds number	Re_{gas}	3000	
Average liquid Reynolds number	Re_{liq}	10000	
Particle diameter in channels	$D_{particle}$	20	μm
Characteristic pore diameter [39]	$D_{pore} = 4\sqrt{\kappa/\varepsilon}$	20	Mm
Genuchten model coefficients	m, n, p_{cb}	0.6489, 2.848, 8200	- . - . Pa

3.1 Nominal conditions

3.1.1 Mass Flow

451 In Figure 3-1, the distribution of liquid phase mass flow rate per channel length is depicted. For comparison
 452 both the distributions predicted by the single- and two-phase models have been plotted. At a first glans, both
 453 models seem to predict the same trend. The highest values are found in the two shortest channels. From here
 454 on and towards the longest channel in the center of the flow field, the mass flow rate per channel length then
 455 decreases. It is worth noting that reversed flow does not occur and hence no local mass starvation occurs.
 456 Moreover, the interdigitated flow field shows significantly less maldistribution than what is observed in the
 457 modeling study by Nie and Chen [30] on parallel-straight channel for PEMEC.

458 A comparison between the two predicted distributions reveals that the added gas phase changes the
 459 distribution slightly. Between channels 2 and 8 it appears that the distribution becomes less uniform. This
 460 suggests that the added gas phase hinders the transport of the liquid phase across the flow field. One possible
 461 explanation could be that the added gas lowers the relative permeability, which then increases the liquid phase
 462 resistance through the porous medium. This shift in the balance between the effect of the channel and porous
 463 medium resistance could cause the liquid phase to distribute differently [40].

464

Figure 3-1: Bar graph of the mass flow rates per channel length for each individual outlet channel

Figure 3-2: Bar graph of the mass quality distribution among the outlet channels

465 An examination of the mass quality in Figure 3-2 shows a parabolic distribution between the channels. In the
 466 shortest channels, a significant higher amount of the liquid phase is being transported relative to the amount
 467 of gas phase. Hence, a much higher local average water stoichiometry can be seen, since they are directly
 468 proportional. Moreover, this further implies that a lower gas volume fraction can be expected here.

469 From these preliminary observations, it could be hypothesized that an improved mass flow distribution could
 470 be obtained by shortening the distance between the longest channels and/or expanding the distance between
 471 the shortest channels. This would increase the resistance between the shortest channels relative to resistance
 472 between the longest channels and hence force more flow through the longest channels at the center of the

473 flow field. Meanwhile, the question remains how large these differences should be and if they result in a
474 critical land area thickness, which cannot support the mechanical compression exerted from the cathode.

475 As shown in a preliminary study of the single-phase flow distribution in a circular-planar, interdigitated flow
476 field by Olesen and Kær [40], maldistribution between channels is strongly dependent on the permeability of
477 the GDL. For the geometry studied in this work, a transition point in the dependence of the viscous
478 permeability was identified. Below this transition point only minor improvements are seen in the uniformity of
479 the water distribution, whereas above a significant increase in channel maldistribution results with increasing
480 permeability.

481 For the Ti-felt considered in this work, values slightly higher than this transition point are seen. This implies that
482 the distribution between channels should mainly be dominated by the transport losses within the GDL. Since
483 the transport within the GDL follows Darcy's law, this further implies that the overall mass flow maldistribution
484 likewise does so. Provided that the mass flow between each pair of interdigitated channels could be viewed as
485 a one-dimensional transport process, the mass flow rate would be inversely proportional to the land area
486 width, or conversely on a mass flow rate per channel length basis, inversely proportional to the land area size.
487 In view of this, a more uniform mass flow distribution would therefore be obtainable if all land areas had the
488 same in-plane cross sectional area. However, this requires that single-phase like conditions prevail for the
489 liquid phase. In other words, the presence of the gas phase should not significantly alter the distribution of the
490 liquid phase. Interestingly, this seems to be the case under the nominal conditions from the mass flow rate
491 distribution in Figure 3-1.

492 Nonetheless, the importance of two-phase flow phenomena cannot be neglected in all cases. The higher the
493 amount of gas is relative to the land area size and liquid phase mass flow rate, the more the distribution of
494 water is affected by capillary pressure action and relative permeability changes, because of the dependence on
495 gas volume fraction. For much wider land areas it could therefore be imagined that a higher gas volume
496 fraction in the direction of the flow would be obtained. Under these circumstances, a much larger resistance to
497 water transport would be seen due to a decrease in relative permeability of the liquid phase. It is therefore not
498 fully clear where the optimum lies, since equal land area sizes would make some areas much wider and
499 therefore impose some differences in transport resistance. Still, an improved distribution should be obtainable
500 by approaching more equal land area sizes.

