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Short communication

A simple, mathematical model of thermal coupling in fuel cell stacks

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Abstract

The authors develop a model of steady state thermal transfer in polymer electrolyte membrane fuel cell stacks. The model is appropriate for straight coolant channel unit cell designs and considers quantities averaged over the cross-channel direction, ignoring the impact of the gas and coolant channel geometries. At steady state and under the assumption that the membrane and electrodes are infinitesimally thin, a simple description can be made of the temperature distribution in the cells. The model provides estimates on two important quantities: the local temperature difference between coolant and membrane, and the spread of heat from an anomalously hot cell to its neighbours in a stack environment. The former question is easy to address after the model is presented. The latter requires small argument Laplace transform asymptotics that correspond to a large scaled heat transfer coefficient to the coolant channels. Results of computational approximation of the model are also shown and compared to the asymptotics.

Keywords: Fuel cell stacks; Thermal management

1. Introduction

A polymer electrolyte membrane fuel cell (PEMFC) is an electrochemical device in which the energy of the chemical reaction is converted directly into electricity. By combining hydrogen fuel with oxygen from air, electricity is formed without combustion of any form. Water and heat are the only byproducts when hydrogen is used as the fuel source. Further details of general fuel cell operation can be found in [1].

Computational modelling of fuel cell operation has been seen as a way to perform design optimization more efficiently than by experimental testing in certain situations. Early low-dimensional averaged models of unit cell performance were developed in [2] and elsewhere. A modern version of this kind of model was recently developed by our group [3]. Three-dimensional computational models have been developed in [4–8], for example. These are finite volume computational tools that describe the coupled mass transport and electrochemistry in unit cells.

A few authors [9,10] have concentrated specifically on computational models of heat transfer in fuel cells. Accurate approximation of temperature profiles is of interest in the application since current fuel cell membranes degrade if the temperature increases 10–20 °C past standard operating points. Thermal profiles also determine (and are affected) by where condensation occurs, which also has a large impact on performance. Despite the importance, there have been few attempts to model the effects of cell-to-cell coupling in a stack environment. A first attempt was made in our own work [11]. The present paper can be viewed as a mathematical analysis of a simplified version of the model presented there that gives insight into the way heat is spread from anomalously hot cells in a stack.

The main simplification of the model is that it considers heat transfer only in an averaged sense over the cross-channel geometry, as discussed in Section 2.2. This simplification limits the model to qualitative accuracy. Another significant limitation to the model is that it does not couple the computed temperature profiles to performance. This means that it cannot predict phenomena of local thermal runaway, caused by such mechanisms as the feedback loop between membrane

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drying and heat production. However, the ability of the model to predict the spread of heat in a stack environment does give insight in to designs where such runaway conditions can occur and how to develop designs that can suppress them. Currently, there is no experimental data to validate the model, which was developed in part to allow experimentalists to investigate what kind of measurements would give useful insight into quantitative aspects of heat transfer in fuel cell stacks. Such experiments are currently being undertaken.

In Section 2, we develop the basic model. In Section 3, we nondimensionalize the equations and present two alternate reformulations of the equations, one suitable for computation and the other for analysis. In Section 4, we present the small argument Laplace transform analysis that leads to an approximate analytic formula for the extent of the spreading of heat from an anomalously hot cell in a stack. In Section 5, we compare computational and analytic solutions. Most of the notation and values of physical parameters are given in Section 2.

2. Basic model

We consider a unit fuel cell as shown in Fig. 1, which is not drawn to scale. The electrodes and membrane together (known collectively as the membrane electrode assembly or MEA) are thinner than the plates. We model cells with straight (in x) coolant channels such as the Ballard Mk 9 hardware, although other designs such as serpentine channels are in use [5].

Unit cells are stacked together in series to make a fuel cell stack. The anode plate of one cell is put against the cathode plate of the next. The combined plate is known as a *bipolar* plate. A schematic is shown in Fig. 2. We will use subscripts j to indicate the cell number in the stack.

