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Computationally-efficient hybrid strategy for mechanistic modeling of fuel cell stacks

A.K. Sharma [a], E. Birgersson [a, *], S.H. Khor [b]

[a] Department of Chemical and Biomolecular Engineering, National University of Singapore, Singapore 117576, Singapore
[b] Department of Mechanical Engineering, National University of Singapore, Singapore 117575, Singapore

HIGHLIGHTS

- A hybrid strategy is proposed for mechanistic modeling of fuel cell stacks.
- The strategy is verified with the full set of equations for a 10-cell stack.
- The strategy preserves geometrical resolution and captures essential physics.
- In particular, captures redistribution of current and heat flux across the cells.
- 80% reductions in computational cost; allows for simulation of large stacks.

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ABSTRACT

In general, detailed mechanistic models for fuel cell stacks that seek to capture the local transport phenomena are computationally expensive. In this context, we propose a hybrid modeling strategy, in which the steady-state conservation equations are solved iteratively in two separate groups: The first comprises asymptotically-reduced governing equations for momentum, mass, and species, which are solved as a transient-like propagation problem; the second comprises the full set of equations for energy and charge, which are solved as an elliptic stationary problem. Physically, the segregation is justified by the nature of the dependent variables; in essence, the first group covers local variables on the cell level and the second involves global variables on the stack level. We demonstrate the methodology for a steady-state detailed mechanistic model of a proton exchange membrane fuel cell stack comprising 2 to 350 cells subjected to non-uniform operating conditions across the cells; e.g., a stack comprising 350 cells takes less than an hour to solve. The proposed methodology is generic and can also be employed for other systems where transport phenomena occur on different length scales and involve some form of slenderness.

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1. Introduction

Mathematical modeling and simulation have found widespread use in the research and development of fuel cells; however, the majority of detailed mechanistic models that provide geometrical resolution and resolve the essential physics have focused on the cell level so far [1–8]. At the stack level, only a few detailed mechanistic models can be found [9–18], which are limited to small stacks of up to around 5 to 10 cells. Modeling of larger stacks generally involves simplifications [19–37] with a loss in the level of detail and resolution of the salient features of the electrochemical and transport phenomena.

In essence, detailed mechanistic models typically consider conservation of mass, momentum, species, energy and charge in the form of a system of coupled nonlinear elliptic partial differential equations (PDEs) with the relevant boundary conditions and constitutive relations to ensure a well-posed problem. While these models can be solved reasonably fast and efficiently for a single cell, the associated computational cost for stacks quickly becomes prohibitive because of the large number of functional domains-separator plates (sp), gas flow fields (ff), coolant flow fields (cff), porous backings (pb), catalyst layer (cl), electrolyte (el) – in each and every cell in a stack (see Fig. 1). One strategy to deal with such large simulations is to deploy clusters of computers or other types of parallel computing environments to speed up calculations, yet these simulations still take on the order of hours or days for fuel cell stacks [1,7,12,25,28,38–40]. Another possible strategy to reduce the overall complexity and associated computational cost of a stack

* Corresponding author. Tel.: +65 6516 7132; fax: +65 6775 4710.
E-mail address: chebke@nus.edu.sg (E. Birgersson).

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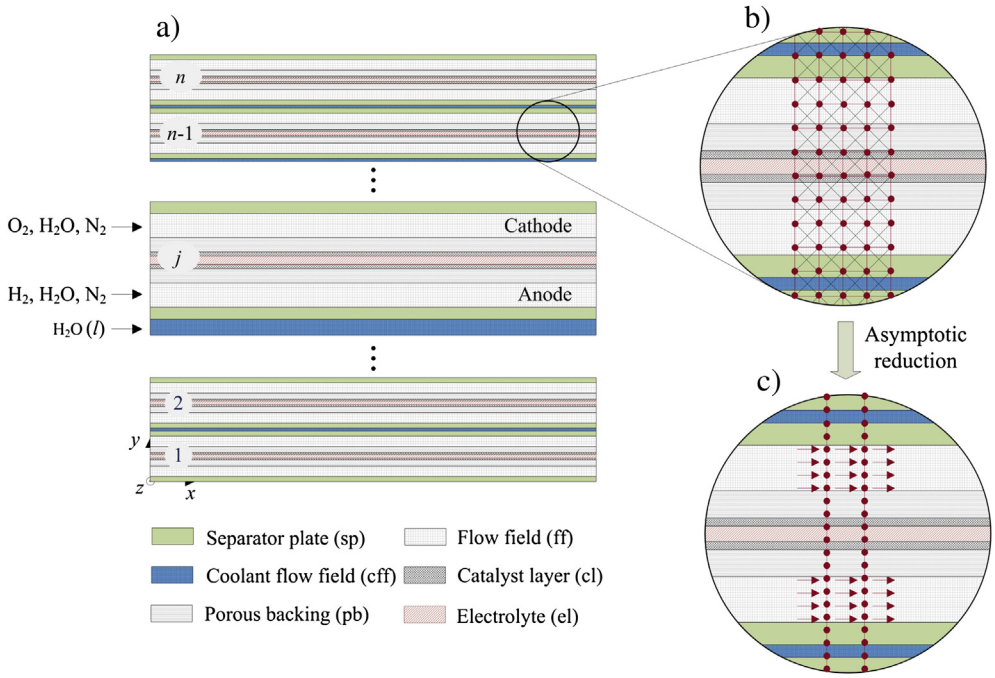