501 To verify the validity of this line of reasoning, the ratio of land areas for the present design could be calculated.
502 Between the shortest channels the land area is $1.069 \times 10^{-4} \text{ m}^2$, and between the longest channels the land area is
503 $4.236 \times 10^{-4} \text{ m}^2$. Indeed, this gives a ratio of land areas of 3.96, which approximately equals the observed ratio of
504 mass flow rates per channel length for the longest and shortest channels, as can be seen from Figure 3-1. In
505 order to make the land areas equal, the average width between the longest channels would have to be
506 reduced to 1.3 mm from the original 5 mm. This further means that additional interdigitated channels would
507 have to be added to account for the decreased land area width.

508 In order to identify the minimum land area width, which can support the imposed mechanical stress, the
509 compressive strength of the BP can be evaluated. This parameter essentially determines the materials ability to

510 withstand deformation due to compression. For a high pressure PEM electrolysis cell, a suitable material could
511 be vinyl ester. This polymeric material has a compressive strength of 76 MPa [41]. Even for a flow field open
512 ratio of 0.5, which corresponds to a land area width of equal size as the channel width, the material could
513 withstand a cathode operating pressure of up to 380 bars. If a safety factor of 1.5 is included the number
514 reduces to 253 bars. Hence, from a material mechanical point of view, it seems feasible to decrease the land
515 area for example by lowering the average distance between the longest channels. Even for land area
516 thicknesses of down to 1 mm, which corresponds to the channel width, the mechanical strength would be
517 enough to sustain the intended conditions of up to 200 bars.

518 It should be noted that the selected value for the safety factor reflects a certain risk of statistical failure and
519 that stress concentrations may form near corners which could cause fractures. Further analysis of filling radii
520 and land area heights would however require a detailed finite element analysis.

521 3.1.2 Volume Fraction

522 In Figure 3-3 and Figure 3-4, the in-plane distribution of gas volume fraction is depicted at two different
523 locations. In Figure 3-3, the gas volume fraction inside the channel structure is shown. At the inlet it is seen
524 how only the liquid phase enters the anode and distributes across the inlet manifold. In each inlet channel, a
525 small amount of gas volume fraction is visible. Because the liquid phase is convectively transported through the
526 GDL, the gas phase is pushed towards the outlet channels. However, a small amount of gas flows out of the
527 GDL and into the inlet channels and then re-enters the GDL further down the channel.

528 Between the outlet channels, large variations in the resulting gas volume fraction can be observed. In the
529 shortest channels, regions with low gas volume fraction are visible; from here and towards the longest
530 channels, the amount of gas volume fraction then gradually increases. It should be noted that this distribution
531 is in agreement with the observed phase mass flow ratio distribution. In the outlet manifold, the two-phase
532 flow streams from each individual outlet channel mix together. At the outlet, this results in a final gas volume
533 fraction of 0.26.

Figure 3-3: In-plane gas volume fraction distribution at $y^*=y/h_{\text{channel}} = 0.5$ inside the channel

Figure 3-4: In-plane gas volume fraction distribution at $y^*=y/t_{\text{GDL}} = 0.5$ inside the GDL

In Figure 3-4, the gas volume fraction distribution inside the GDL is portrayed. While regions of low gas volume fraction form underneath the inlet channels, the opposite is seen for the outlet channels. Along the outlet channels a skewed, parabolic distribution of the gas volume fraction forms. At both ends of the channels, the gas volume fraction is high and then gradually decreases along the channel length. The highest amount of gas volume fraction is seen near the end of outlet channels.

Further variation in the gas volume fraction can be identified between each channel. Underneath the shortest channels, regions of lower gas volume fraction are visible. This distribution coincides with the distribution found above in the outlet channels. Hence, the gas volume fractions inside the GDL and above are directly coupled. This is an effect that would not have been seen, if a constant gas volume fraction or capillary pressure would have been specified as a boundary condition.

3.1.3 Velocity

The in-plane distribution of phase velocity within the GDL is depicted in Figure 3-5 and Figure 3-6 for the liquid and gas phase, respectively. Throughout Figure 3-5, large variations can be observed in the liquid phase velocity; particularly between the shortest and longest channels. Along the channel length, a parabolic distribution can furthermore be seen. The lowest liquid phase velocity is located at the center and then gradually increases along the channel length in both directions.

A quite different velocity distribution is seen in Figure 3-6 for the gas phase. Clearly, the dominating mechanisms behind the movement of gas and liquid are different. While the variations in gas phase velocity under nominal conditions predominantly are caused by capillary pressure and turbulent dispersion forces, the variations in liquid phase velocity appear mainly to be due to the circular shape of the flow field and the differences in land to channel area.

