



















Now, returning to the question about current density depletion in the middle of the channel, we see that the answer is directly coupled to the depletion of the oxygen concentration in the middle of the channel, as can be inferred from Figure 4. Clearly, the convective flow of oxygen driven by natural convection into the cathode channel is not high enough to penetrate deeper into the cathode flow field to produce electricity. This mass transport limitation can be reduced by shortening the cathode flow field, so that the oxygen still can reach to the middle, as can be seen in Figure 4a.

### Orientation and Gravitational Effects

The flow arising from natural convection depends on the coupling between transport of mass, energy and momentum and the variation of the density. The orientation of the fuel cell/stack can therefore be expected to have an impact on the performance. To study if this is the case, let us return to case b and introduce three different orientations: vertical ( $90^\circ$ , base-case); tilted ( $45^\circ$ ); horizontal ( $0^\circ$ ), as shown in Figure 5.

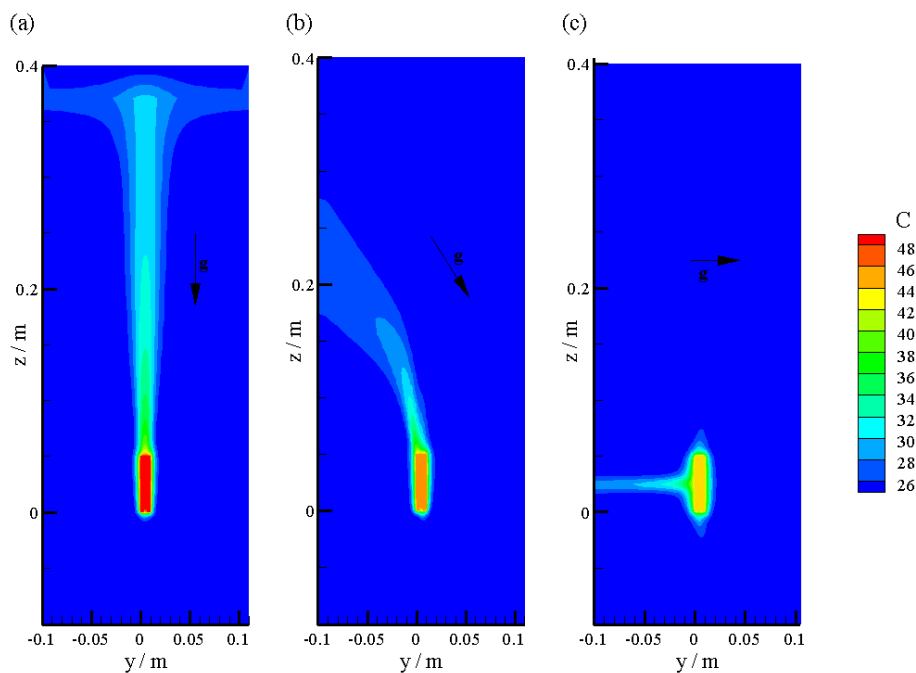


Figure 5. Temperature distribution ( $^\circ\text{C}$ ) for different gravitational orientations: a) vertical ( $90^\circ$ ); b) tilted ( $45^\circ$ ); c) horizontal ( $0^\circ$ )

Before we look into cell performance, let us have a closer look at the temperature distribution, which is one of the driving forces for the density variations and buoyant flow. As shown in Figure 5, the temperature distribution is similar to the thermal plume that Fabian et al. [34] observed experimentally. Focusing on case a, and the immediate vicinity of the cell, as depicted in Figure 6, we find that the average velocity is around  $2 \times 10^{-2} \text{ m s}^{-1}$  at the cathode inlets arising from buoyancy flowing from bottom to the top. For tilted case, a slightly lower velocity is observed flowing at the bottom of the cathode channel with the average velocity of around  $8 \times 10^{-3} \text{ m s}^{-1}$ . In contrast, for the horizontal placement, the inlet velocity is around one order-of-magnitude lower with an average flow velocity of  $3 \times 10^{-3}$ . In addition, the maximum velocity due to natural convection in the surrounding is around  $5 \times 10^{-2} \text{ m s}^{-1}$ , which is similar to the velocities predicted by Lister et al. [14].