We make the following assumptions:

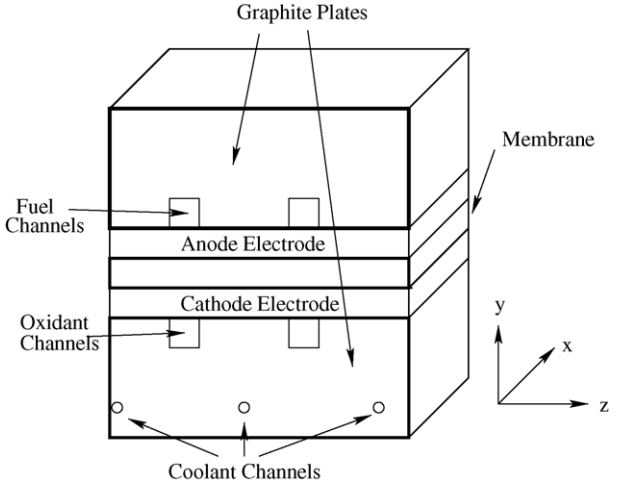

Fig. 1. Schematic of unit fuel cell.

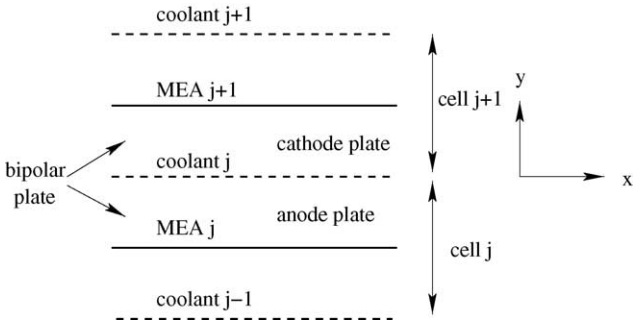

Fig. 2. Cross-section (x–y) of stacked unit cells.

1. The MEAs can be taken to be infinitesimally thin. The effect of MEA structure can be added as done in [11]. These effects are not insignificant (the majority of the heat is produced in the cathode electrode due to the ORR overpotential). However, we choose to neglect these effects for simplicity in the current model which aims at qualitative description of stack level thermal coupling.
2. Heat is generated only in the MEA layer and that the heat flux Q^j is given and constant in x and z for each unit cell but that it may vary between cells in the stack.
3. Heat is removed only by the coolant and that local (y–z plane) conduction to the coolant is dominant. That is, heat conduction in the x-direction of the plates can be neglected. This will be true except in an asymptotically small region near cell inlet and outlet where corrections are needed to match to given insulating or radiative conditions. We neglect these small end effects.
4. The geometric effects of the gas channels can be ignored and the thermal transport from electrodes to coolant channels through the plates can be described approximately by a one-dimensional conjugate heat transfer process with standard transfer coefficients.

We also neglect stack end effects (for example, convection from end cell surfaces). These effects are known to be important [12], but our work here concentrates on the thermal coupling effects of cells away from stack ends.

Assumptions 1 and 2 above are made just for the convenience of the analytic investigations of this paper. Some preliminary results of a more complete model are given in [11], where the temperature distribution through the MEA is modelled and approximate heat fluxes from membrane resistance, condensation and overpotential losses varying (in x) are used from an existing performance model.

Assumptions 3 and 4 are what lead to great simplifications in the model equations. They are discussed in more details in Sections 2.1 and 2.2. We take all quantities to be averaged over the cross-channel z-direction and use $T^j(x)$ to denote the average coolant temperatures, $\beta_j(x)$ for plate temperatures at the coolant and $\theta_j(x)$ for MEA temperatures. All temperatures are taken relative to the inlet coolant temperature. We arrive at a system of ordinary differential algebraic equations (DAE) in these variables below.

We use the following physical constants:

c: Coolant heat capacity ($\mathrm{J\,kg^{-1}\,K^{-1}}$).
Q_c: Coolant flux per unit z in each cell ($\mathrm{kg\,s^{-1}\,m^{-1}}$).
A: Coolant transfer factor $5600\,\mathrm{W\,m^{-2}\,K^{-1}}$ derived in Section 2.2.
κ: Bipolar plate thermal conductivity. Considerable variability in this value can be found for different plate construction. Varying values for through plane y and in-plane x–z are also reported. We take the single value $1.29\,\mathrm{W\,m^{-1}\,K^{-1}}$ [13] that corresponds to graphite 20–40 mesh as a base value for this study.
L: Single plate thickness (1 mm).
L_c: Cell length (1 m).
Q: Heat flux $7000\,\mathrm{W\,m^{-2}}$ as a base value. This roughly corresponds to a current density of $10{,}000\,\mathrm{A\,m^{-2}}$ (or $1\,\mathrm{A\,cm^{-2}}$) at about 50% overall efficiency.
T_Δ: Target coolant temperature increase from inlet to outlet for an average cell. We take $T_\Delta = 15\,\mathrm{K}$. This determines cQ_c as shown below.