555 When taking a closer look at the gas phase velocity distribution, narrow high velocity zones become apparent
 556 near the inlet channels. These zones are most prominent near the start of channel and then gradual fade out
 557 along the channel length. It turns out that these zones indicate where the gas phase flows into the inlet
 558 channels and thus opposite the liquid phase flow. Further down the channel length, the gas phase then re-
 559 enters the GDL. This redistribution along the inlet channel length is what causes the observed skewed,
 560 parabolic distribution in gas volume fraction as well as the higher gas velocities downstream of the inlet
 561 channels. This phenomenon is initiated by the turbulent dispersion force and reinforced by the fact that the gas
 562 phase relative permeability lowers at higher gas volume fractions. This in turn means that the gas phase easier
 563 can flow through the GDL downstream of the channel.

Figure 3-5: In-plane true liquid velocity distribution inside the GDL at $y^*=y/t_{GDL}=0.5$

Figure 3-6: In-plane true gas velocity distribution inside the GDL at $y^*=y/t_{GDL}=0.5$

564 3.1.4 Temperature

565 In Figure 3-7 and Figure 3-8, the predicted in-plane liquid phase temperature distributions of the interdigitated
 566 channel structure and GDL are illustrated, respectively. At the manifold inlet in Figure 3-7, the liquid phase
 567 enters at a temperature of approximately 340 K. After the GDL, the resulting two-phase flow streams mix and
 568 the combined flow leaves the manifold outlet at a temperature of 343.15 K, as specified. Within the channels,
 569 the highest temperature is reached in the longest channel. Here the temperature becomes 345 K,
 570 approximately 2 K higher than the outlet temperature. From the longest to the shortest outlet channel, a
 571 gradual decrease in temperature is visible. This variation is partly a reflection of the difference in active surface
 572 area between inlet and outlet channels, and partly due to the difference in mass flow and hence thermal
 573 capacity of the flow.

Figure 3-7: In-plane temperature distribution inside channels at $y^*=y/t_{\text{chan}} = 0.5$, under nominal conditions

Figure 3-8: In-plane temperature distribution inside the GDL at $y^*=y/t_{\text{GDL}} = 0.5$, under nominal conditions

Inside the GDL, as shown in Figure 3-8, the same trend in the temperature distribution can be seen as within the channels; the highest temperature is found underneath the longest channels. Between inlet and outlet channel a large temperature gradient is visible. A further variation can be identified along the channel length. This seems to be in accordance with the observed velocity and gas volume fraction distributions. Both a high velocity and a low gas volume fraction mean better cooling. The more liquid phase, the higher the thermal capacity and the better the effective heat conduction becomes. Consequently, the highest temperatures are to be expected where the liquid velocity is lowest and the gas volume fraction the highest relative to amount of heat being dissipated.

3.2 Effect of Stoichiometry

3.2.1 Channel mass flow

The standard deviation in liquid mass flow per channel length as function of water stoichiometry is depicted in Figure 3-9. For the single- and two-phase simulation cases, the same trend appears. As the water stoichiometry increases, correspondingly does the standard deviation. Below a water stoichiometry of 350, the standard deviation increases due to the presence of the gas phase when compared with the single-phase case, whereas above the two-phase flow decreases the standard deviation compared with single-phase conditions. With this in mind, it would seem that the gas phase hinders distribution of water below a water stoichiometry of 350, but improves it slightly above.

Figure 3-9: Standard deviation in liquid mass flow rate per channel length for outlet channels.

Figure 3-10: Mean, maximum and standard deviation in gas volume fraction throughout the GDL.

3.2.2 Gas volume fraction

In Figure 3-10, the mean, maximum and standard deviation in gas volume fraction are depicted for the GDL. For each statistical parameter, the same inversely proportional dependence on water stoichiometry is seen. In particular, it is noticeable that the standard deviation is nearly halved in the simulated range of water stoichiometry. This is a clear indication that the gas volume fraction distributes more uniformly with increasing water stoichiometry. However, the extent of this apparent effect also seems to diminish with increasing water stoichiometry. Consequently, a substantial increase in water stoichiometry is necessary to further lower the standard deviation in gas volume fraction above a water stoichiometry of 500.

It can further be noticed that the gas volume fraction exceeds a maximum value of 0.5 at a water stoichiometry below 350. Hence, low stoichiometry operation will cause a significantly increased pressure loss relative to single-phase conditions as well as poorer heat removal.

3.2.3 Temperature

From the temperature variation shown in Figure 3-11, a decrease in maximum temperature is seen as function of water stoichiometry. This is comparatively the same tendency as for the gas volume fraction. With this in mind, it appears that the presence of the gas phase significantly increases the formation of hotspots. From the single-phase simulation it appears that the water stoichiometry in itself results in an increase in maximum temperature due to a non-uniform mass flow distribution. Meanwhile, this is much more pronounced in the case of the two-phase flow.