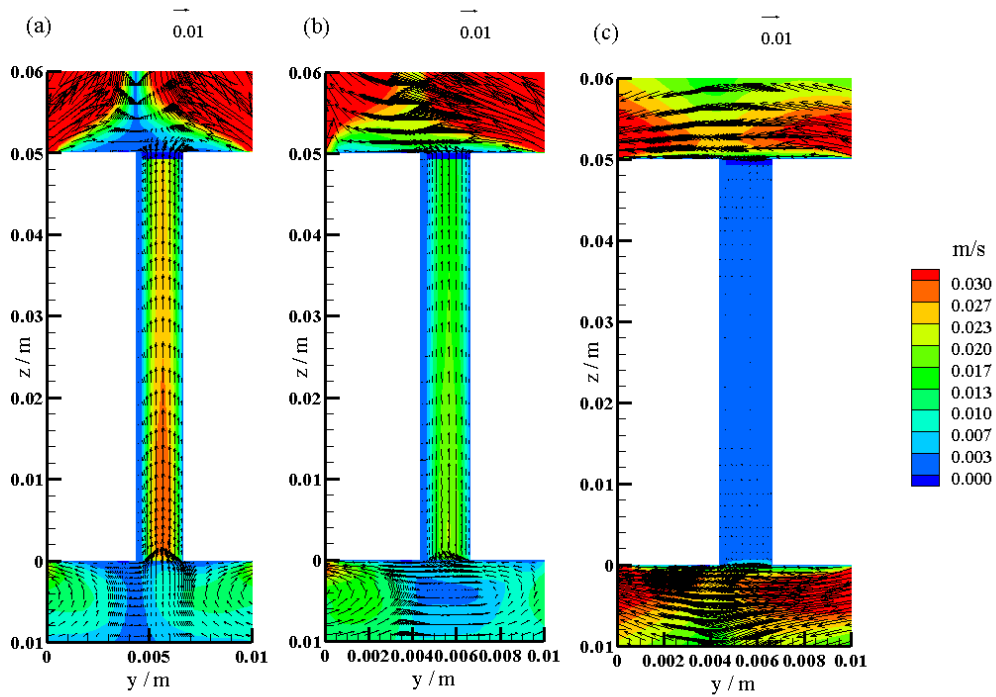


Figure 6. Velocity vector and contour ( $\text{ms}^{-1}$ ) at the cathode and its immediate ambient for different gravitational orientations: a) vertical ( $90^\circ$ ); b) tilted ( $45^\circ$ ); c) horizontal ( $0^\circ$ )

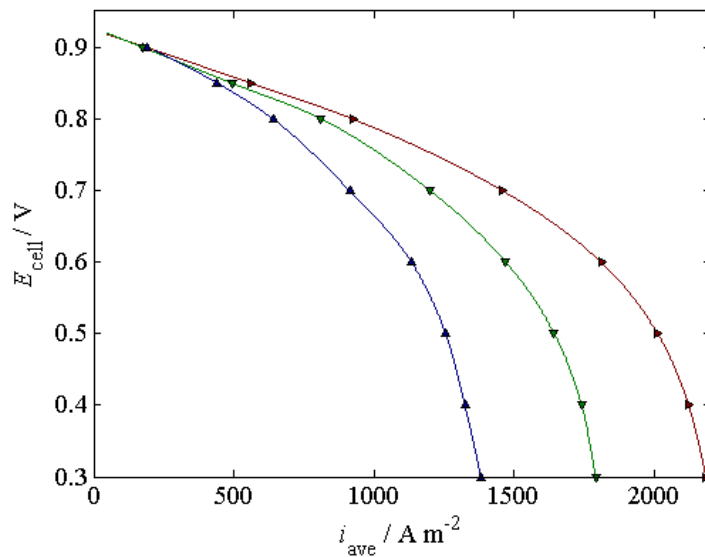


Figure 7. Polarization curves for different gravitational orientations: [►] vertical ( $90^\circ$ ); [▼] tilted ( $45^\circ$ ); and [▲] horizontal ( $0^\circ$ )