Fig. 1. Schematic for a PEMFC stack comprising n cells, denoted by j (a); mathematical nature of the governing equations for the full stack model (b) and reduced stack model (c): elliptic PDEs (⊠), parabolic PDEs (→) and ODEs (|).

model is to address the underlying mathematical nature of the system of equations. Care has to be taken though so as not to reduce the fidelity of model predictions especially when reductions sacrifice leading-order phenomena or dimensionality. This strategy was demonstrated in Refs. [41], where a leading-order reduced mathematical model for a proton exchange membrane fuel cell (PEMFC) stack was derived and shown to cut down the computational cost by 2–3 orders of magnitude (depending on stack size). The leading-order solution was, however, found to be unable to capture the redistribution of physical quantities for stacks subjected to significant perturbations between cells—a key phenomenon in fuel cell stacks [42–44].

In light of the promise the reduced model [41] holds in terms of computational efficiency even for large stacks of hundreds of cells or more, we shall here seek to overcome its main limitation by exploring a hybrid strategy that exploits the inherent nature of the dependent variables. In short, we shall argue that the dependent variables exist either locally in each cell or globally throughout the stack whence their PDEs can be split up into two separate groups. The local variables can now be solved at leading order with a space-marching algorithm whilst the global are allowed to retain their elliptic nature; iteration between the two groups then links them together into a complete stack model. We demonstrate the proposed strategy for the steady-state operation of a 10-cell PEMFC stack subject to non-uniform operating conditions for the individual cells.

The layout of the paper is as follows. First, we introduce the mathematical formulation for the full and proposed hybrid model for a PEMFC stack, which is then followed by a summary of the hybrid coupling methodology. After a description of numerics necessary to solve the models, the results of the hybrid model for both the global and local behavior are verified against those of the full model. The savings in computational cost in terms of memory usage and computing time are then discussed. Finally, we draw conclusions and highlight how the present approach can be adapted to other systems.

2. Mathematical formulation

Let us start by turning our attention towards a typical fuel cell stack as illustrated schematically in Fig. 1, which comprises several single cells connected in series; each cell further contains several functional layers. A detailed mechanistic model needs to consider coupled transport phenomena – mass, momentum, species, energy, and charge – in all of the relevant length scales that can be found in the stack. Since the cells in a stack are connected via impermeable graphite or metallic plates, transport of mass, momentum, and species is confined to individual cells; in contrast, the transport of energy and charge occurs across the cells and throughout the entire stack. Thus, the transport phenomena in the fuel cell stack, from the viewpoint of their scales of occurrence, can be classified into two categories:

- *Local to a cell:* conservation of mass, momentum and species. At this scale, the inherent slenderness in the functional layers of the cell and the relatively impermeable nature of all layers except for the flow field can be exploited to reduce the elliptic PDEs to parabolic counterparts and even ordinary differential equations (ODEs) with significant savings in computational cost [41,45–48].
- *Global to the stack:* conservation of energy and charge. At this scale, we retain the elliptic nature of the PDEs since there is no slenderness that can be exploited at leading-order. (*N.B.*: It should be possible to still reduce the equations, but we shall not pursue that here; see the Conclusions section for a short discussion.)

This in turn suggests that a hybrid modeling strategy based on these two groups should be feasible and allow for significant reduction in computational cost without sacrificing the fidelity of model predictions for the stack. We shall justify the strategy a *posteriori* by comparing the model predictions from the hybrid strategy with solutions from the full non-reduced set of equations.

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