Interestingly, the opposite behavior is seen in the mean temperature; as the water stoichiometry increases, so does the average temperature. Although this might seem odd at first sight, it must be remembered that an increasing mass flow reduces the required temperature difference needed for cooling. Hence, the average temperature has to increase with water stoichiometry. In fact, it will asymptotically approach the outlet temperature. What furthermore may be surprising is that the mean temperature is nearly equal for single- and

614 two-phase flow. Despite the formation of hotspots, the overall impact on the mass-averaged temperature is
 615 almost negligible.

Figure 3-11: The mean and maximum temperatures throughout the GDL, as predicted by the single- and two-phase models

Figure 3-12: Back pressure as a function of water stoichiometry for single- and two-phase flow

616 Finally, it should be noted that the simplification of a uniformly distributed current density, inherently is
 617 affected by the maldistribution of temperature and not to mention two-phase flow. Areas where a high
 618 temperature is seen, an equivalent high current density would be produced for the same applied voltage
 619 difference. The impact of the maldistribution on current density can only be revealed fully by modeling a whole
 620 cell. Meanwhile, the standard deviation in temperature inside the GDL is fairly low, which would suggests that
 621 overall the current density would be fairly uniform.

622 **3.2.4 Back pressure**

623 The back pressure as a function of water stoichiometry is shown in Figure 3-12. While the required differential
 624 pressure for the single-phase model increases from 1.58 to 7.06 kPa, the differential pressure for the two-
 625 phase model increases from 3.3 to 9.92 kPa. At low water stoichiometry, roughly a factor of two in difference
 626 can be seen between single- and two-phase flows. As the water stoichiometry increases, this difference
 627 increases slightly. However, the extent is significantly less than the absolute increase in both the single- and
 628 two-phase pressures. This corresponds well to the fact that the mean gas volume fraction decreases in the GDL
 629 and hence less gas hinders liquid phase transport.

630 **3.3 Particle diameter**

631 **3.3.1 Channel mass flow**

632 The effect of particle diameter on the standard deviation in mass flow per channel length is depicted in Figure
 633 3-13. From the graph it is apparent that the mass flow distribution is sensitive to particle diameter and as such
 634 the forces related to the particle size. As the particle size grows, mass flow maldistribution increases relative to
 635 single-phase conditions. The increased maldistribution can to a high extent be attributed to the change in drag

636 force. The larger the particle diameter, the slower the gas bubbles move relative to the liquid phase. In turn,
 637 this effect causes a higher gas phase hold-up.

Figure 3-13: Standard deviation in mass flow per channel length as function of particle diameter

Figure 3-14: Mean, maximum and standard deviation in gas volume fraction inside the GDL as function of particle diameter

638 **3.3.2 Gas volume fraction**

639 The change in gas volume fraction as function particle diameter is shown in Figure 3-14. While the mean and
 640 standard deviation show a minor dependence, a considerable impact is observed in the maximum gas volume
 641 fraction. Above a particle diameter of 40 micrometer, an excessive amount of gas forms near the beginning of
 642 the outlet channels, where the land area is the widest and the channel flow lowest. This build-up of gas in turn
 643 lowers the rate of heat removal, because of the lowered liquid mass flow rate and decreased heat conductivity.

644 **3.3.3 Temperature**

645 In Figure 3-15, the impact on the temperature distribution is shown. As expected from the gas volume fraction,
 646 a substantial impact is likewise seen on the maximum temperature. The temperature increases with nearly 2°C
 647 when doubling the particle size from 20 to 40 micrometer. Interestingly, the location of this temperature
 648 increase coincides with the maximum gas volume fraction. At the same time as this large increase in maximum
 649 temperature is seen, a negligible effect on the mean temperature is found. This means that the effect is
 650 restricted to fairly local areas.

651 The observed large impact of particle diameter on temperature underlines the importance of accurately
 652 determining it. As such particle diameter does not significantly impact the average values of the temperature
 653 or gas volume fraction; hence it would, to some extent, make sense only to determine an appropriate average
 654 size. Else, the effect of particle coalescence and break-up could be accounted for using a multiple size group
 655 model. In this framework, a population balance is formulated which keeps track of the particle size distribution.

Figure 3-15: Mean and maximum temperature inside the GDL as a function of particle diameter.

4 Conclusion

In the present work, the flow and heat maldistribution in a circular-planar, interdigitated, anode flow field of a high pressure PEM electrolysis cell was studied. For this purpose, a comprehensive computational fluid dynamics model of the gas-liquid, two-phase flow was developed. In order to clearly identify the effect of two-phase flow and geometry, a single-phase model was solved in addition as a reference.