In free-breathing fuel cell, the velocity is highly nonlinear as it is functions of buoyancy flow due to temperature gradient, flow channel geometry and orientations as well as mass transfer driving force due to oxygen consumption. Note that in this simulation, the air flow rate is not fixed; instead we prescribe ambient condition, i.e., constant ambient pressure, temperature and mass fraction, to allow for natural convection air flow due to the factors mentioned above. Moreover, the three-dimensional simulation is able to capture the

effect of channel-rib geometry to the incoming air flow and species distribution in the catalyst layer. Closer inspection reveals that rib adds flow resistant to the incoming air to flow channel: small boundary layer is observed at the wall between rib-ambient. In the catalyst layer, the three-dimensionality effect of rib is also seen: oxygen concentration bellow rib area is slightly lower than that bellow channel; this is mirrored by no-uniform current generation and temperature distribution.

The impact of orientation on fuel cell performance is highlighted in Figure 7. The highest performance can be achieved by vertical alignment of the cell, followed by tilted case and finally the horizontal one for the operating conditions considered here. On closer inspection, we note that by changing gravitational orientation, the cell performance can improve by up to ~ 35%; that is by changing cell orientation from horizontal with limiting current of ~ 1300 A m<sup>-2</sup> improves to around 2300 A m<sup>-2</sup> as the cell is arranged vertically.

### Thermal Management: Single Cell and Stack

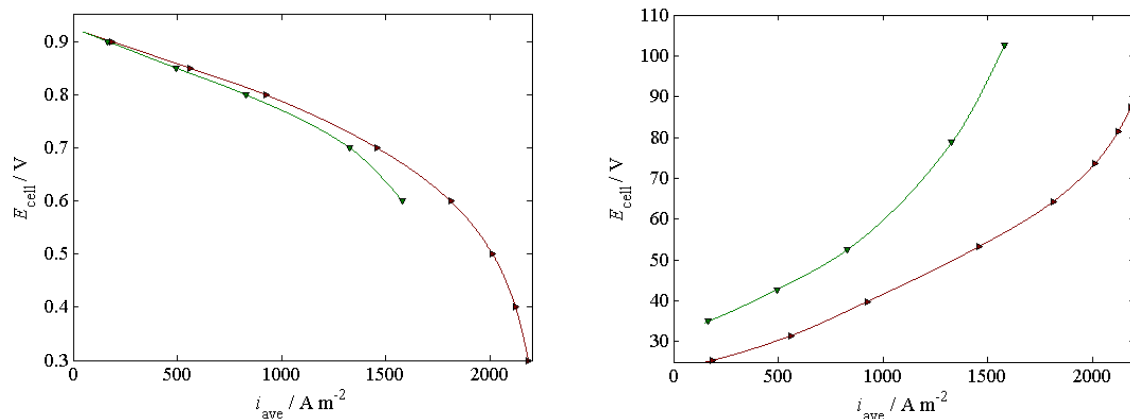


Figure 8. Comparison of (a) polarization curve and (b) average temperature for single cell [►] and stack comprises of 12 cells [▼] with free air-breathing

One key component in control strategies of a fuel cell stack or single cell is thermal management. This is especially important for the former as every cell can generate a significant amount of heat, which needs to be removed from the stack. For the case of a fuel cell single cell or stack operating at natural convection conditions, the removal rate is limited by the natural convection to and from the cell/stack. Generally, this only allows for the operation of small stacks of a few cells. Here, we simulate the thermal envelope for both a single cell and a stack comprising of twelve cells, the results of which are shown in Figure 8.

The temperature increase for the stack is much higher than the single cell as expected. The overall temperature increase for the latter is around 23°C at operating cell voltage of 0.7 V (see Figure 9a), which is in agreement with experimental data from Fabian et al. [34]. For the former, the stack temperature is around 55°C higher than the ambient air (Figure 9b). The higher temperature inside each cell of the stack leads to a lower water content in the membranes and thus an increase in ohmic resistance, which in turn manifests itself in a lower performance. In this case, the overall current density that is generated by the stack is around 20% lower than that of the single cell. As we proceed to higher current densities, the single cell performance can sustain up to more than 2000 A m<sup>-2</sup>; whereas for stack, the performance is only able to generate current density up to ~ 1600 A m<sup>-2</sup>, after which the performance drops to zero as temperature inevitably rise to more than 100°C which

indicates that membrane start to failure. To improve performance of the stack, one needs to carefully design it to maximize the buoyant flow and perhaps introduce additional cooling channels or add fan to forced more air flows to the cathode.