The coolant temperature increases according to how much heat it absorbs locally:

$$cQ_c\frac{dT_j}{dx} = A(\beta_j - T_j), \tag{1}$$

where the RHS above describes the local heat flux in to the coolant, expressed by the flux from the edge of coolant channel to its average temperature. We now consider two heat flux balances, the first at the MEA and the second at the coolant:

$$Q_j = \frac{\kappa}{L}(\theta_j - \beta_j) + \frac{\kappa}{L}(\theta_j - \beta_{j-1}) \tag{2}$$

$$A(\beta_j - T_j) = \frac{\kappa}{L}(\theta_j - \beta_j) + \frac{\kappa}{L}(\theta_{j+1} - \beta_j) \tag{3}$$

Here, we have used simple expressions for one-dimensional steady heat conduction. The two terms on the right-hand side of (2) represent heat flux leaving the MEA up and down, respectively. In (3), the two terms on the right-hand side represent the heat flux flowing from cell j and cell $j+1$, respectively, into coolant channel j.

We have boundary conditions

$$T_j(0) = 0 \tag{4}$$

for each j (recall temperatures are all relative to the coolant inlet temperature common to all cells since the flow is from a common source distributed by a header). Eqs. (1)–(3) are a first-order DAE to be solved from inlet $x = 0$ with conditions (4) to outlet $x = L_c$. In the theoretical analysis that follows, we assume a stack with an infinite number of cells. In computations, we can consider a finite stack, periodic in j. These are conveniences in this paper where we are not explicitly considering stack end effects.

If we consider a uniform stack ($Q_j = Q$ for all j), then Eqs. (1)–(3) have a simple solution common to all cells j. By integrating (1) from inlet to outlet and specifying the target temperature increase, we obtain the value

$$cQ_c = \frac{L_c Q}{T_\Delta} \tag{5}$$

for the combination cQ_c, which can be considered to be the thermal carrying capacity of the coolant flow, per unit width. $T(x)$ is linear from 0 to T_Δ. At every x, the plate temperature by the coolant β is larger than the coolant by

$$\frac{Q}{A} \approx 1.25\,\mathrm{K}$$

and the MEA temperature θ is larger than this plate temperature by

$$\frac{LQ}{2\kappa} \approx 2.71\,\mathrm{K}$$

using the base parameters above. The main objective of this work is to determine how anomalously large heating in one cell in a stack of cells at base conditions will be distributed through the stack.

2.1. Heat removal

In this section, we show that the heat removal by thermal conduction through the graphite plates in-plane x–z is negligible as well as the heat removed by the reactant gas streams.

We consider the oxidant stream with pure air. At inlet, the molar flow rate of oxygen per unit z is

$$\mathcal{S}\frac{IL_c}{4\mathcal{F}},$$

where $\mathcal{S}$ is the *stoichiometric* flow rate (the dimensionless flow rate to the minimum to generate the desired current). We take $\mathcal{S} = 2$. I is the current density of the cell which we take to be $10{,}000\,\mathrm{A\,m^{-2}}$ and $\mathcal{F}$ is Faraday's constant ($96485\,\mathrm{C\,mol^{-1}}$). The heat removed by the gas stream at constant pressure is approximately

$$\frac{1}{X_o}\mathcal{S}\frac{IL_c}{4\mathcal{F}}c_N T_\Delta,$$

where $X_o \approx 0.2$ is the molar fraction of oxygen in air and c_N is the specific heat capacity of nitrogen $c_N = 29.1\,\mathrm{J\,mol^{-1}\,K^{-1}}$ [13]. The heat removed by the coolant per unit width is QL_c. The ratio of heat removal by the cathode gas stream to the coolant is then approximately

$$\frac{\mathcal{S}}{X_o}\frac{Ic_N T_\Delta}{Q4\mathcal{F}} \approx 0.016.$$

This is small enough to be neglected.