From the obtained simulation results, the following conclusion can be drawn:

- The investigated design of the circular-planar, interdigitated flow field causes flow maldistribution. Although the extent increases as function of water stoichiometry, no mass transport limitation or reversed flow is seen.
- At a low water stoichiometry and under nominal conditions, the maldistribution in the flow of the liquid phase is adversely affected by the presence of the gas phase. Relative to single-phase conditions, this leads to an excessive formation of hotspots. A water stoichiometry above 350 at a current density of 1 A/cm^2 is necessary to avoid that the difference between maximum and mean temperature exceeds 4°C .
- It is found that the extent of mass flow maldistribution can be reduced by approaching equal in-plane cross sectional land area sizes. This means that the land area width between the longest channels must be narrower than the width between the shortest channels. Indeed, if the overall mass flow maldistribution is dominated by the pressure losses within the GDL due to a low permeability, a more uniform distribution should be seen. However, it should be noted that the exact deviation from equal land areas depends on the extent of capillary pressure action and relative permeability of the GDL in question.

- For BP plates made from vinyl ester and under nominal conditions, the suggested geometrical changes do not lead to a critical land area width, which cannot sustain the compression forces exerted by cathode operating pressure.
- To minimize the formation of hotspots where the land areas are the widest, the extent of channel bending should be reduced.

To validate model predictions different experimental approaches can be taken. The simplest being a measurement of the anode back pressure, similarly as in the study by Nie and Chen [6]. However, such a type of validation does not give any details about the two-phase flow distribution inside channels or within the GDL; essentially, it only gives a lumped effect. A better approach would be to use a transparent BP similarly as done by Su et al. [18]. This approach allows for the use of direct imaging techniques, which enable direct bubble tracking through the use of edge detection algorithms by means of MATLAB or NI Vision. Furthermore, this techniques makes it is possible to determine of the bubble size distribution within a confined area of the channel flow field. In addition, a thermographic camera could be added to determine the temperature distribution within the flow field and highlight hotspot formation. Meanwhile, to get the two-phase distribution within the GDL, neutron radiography is necessary. This technique has among others been applied by Owejan et al. [25].

In our future work, we intend to construct a cell with a transparent BP and then determine the bubble size distribution, track gas particles as well as measure the temperature distribution using a thermographic camera. Furthermore, the proposed improvements to the flow field will be implemented and tested in an operating electrolysis cell. The obtained results will then be compared to the previous design and potential new design improvements could further be proposed.

In regard to modeling, our future work will also include the application of a multiple size group model that takes particle coalescence and breakup into account. The implementation of such a model can be validated using the proposed measurement of the particle size distribution using a direct imaging technique. Furthermore, phase change will be included for studies at low anode pressures. Similarly, the presence of the bipolar plate will be added to improve model predictions of cooling phenomena.

5 Acknowledgement

This work was partially supported by the Danish Energy Technology Development and Demonstration program EUDP through the HyProvide project, and by the Innovation Fund Denmark through the e-STORE project. The authors would in addition like to thank the members of the Fuel Cells and Battery Systems Research Group at the Department of Energy Technology for their input.

6 References

- [1] Hedegaard K, Ravn H, Juul N, Meibom P. Effects of electric vehicles on power systems in Northern Europe. *Energy* 2012;48:356–68. doi:10.1016/j.energy.2012.06.012.

- 713 [2] Gutiérrez-Martín F, Guerrero-Hernández I. Balancing the grid loads by large scale integration of
714 hydrogen technologies: The case of the Spanish power system. *Int J Hydrogen Energy* 2012;37:1151–61.
715 doi:10.1016/j.ijhydene.2011.09.116.
- 716 [3] Pickard WF, Shen AQ, Hansing NJ. Parking the power: Strategies and physical limitations for bulk energy
717 storage in supply–demand matching on a grid whose input power is provided by intermittent sources.
718 *Renew Sustain Energy Rev* 2009;13:1934–45. doi:10.1016/j.rser.2009.03.002.
- 719 [4] Carmo M, Fritz DL, Mergel J, Stolten D. A comprehensive review on PEM water electrolysis. *Int J*
720 *Hydrogen Energy* 2013;38:4901–34. doi:10.1016/j.ijhydene.2013.01.151.
- 721 [5] Zeng K, Zhang D. Recent progress in alkaline water electrolysis for hydrogen production and
722 applications. *Prog Energy Combust Sci* 2010;36:307–26. doi:10.1016/j.pecs.2009.11.002.
- 723 [6] Onda K, Kyakuno T, Hattori K, Ito K. Prediction of production power for high-pressure hydrogen by high-
724 pressure water electrolysis. *J Power Sources* 2004;132:64–70. doi:10.1016/j.jpowsour.2004.01.046.
- 725 [7] Bensmann B, Hanke-Rauschenbach R, Peña Arias IK, Sundmacher K. Energetic evaluation of high
726 pressure PEM electrolyzer systems for intermediate storage of renewable energies. *Electrochim Acta*
727 2013;110:570–80. doi:10.1016/j.electacta.2013.05.102.
- 728 [8] O’Hayre R, Cha SW, Colella W, Prinz FB. *Fuel Cell Fundamentals*. 2nd ed. John Wiley & Sons, Inc.; 2009.
- 729 [9] Li X, Sabir I. Review of bipolar plates in PEM fuel cells: Flow-field designs. *Int J Hydrogen Energy*
730 2005;30:359–71. doi:10.1016/j.ijhydene.2004.09.019.
- 731 [10] Li H, Tang Y, Wang Z, Shi Z, Wu S, Song D, et al. A review of water flooding issues in the proton exchange
732 membrane fuel cell. *J Power Sources* 2008;178:103–17. doi:10.1016/j.jpowsour.2007.12.068.
- 733 [11] Nguyen T V. A Gas Distributor Design for Proton-Exchange-Membrane Fuel Cells. *J Electrochem Soc*
734 1996;143:L103. doi:10.1149/1.1836666.
- 735 [12] Wang X-D, Duan Y-Y, Yan W-M, Peng X-F. Effects of flow channel geometry on cell performance for PEM
736 fuel cells with parallel and interdigitated flow fields. *Electrochim Acta* 2008;53:5334–43.
737 doi:10.1016/j.electacta.2008.02.095.
- 738 [13] Yan W-M, Mei S-C, Soong C-Y, Liu Z-S, Song D. Experimental study on the performance of PEM fuel cells
739 with interdigitated flow channels. *J Power Sources* 2006;160:116–22.
740 doi:10.1016/j.jpowsour.2006.01.063.
- 741 [14] Wang L, Liu H. Performance studies of PEM fuel cells with interdigitated flow fields. *J Power Sources*
742 2004;134:185–96. doi:10.1016/j.jpowsour.2004.03.055.