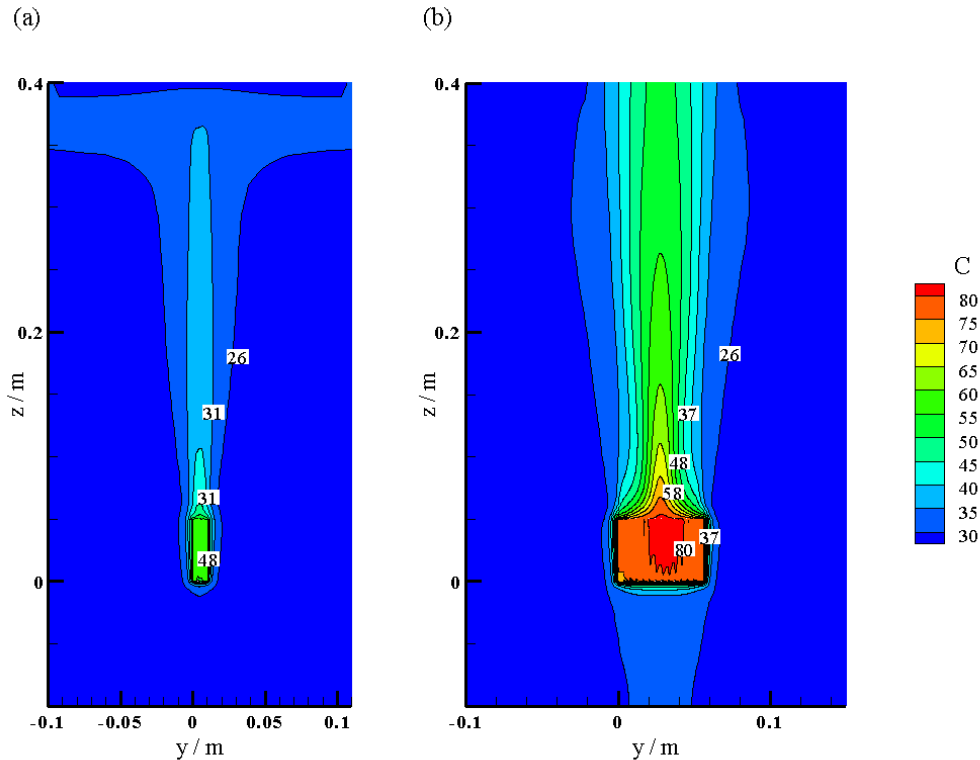


Figure 9. Temperature contours ( $^{\circ}\text{C}$ ) for a) single cell; b) stack comprising 12 cells with its immediate ambient

## Concluding Remarks

A numerical study of a free air-breathing PEM fuel cell was carried out for both a single cell and a stack. It is shown that the cathode flow field design plays an important role in determining the mass transport limitations that arise along the cathode; a short length allows for more oxygen to be transported into the cathode. Furthermore, orientation of the cell/stack with respect to gravity also needs to be considered to ensure adequate airflow; for conditions considered here, a vertical alignment of the cell gave a better performance than tilting the cell at an angle or even positioning it horizontally. Finally, the simulation results indicate that stacks, even when only comprising of a few cells, can heat up significantly relative to the ambient conditions.