We now approximate the heat transferred per unit width by plate conduction, which can be found to be

$$\frac{2L\kappa}{L_c}T_\Delta.$$

The ratio of this heat transfer to that of the coolant is

$$\frac{2L\kappa}{QL_c^2}T_\Delta \approx 3.7\times 10^{-7}, \tag{6}$$

which can be neglected even if the in-plane conductivity of the plates is two orders of magnitude larger than through plane which has been reported [12]. This justifies the neglect of the in-plane thermal transport in the plates away from cell ends.

2.2. Averaging over cross-plane

The cross-plane (y–z) geometry is shown in Fig. 3. We discuss briefly here the reasoning that leads to the one-dimensional approximation of the cross-plane transport used in the model equations above. If the effect of the gas channel geometries are neglected and the temperatures at the MEA (θ) and the temperatures at the coolant channel edge and centre line of the bipolar plates (β) can be taken to be constant in z, we are led to formulas (2) and (3). These assumptions clearly are not rigorously valid and are made for the convenience of the simplified analysis to follow. The results we obtain are limited to *qualitative* accuracy only.

If we consider a net average thermal flux density Q coming from the MEAs above and below the coolant channel shown in Fig. 3, we see that the average thermal flux density into the coolant is

$$Q\frac{L_w}{\pi D},$$

where L_w is the MEA width associated with one channel (that is, the cell width divided by the number of channels). We assume the flux into the coolant is uniform around its circumference and that the coolant flow is laminar. Using standard conjugate heat transfer theory [14], we find

$$Q\frac{L_w}{\pi D} = N_u\frac{\kappa_o}{D}(\beta_j - T_j),$$

where N_u is a dimensionless number that depends on the coolant channel shape, 48/11 for the case of the circular channels considered here, L_w is the spacing between the channels which we take to be 1 mm and κ_o is the conductivity of the coolant taken to be $0.41\,\mathrm{W\,m^{-1}\,K^{-1}}$ [12]. This leads to the value

$$A = N_u\frac{\pi\kappa_o}{L_w} \approx 5600\,\mathrm{W\,m^{-2}\,K^{-1}}$$

used in the model above.

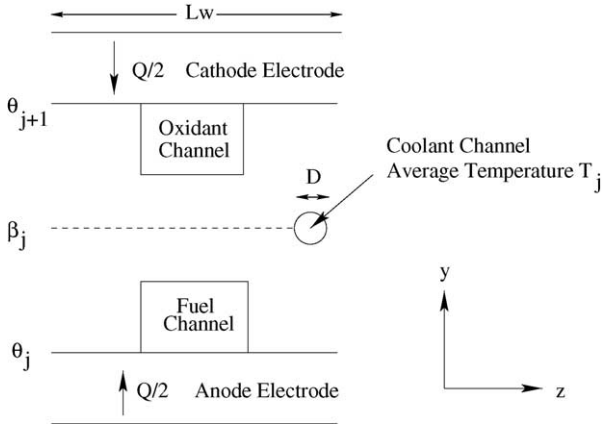

Fig. 3. Cross-plane (y–z) view of a unit cell. The channel structure repeats in the z-direction. Unit cells are stacked in the y-direction.

3. Nondimensionalization and formulations

We solve (2) for θ_j:

$$\theta_j = \frac{1}{2}\left(\beta_j + \beta_{j-1} + \frac{LQ_j}{\kappa}\right), \tag{7}$$

and use this result in (3) to obtain

$$\beta_{j+1} - \left(2 + \frac{2LA}{\kappa}\right)\beta_j + \beta_{j-1} + \frac{2LA}{\kappa}T_j = -\frac{L}{\kappa}(Q_j + Q_{j+1}). \tag{8}$$

This equation with (1) is used for the numerical computations described in Section 5. Values of the MEA temperatures θ^j are post-processed using (7).

We further combine (1) with (3) to eliminate the coolant temperatures T_j and obtain an equation for the plate temperatures β alone:

$$-\frac{cQ_c}{W}\{\dot\beta_{j+1} - 2(1+W)\dot\beta_j + \dot\beta_{j-1}\} = \frac{\kappa}{L}(\beta_{j+1} - 2\beta_j + \beta_{j-1}) + (Q_j + Q_{j+1}), \tag{9}$$

where the dot denotes differentiation with respect to x, and $W = LA/\kappa$, a dimensionless ratio of the temperature increase through the plates to that of the plates to the coolant.

