Supplementary Electronic Information 1

The analytic sensitivities of the objective function f, with respect to any of the design variables p_i, can be obtained using functional analysis as

$$\begin{aligned}\frac{df(\mathbf{u},\mathbf{p})}{dp_i} &= \frac{\partial f(\mathbf{u},\mathbf{p})}{\partial u_j}\frac{\partial u_j}{\partial p_i} + \frac{\partial f(\mathbf{u},\mathbf{p})}{\partial p_i} \\ &= \frac{1}{H}\int_0^H \int_0^L \left(\frac{\partial(\boldsymbol{\nabla}\cdot\mathbf{i})}{\partial u_j}\frac{\partial u_j}{\partial p_i} + \frac{\partial(\boldsymbol{\nabla}\cdot\mathbf{i})}{\partial p_i}\right) dxdy \end{aligned} \quad (1)$$

where $\mathbf{u}$ is the vector of unknowns solved for by the analysis program, $\mathbf{p}$ is the vector of design parameters, $i = 1,\dots,8$, $j = 1,\dots,5$, $\frac{\partial(\boldsymbol{\nabla}\cdot\mathbf{i})}{\partial u_j}$ and $\frac{\partial(\nabla\cdot\mathbf{i})}{\partial p_i}$ are obtained by analytical differentiation of the nonlinear expression $\boldsymbol{\nabla}\cdot\mathbf{i}$ with respect to the solution vector and the design variables respectively and, finally, the term $\frac{\partial u_j}{\partial p_i}$ is unknown and represents the change of the solution vector with respect to the design variables. This latter vector can be obtained by noticing that the residual of the governing equations has to be zero at the solution and that any perturbation in the parameters of the system should result in no variation of the residual if the governing equation is to be satisfied. Therefore, the total derivative of the residual has to be zero. Then, $\frac{\partial u_j}{\partial p_i}$ is computed by solving the system of partial differential equations given by

$$\frac{\partial R(\mathbf{u},\mathbf{p})}{\partial u_j}\frac{\partial u_j}{\partial p_i} = -\frac{\partial R(\mathbf{u},\mathbf{p})}{\partial p_i} \quad (2)$$

where $\frac{\partial R(\mathbf{u},\mathbf{p})}{\partial u_j}\frac{\partial u_j}{\partial p_i}$ and $\frac{\partial R(\mathbf{u},\mathbf{p})}{\partial p_i}$ represent the derivatives of the governing equations in (1) in the main text with respect to the solution vector and the design variables respectively. These are obtained using functional analysis. Note that $\frac{\partial R(\mathbf{u},\mathbf{p})}{\partial u_j}\frac{\partial u_j}{\partial p_i}$ is a directional derivative and therefore results in a differential equation with the vector $\frac{\partial u_j}{\partial p_i}$ as the unknown [1, 2]. A more detailed explanation of the methodology used to solve the fuel cell governing equations and the sensitivity equations is given in reference [3].

References

[1] D. G. Luenberger, *Optimization by vector space methods*, John Wiley & Sons, New York, 1969.

[2] K. Yosida, *Functional analysis*, Springer-Verlag, Berlin, 1965.

[3] M. Secanell *Computational Modeling and Optimization of Proton Exchange Membrane Fuel Cells* PhD thesis, University of Victoria, 2007.