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## References

- [1] S. Hamel, and L.G. Frechette, "Critical importance of humidification of the anode in miniature air-breathing polymer electrolyte membrane fuel cells," *Journal of Power Sources*, Vol. 196, pp. 6242-6248, 2011.
- [2] Z.R. Williamson, D. Kim, D.K. Chun, T. Lee, and C.W. Squibb, "Experimental evaluation of cell temperature effects on miniature air breathing PEM fuel cells," *Applied Thermal Engineering*, 2011, doi: 10.1016/j.applthermaleng. 2011. 06.10.
- [3] C.K. Poh, Z. Tian, N. Bussayajarn, Z. Tang, F. Su, S.H. Lim, Y.P. Feng, D. Chua, and J. Lin, "Performance enhancement of air-breathing proton exchange membrane fuel cell through utilization of an effective self-humidifying platinum-carbon catalyst," *Journal of Power Sources*, Vol. 195, pp. 8044-8051, 2010.
- [4] K.I. Lee, S.W. Lee, M.S. Park, and C.N. Chu, "The development of air-breathing proton exchange membrane fuel cell (PEMFC) with a cylindrical configuration," *International Journal of Hydrogen Energy*, Vol. 35, pp. 11844-11854, 2010.
- [5] N. Bussayajarn, H. Ming, K.K. Hoong, W.Y.M. Stephen, and C.S. Hwa, "Planar air breathing PEMFC with self-humidifying MEA and open cathode geometry design for portable applications," *International Journal of Hydrogen Energy*, Vol. 34, pp. 7761-7767, 2009.
- [6] P.W. Li, T. Zhang, Q.M. Wang, L. Schaefer, and M.K. Chyu, "The performance of PEM fuel cells fed with oxygen through the free-convection mode," *Journal of Power Sources*, Vol. 114, pp. 63-69, 2003.
- [7] T. Mennola, M. Noponen, M. Aronniemi, T. Hottinen, M. Mikkola, O. Himanen, and P. Lund, "Mass transport in the cathode of a free-breathing polymer electrolyte membrane fuel cell," *Journal of Applied Electrochemistry*, Vol. 33, pp. 979-987, 2003.
- [8] A. Schmitz, C. Ziegler, J.O. Schumacher, M. Tranitz, E. Fontes, and C. Hebling, "Modelling approach for planar self-breathing PEMFC and comparison with experimental results," *Fuel Cells*, Vol. 4, pp. 358-364, 2004.
- [9] Y. Wang, Y.J. Sohn, W.Y. Lee, J. Ke, and C.S. Kim, "Three-dimensional modeling and experimental investigation for an air-breathing polymer electrolyte membrane fuel cell PEMFC," *Journal of Power Sources*, Vol. 145, pp. 563-571, 2005.
- [10] Y. Wang, T.H. Yang, W.Y. Lee, J. Ke, and C.S. Kim, "Three-dimensional analysis for effect of channel configuration on the performance of a small air-breathing proton exchange membrane fuel cell (PEMFC)," *Journal of Power Sources*, Vol. 145, pp. 572-581, 2005.
- [11] Y. Wang, J. Ke, W.Y. Lee, T.H. Yang, and C.S. Kim, "Effects of cathode channel configurations on the performance of an air-breathing PEMFC," *International Journal of Hydrogen Energy*, Vol. 30, pp. 1351-1361, 2005.
- [12] Y. Wang, and M. Ouyang, "Three-dimensional heat and mass transfer analysis in an air-breathing proton exchange membrane fuel cell," *Journal of Power Sources*, Vol. 164, pp. 721-729, 2007.
- [13] Y. Tabe, S.K. Park, K. Kikuta, T. Chikahisa, and Y. Hishinuma, "Effect of cathode separator structure on performance characteristics of free-breathing PEMFCs," *Journal of Power Sources*, Vol. 162, pp. 58-65, 2006.
- [14] S. Lister, J.G. Pharoah, G. McLean, and N. Djilali, "Computational analysis of heat and mass transfer in a micro-structured PEMFC cathode," *Journal of Power Sources*, Vol. 156, pp. 334-344, 2005.
- [15] J.J. Hwang, "Species-electrochemical modeling of an air-breathing cathode of a planar fuel cell," *Journal of the Electrochemical Society*, Vol. 153, pp. A1584-A1590, 2006.