We now scale the equations and variables. Dimensionless variables are denoted by hats.

Flux: We scale the fluxes to make them order unity:

$$Q_j = Q\hat Q_j,$$

where Q is the representative value of the previous section.

Temperature: The scaling of temperature is dictated by the thermal scaling above

$$\beta_j = \frac{QL}{\kappa}\hat{\beta}_j.$$

Length: The natural length scaling follows:

$$x = \frac{cQ_cL}{W\kappa}\hat{x},$$

where the length scale above can be further simplified to

$$\frac{L_cQ}{T_\Delta A}$$

with our parameters. In Section 4, an asymptotic theory for large $\hat{x}$ is presented. We have $\hat{x} \in [0, AT_\Delta/Q] \approx [0, 12]$ for the base parameters and numerical experiments show the asymptotics are valid at outlet. The asymptotic regime corresponds to large AT_Δ/Q which can be considered to be a scaled coolant channel thermal transfer coefficient.

In scaled variables, dropping the hats, (9) becomes

$$\{\dot{\beta}_{j+1} - 2(1+W)\dot{\beta}_j + \dot{\beta}_{j-1}\} + \beta_{j+1} - 2\beta_j + \beta_{j-1} = -(Q_j + Q_{j-1}). \tag{10}$$

This equation is considered analytically in the next section.

4. Analysis

Consider now (8) at $x = 0$, where $T_j(0) = 0$ for all j. Let b_j denote $\beta_j(0)$. We obtain under our scaling:

$$b_{j+1} - 2(1+W)b_j + b_{j-1} = -(Q_j + Q_{j+1}). \tag{11}$$

We take the Laplace transform of (10):

$$\begin{aligned}(s+1)\tilde{\beta}_{j+1} - 2(s+sW+1)\tilde{\beta}_j + (s+1)\tilde{\beta}_{j-1} &= b_{j+1} - 2(1+W)b_j + b_{j-1} - \frac{1}{s}(Q_j + Q_{j+1}) \\ &= -\frac{1}{s}(s+1)(Q_j + Q_{j+1}),\end{aligned} \tag{12}$$

where we have used tildes for the Laplace transform and where (11) was used. After dividing by $s+1$, we obtain:

$$\tilde{\beta}_{j+1} - 2\left(1 + \frac{sW}{s+1}\right)\tilde{\beta}_j + \tilde{\beta}_{j-1} = -\frac{1}{s}(Q_j + Q_{j+1}). \tag{13}$$

We now consider an anomalous cell ($j = 0$) in an infinite stack generating uniformly more heat than any other, so $Q_0 = 1$ but $Q_j = 0$ for all other j. Resulting temperatures are increases from base temperatures. Eq. (13) has a solution of the form:

$$\tilde{\beta}_j(s) = C(s)G^{|j+1/2|}.$$

This can be seen by inserting the form above into Eq. (13) for coolant channels not adjacent to the anomaly (j not equal to 0 or -1). For these cells, the right-hand side of (13) is zero and

$$C(s)G^{1/2}\left\{G^{j+1} - 2\left(1 + \frac{sW}{s+1}\right)G^j + G^{j-1}\right\} = 0$$

for $j > 0$ and a similar expression for $j < -1$. This relationship can be satisfied for all $j > 0$ (and the equivalent relationship for $j < -1$) if $G(s)$ solves

$$G^2 - 2\left(1 + \frac{Ws}{1+s}\right)G + 1 = 0 \tag{14}$$

with $|G| < 1$. Consider (13) at $j = 0$ (or equivalently at $j = -1$) to determine $C(s)$:

$$C(s)G^{-1/2}\left(G^2 - 2\left(1 + \frac{sW}{1+s}\right)G + G\right) = -\frac{1}{s}.$$