743 [15] Hu G, Fan J, Chen S, Liu Y, Cen K. Three-dimensional numerical analysis of proton exchange membrane
744 fuel cells (PEMFCs) with conventional and interdigitated flow fields. J Power Sources 2004;136:1–9.
745 doi:10.1016/j.jpowsour.2004.05.010.

746 [16] Wang X-D, Duan Y-Y, Yan W-M, Weng F-B. Effect of humidity of reactants on the cell performance of
747 PEM fuel cells with parallel and interdigitated flow field designs. J Power Sources 2008;176:247–58.
748 doi:10.1016/j.jpowsour.2007.10.065.

749 [17] Natarajan D, Van Nguyen T. Three-dimensional effects of liquid water flooding in the cathode of a PEM
750 fuel cell. J Power Sources 2003;115:66–80. doi:10.1016/S0378-7753(02)00624-9.

751 [18] SU A, WENG F, HSU C, CHEN Y. Studies on flooding in PEM fuel cell cathode channels. Int J Hydrogen
752 Energy 2006;31:1031–9. doi:10.1016/j.ijhydene.2005.12.019.

753 [19] Berning T, Odgaard M, Kær SK. Water balance simulations of a polymer-electrolyte membrane fuel cell
754 using a two-fluid model. J Power Sources 2011;196:6305–17. doi:DOI: 10.1016/j.jpowsour.2011.03.068.

755 [20] Yi JS, Nguyen T V. An Along-the-Channel Model for Proton Exchange Membrane Fuel Cells. J
756 Electrochem Soc 1998;145:1149–59.

757 [21] Wood DL, Yi JS, Nguyen T V. Effect of direct liquid water injection and interdigitated flow field on the
758 performance of proton exchange membrane fuel cells. Electrochim Acta 1998;43:3795–809.
759 doi:10.1016/S0013-4686(98)00139-X.

760 [22] Yi JS, Nguyen T Van. Multicomponent Transport in Porous Electrodes of Proton Exchange Membrane
761 Fuel Cells Using the Interdigitated Gas Distributors Ø F w I y K 1999;146:38–45.

762 [23] He W, Yi JS, Nguyen T Van. Two-Phase Flow Model of the Cathode of PEM Fuel Cells Using Interdigitated
763 Flow Fields 2000;46:2053–64.

764 [24] Kazim a, Liu HT, Forges P. Modelling of performance of PEM fuel cells with conventional and
765 interdigitated flow fields. J Appl Electrochem 1999;1409–16.

766 [25] Owejan JP, Trabold T a., Jacobson DL, Baker DR, Hussey DS, Arif M. In situ investigation of water
767 transport in an operating PEM fuel cell using neutron radiography: Part 2 - Transient water
768 accumulation in an interdigitated cathode flow field. Int J Heat Mass Transf 2006;49:4721–31.
769 doi:10.1016/j.ijheatmasstransfer.2006.07.004.

770 [26] Yan W-M, Chen C-Y, Mei S-C, Soong C-Y, Chen F. Effects of operating conditions on cell performance of
771 PEM fuel cells with conventional or interdigitated flow field. J Power Sources 2006;162:1157–64.
772 doi:10.1016/j.jpowsour.2006.07.044.