- [16] J.J. Hwang, S.D. Wu, R.G. Pen, P.Y. Chen, and C.H. Chao, "Mass/electron co- transports in an air-breathing cathode of a PEM fuel cell," *Journal of Power Sources*, Vol. 160, pp. 18-26, 2006.
- [17] R. O'Hayre, T. Fabian, S. Litster, F.B. Prinz, and J.G. Santiago, "Engineering model of a passive planar air breathing fuel cell cathode," *Journal of Power Sources*, Vol. 167, pp. 118-129, 2006.
- [18] B.P.M. Rajani, and A.K. Kolar, "A model for a vertical planar air breathing PEM fuel cell," *Journal of Power Sources*, Vol. 164, pp. 210-221, 2007.
- [19] Y. Zhang, and R. Pitchumani, "Numerical studies on an air-breathing proton exchange membrane PEM fuel cell," *International Journal of Heat and Mass Transfer*, Vol. 50, pp. 4698-4712, 2007.
- [20] Y. Zhang, A. Mawardi, and R. Pitchumani, "Numerical studies on an air-breathing proton exchange membrane PEM fuel cell stack," *Journal of Power Sources*, Vol. 173, pp. 264-276, 2007.
- [21] L. Matamoros, and D. Bruggemann, "Concentration and ohmic losses in free-breathing PEMFC," *Journal of Power Sources*, Vol. 173, pp. 367-374, 2007.
- [22] M. Paquin, and L. Frechete, "Polarization study of a PEMFC with four reference electrodes at hydrogen starvation conditions," *Journal of Power Sources*, Vol. 180, pp. 440-451, 2008.
- [23] X.Q. Xing, K.W. Lum, H.J. Poh, and Y.L. Wu, "Geometry optimization for proton-exchange membrane fuel cells with sequential quadratic programming method," *Journal of Power Sources*, Vol. 186, pp. 10-21, 2009.
- [24] M.A.R.S. Al-Baghdadi, "Performance comparison between airflow-channel and ambient air-breathing PEM fuel cells using three-dimensional computational fluid dynamics models," *Renewable Energy*, Vol. 34, pp. 1812-1824, 2009.
- [25] P.M. Kumar, and A.K. Kolar, "Effect of cathode design on the performance of an air-breathing PEM fuel cell," *International Journal of Hydrogen Energy*, Vol. 35, pp. 671-681, 2010.
- [26] P.M. Kumar, and A.K. Kolar, "Effect of cathode channel dimensions on the performance of an air-breathing PEM fuel cell," *International Journal of Thermal Sciences*, Vol. 49, pp. 844-857, 2010.
- [27] A.P. Sasmito, K.W. Lum, E. Birgersson, and A.S. Mujumdar, "Computational study of forced air-convection in open-cathode polymer electrolyte fuel cell stacks," *Journal of Power Sources*, Vol. 195, pp. 5550-5563, 2010.
- [28] A.P. Sasmito, E. Birgersson, K.W. Lum, and A.S. Mujumdar, "Fan selection and stack design for open-cathode polymer electrolyte fuel cell stacks," *Renewable Energy*, Vol. 37, pp. 325-332, 2012.
- [29] A.P. Sasmito, E. Birgersson, and A.S. Mujumdar, "Numerical evaluation of various thermal management strategies for polymer electrolyte fuel cell stacks," *International Journal of Hydrogen Energy*, Vol. 36, pp. 12991-13007, 2011.
- [30] A.P. Sasmito, and A.S. Mujumdar, "A novel flow reversal concept for improved thermal management in polymer electrolyte fuel cell stacks," *International Journal of Thermal Sciences*, Vol. 54, pp. 242-252, 2012.
- [31] A.P. Sasmito, and A.S. Mujumdar, *Transport Phenomena Models for Polymer Electrolyte Fuel Cell Stacks: Thermal, Water and Gas Management - From Fundamentals to Applications*, Lambert Academic Publishing, Germany, 2011.
- [32] A.P. Sasmito, E. Birgersson, and A.S. Mujumdar, "Numerical investigation of liquid water cooling for a proton exchange membrane fuel cell stack," *Heat Transfer Engineering*, Vol. 32, pp. 151-167, 2011.
- [33] A.P. Sasmito, and A.S. Mujumdar, "Performance evaluation of a polymer electrolyte

- fuel cell with a dead-end anode: A computational fluid dynamic study,” *International Journal of Hydrogen Energy*, Vol. 36, pp. 12991-13007, 2011.
- [34] T. Fabian, J.D. Posner, R. O’Hayre, S.W. Cha, J.K. Eaton, F.B. Prinz, and J.G. Santiago, “The role of ambient conditions on the performance of a planar air-breathing hydrogen PEM fuel cell,” *Journal of power Sources*, Vol. 161, pp. 168-182, 2006.