In the bracket above add and subtract 1, then use (14) to simplify the expression to

$$C(s)G^{-1/2}(G-1) = -\frac{1}{s},$$

or

$$C(s) = \frac{1}{s}\frac{1}{G^{-1/2} - G^{1/2}},$$

and so the following is an explicit form of the Laplace transform for the plate temperatures:

$$\tilde{\beta}_j(s) = \frac{1}{s}\frac{1}{G(s)^{-1/2} - G(s)^{1/2}}G(s)^{|j-1/2|}. \tag{15}$$

For fixed j, the expression (15) is analytic except on the negative real axis. It has branch points at $s = 0$ and $s = -1/(2+W)$ and has algebraic growth as $|s| \to \infty$. It satisfies the conditions of Watson's lemma [15] and the large x behaviour is determined by the small s asymptotics of the transform. We consider the form of G for s small in (14):

$$G^2 - 2(1+Ws)G + 1 \approx 0,$$

so

$$G \approx 1 + Ws - \sqrt{(1+Ws)^2 - 1} \approx 1 - \sqrt{2Ws}.$$

Now, (15) becomes

$$\tilde{\beta}_j \approx \frac{1}{s^{3/2}\sqrt{2W}}\,\mathrm{e}^{-|(j-1/2)|\sqrt{2Ws}}, \tag{16}$$

where the alternate form $G \approx \mathrm{e}^{-\sqrt{2Ws}}$ has been used in the approximation of $G^{|j-1/2|}$ in order to obtain (16). The ex-

pression above has a known inverse transform:

$$\beta_j \approx \frac{1}{\sqrt{2W}} \left\{ 2\sqrt{\frac{x}{\pi}}\, \mathrm{e}^{-(j-1/2)^2 W/2x} - |j-1/2|\sqrt{2W}\,\mathrm{erfc} \right.$$
$$\left. \times \left(|j-1/2| \sqrt{\frac{W}{2x}} \right) \right\}, \tag{17}$$

where erfc is the complementary error function. Since (16) is accurate to $O(\sqrt{s})$ the expression (17) has errors $O(1/\sqrt{x})$ for fixed j.

The expression (17) is analogous to the solution of the heat equation in a semi-infinite rod forced by a fixed heat flux in at the end (see [16], for example), where x plays the role of time and j of a discretized spatial variable. It is clear the physical models are also similar.

We note that in this setting with one anomalously heated cell, plate temperature increases grow like $\sqrt{x}$. In a uniformly heated stack, base temperatures increase linearly. The expression above shows that the anomalous heat spreads out to a characteristic number of adjacent cells J characterized by

$$J(x) \approx \sqrt{\frac{2x}{W}}.$$

If we consider the spread at the outlet of a cell of length L_c then we obtain, recalling the length scaling:

$$J \approx \sqrt{\frac{2\kappa T_\Delta}{QL}} \approx 2.4 \tag{18}$$

with our parameters. Note that this expression does not depend on A and increases with κ/L. These predictions are verified in the computations shown in the next section.

We remark that we could have used the expression

$$\tilde{\beta}_j \approx \frac{1}{s^{3/2}\sqrt{2W}} - \frac{|j-1/2|}{s}$$

instead of (16) leading to the expression

$$\beta_j \approx \sqrt{\frac{2x}{W\pi}} - |j-1/2|$$

which is asymptotically as accurate as (17). However, this form gives negative (unphysical) values for small x (out of the asymptotic range).

5. Computations

We consider a $2M$-cell periodic stack using M computational cells labelled 1 (anomaly) up to M using symmetry conditions. The computations are based on an implicit discretization of (1) and (8), considered as a linear system of $2M$ unknowns T_j and β_j at the next space step in x. MEA

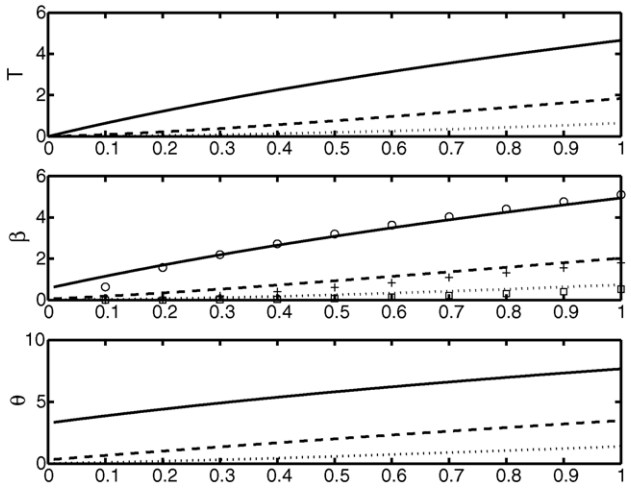

Fig. 4. Temperatures from an anomalously hot centre cell, base conditions. The solid line is the anomalous cell $j = 1$, dashed line is $j = 2$ and dotted line is $j = 3$. Symbols represent the asymptotic solutions.

temperatures θ_j can be reconstructed using (7). We use a grid of $N = 100$ in the channel length discretization.