773 [27] Berning T, Odgaard M, Kær SK. A study of multi-phase flow through the cathode side of an
774 interdigitated flow field using a multi-fluid model. J Power Sources 2010;195:4842–52.
775 doi:10.1016/j.jpowsour.2010.02.017.

- 776 [28] Berning T, Kær SK. Low stoichiometry operation of a proton exchange membrane fuel cell employing the
777 interdigitated flow field - A modeling study. *Int J Hydrogen Energy* 2012;37:8477–89.
- 778 [29] Ito H, Maeda T, Nakano a., Hasegawa Y, Yokoi N, Hwang CM, et al. Effect of flow regime of circulating
779 water on a proton exchange membrane electrolyzer. *Int J Hydrogen Energy* 2010;35:9550–60.
780 doi:10.1016/j.ijhydene.2010.06.103.
- 781 [30] Nie J, Chen Y. Numerical modeling of three-dimensional two-phase gas–liquid flow in the flow field plate
782 of a PEM electrolysis cell. *Int J Hydrogen Energy* 2010;35:3183–97. doi:10.1016/j.ijhydene.2010.01.050.
- 783 [31] Olesen AC, Berning T, Kær SK. The Effect of Inhomogeneous Compression on Water Transport in the
784 Cathode of a Proton Exchange Membrane Fuel Cell. *J Fuel Cell Sci Technol* 2012;9:031010.
785 doi:10.1115/1.4006475.
- 786 [32] Tomadakis MM, Robertson TJ. Viscous Permeability of Random Fiber Structures: Comparison of
787 Electrical and Diffusional Estimates with Experimental and Analytical Results. *J Compos Mater*
788 2005;39:163–88. doi:10.1177/0021998305046438.
- 789 [33] Menter FR. Two-equation eddy-viscosity turbulence models for engineering applications. *AIAA J*
790 1994;32:1598–605. doi:10.2514/3.12149.
- 791 [34] Sato Y, Sekoguchi K. Liquid velocity distribution in two-phase bubble flow. *Int J Multiph Flow* 1975;2:79–
792 95. doi:10.1016/0301-9322(75)90030-0.
- 793 [35] Gostick JT, Fowler MW, Ioannidis MA, Pritzker MD, Volfkovich YM, Sakars A. Capillary pressure and
794 hydrophilic porosity in gas diffusion layers for polymer electrolyte fuel cells. *J Power Sources*
795 2006;156:375–87. doi:10.1016/j.jpowsour.2005.05.086.
- 796 [36] Gostick JT, Fowler MW, Pritzker MD, Ioannidis MA, Behra LM. In-plane and through-plane gas
797 permeability of carbon fiber electrode backing layers. *J Power Sources* 2006;162:228–38. doi:DOI:
798 10.1016/j.jpowsour.2006.06.096.
- 799 [37] Berning T, Odgaard M, Kær SK. A Computational Analysis of Multiphase Flow Through PEMFC Cathode
800 Porous Media Using the Multifluid Approach. *J Electrochem Soc* 2009;156:B1301–11.
- 801 [38] Gurau V, Thomas A, Zawodzinski J, J. Adin Mann J. Two-Phase Transport in PEM Fuel Cell Cathodes. *J*
802 *Fuel Cell Sci Technol* 2008;5:21009. doi:10.1115/1.2821597.
- 803 [39] Nam JH, Kaviany M. Effective diffusivity and water-saturation distribution in single- and two-layer
804 PEMFC diffusion medium. *Int J Heat Mass Transf* 2003;46:4595–611. doi:DOI: 10.1016/S0017-
805 9310(03)00305-3.
- 806 [40] Olesen AC, Kær SK. Flow Maldistribution in the Anode of A Polymer Electrolyte Membrane Electrolysis
807 Cell Employing Interdigitated Channels. *Proc. 55th Conf. Simul. Model. (SIMS 55), Model. Simul. Optim.*
808 21-22 Oct. 2014, Aalborg, Denmark, Linköping Electronic Conference Proceedings; 2014, p. 241–9.

809 [41] Inc. B. Data sheet for vinyl ester bipolar plate material - BMC 940 2001.
810 http://www.bulkmolding.com/datasheets/informational/bmc_940.pdf (accessed September 21, 2015).

811

812 **List of Figures**

813 Figure 1: Anode planar-circular flow field

814 Figure 2: Titanium felt deformation strain, viscous permeability and volume porosity as function of deformation
815 pressure

816 Figure 3: Polarization curve and heat generation of a PEMEC per unit area at 70 C, cathode pressure of 1.8 bar
817 and different anode pressures.