As an example, we take a 17-cell stack ($M = 8$) and take $Q_0 = Q$ but all other $Q_j = 0$. This simulates a stack with a centre cell running very hot. On its own (isolated with one coolant channel), it would run T_Δ degrees hotter at outlet than normal. The temperatures computed from the study should be thought of as *increases* from normal temperature profiles. In Fig. 4, we show the results for the base parameters; in Fig. 5, the results if A is doubled from the base case (coolant thermal conductivity doubled); and in Fig. 6, the results if κ/L is doubled (plate conductivity doubled or thickness halved). Note that doubling A has little effect on the solution spread but doubling κ/L spreads out the heat from the anomalous cell to more neighbouring cells. This agrees with the approximate analytic predictions above.

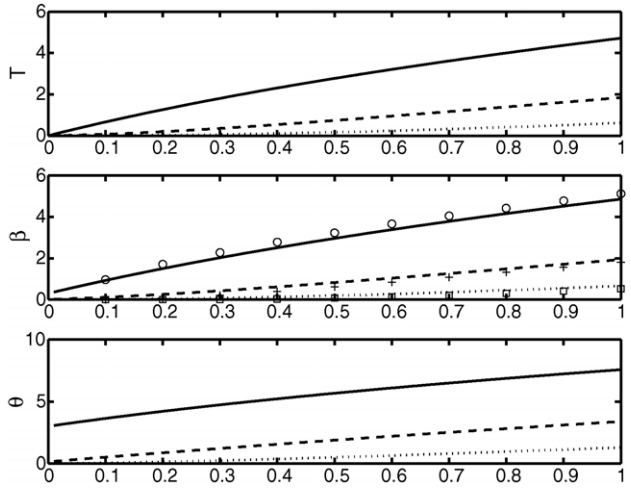

Fig. 5. Temperatures from an anomalously hot centre cell, doubled A. The solid line is the anomalous cell $j = 1$, dashed line is $j = 2$ and dotted line is $j = 3$. Symbols represent the asymptotic solutions.

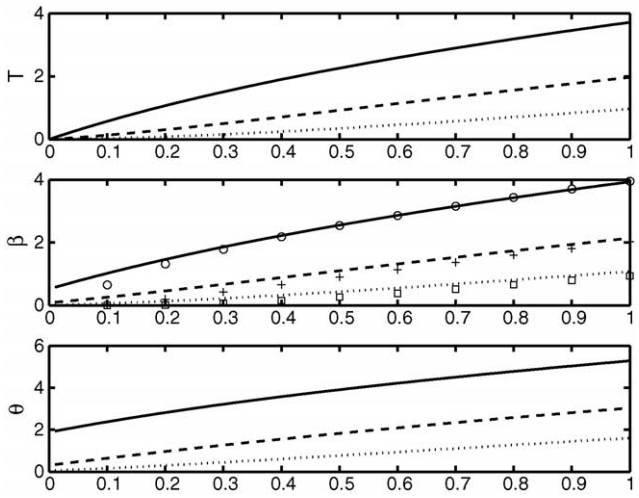

Fig. 6. Temperatures from an anomalously hot centre cell, doubled κ/L. The solid line is the anomalous cell $j = 1$, dashed line is $j = 2$ and dotted line is $j = 3$. Symbols represent the asymptotic solutions.

In Figs. 4–6, the approximate analytic solution for β is shown for the equivalent parameters. The agreement is very good for larger x values, where the analytic results are asymptotically valid.

6. Summary

We have developed models describing the temperature distribution in a fuel cell stack under several assumptions. Approximate analysis of the model leads to an analytic expression (18) for the characteristic number of cells anomalous heat is spread to.

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