818 Figure 4: Bar graph of the mass flow rates per channel length for each individual outlet channel

819 Figure 5: Bar graph of the mass quality distribution among the outlet channels

820 Figure 6: In-plane gas volume fraction distribution at $y^*=y/h_{\text{channel}} = 0.5$ inside the channel

821 Figure 7: In-plane gas volume fraction distribution at $y^*=y/t_{\text{GDL}} = 0.5$ inside the GDL

822 Figure 8: In-plane true liquid velocity distribution inside the GDL at $y^*=y/t_{\text{GDL}} = 0.5$

823 Figure 9: In-plane true gas velocity distribution inside the GDL at $y^*=y/t_{\text{GDL}} = 0.5$

824 Figure 10: In-plane temperature distribution inside channels at $y^*=y/t_{\text{chan}} = 0.5$, under nominal conditions

825 Figure 11: In-plane temperature distribution inside the GDL at $y^*=y/t_{\text{GDL}} = 0.5$, under nominal conditions

826 Figure 13: Standard deviation in liquid mass flow rate per channel length for outlet channels.

827 Figure 13: Mean, maximum and standard deviation in gas volume fraction throughout the GDL.

828 Figure 14: The mean and maximum temperatures throughout the GDL, as predicted by the single- and two-
829 phase models

830 Figure 15: Back pressure as a function of water stoichiometry for single- and two-phase flow

831 Figure 16: Standard deviation in mass flow per channel length as function of particle diameter

832 Figure 17: Mean, maximum and standard deviation in gas volume fraction inside the GDL as function of particle
833 diameter

834 Figure 18: Mean and maximum temperature inside the GDL as a function of particle diameter

837 **List of Tables**

838 Table 1: Superficial Reynolds number as a function of water stoichiometry for a current density of 1 A/cm²

839 Table 2: Nominal operation conditions

840

Symbol	Description	Unit
ϵ	Volume porosity	-
s	Engineering strain	-
P	Pressure	Pa
μ	Dynamic viscosity	Pa s
K	Viscous permeability	m^2
ρ	Density	kg/m^3
β	Inertial Forchheimer coefficient	$1/\text{m}$
u	Superficial velocity	m/s
Q	Heat	J
T	Temperature	K
S	Entropy	J/K
G	Gibbs free energy	J
H	Enthalpy	J
h	Specific enthalpy	J/kg
e	Specific internal energy	J/kg
n	Number of electrons transferred	-
F	Faradays constant = 96485.3365	C/mol
V	Voltage	V
q	Specific heat	J/mol
I	Current	A
j	Current density	A/m^2
A	Area	m^2
D	Diameter	m
λ	Stoichiometric factor	-
M	Molecular weight	kg/mol
$\dot{m}$	Mass flow rate	Kg/s
Re	Reynolds number	-
a	Length	m
b	Width	m
U	True velocity	m/s
S	Source term	
τ	Shear stress	Pa
$\mathbf{g}$	Gravitational acceleration vector	m/s^2
$\mathbf{M}$	Generalized momentum source term	$\text{kg}/\text{m}^2 \text{ s}^2$
k	Kinetic energy	m^2/s^2
ω	Turbulent eddy frequency	$1/\text{s}$
C	Turbulence model constant = 0.09	-
β	Turbulence model constant = 0.09	-
β'	Turbulence model constant = 0.075	-
σ_ρ	Turbulent Schmidt number = 1	-
α	Turbulence model constant = 5/9	-

C_3	Turbulence model constant = 1	-
$C_{\mu p}$	Turbulence model constant = 0.6	
s	Phase saturation or phase volume fraction	-
C_D	Drag coefficient	-
a_{cd}	Interfacial area density for the interphase drag force	1/m
s_{dm}	Maximum packing value	-
C_{cd}	Momentum transfer coefficient for the interphase drag force	-
n	Genuchten model constant	-
m	Genuchten model constant	-
λ	Thermal conductivity	W/m K
$\mathbf{n}$	Normal vector	-
c_p	Specific heat capacity at constant pressure	J/kg K
σ	Surface tension	N/m
σ	Standard deviation	
μ	Mean	
V	Volume	m ³
m	Mass	kg

842

843

844 **Abbreviations**

PEM	Proton exchange membrane
FC	Fuel cell
EC	Electrolysis cell
GDL	Gas diffusion layer
CL	Catalyst layer
MPL	Micro porous layer
BP	Bipolar plate
Ti	Titanium

845

846

847 **Subscripts**

0	Initial conditions
rev	Reversible
irr	Irreversible
cell	Cell conditions
neutral	Thermo-neutral conditions i.e. no heat is produced or consumed
in	Inlet
out	Outlet
H	Hydraulic
T	Turbulence
k	Turbulent kinetic energy
kb	Effect of buoyancy on turbulent kinetic energy
ωk	Effect of buoyancy on turbulent frequency
α	Phase
rel	Relative
D	Drag
TD	Turbulent dispersion
l	Liquid
g	Gas
m	Mixture
c	Capillary
cb	Capillary breakthrough
e	Effective
s	Solid
E	External
c	Cross section

848

849