Dynamic Multi-Fidelity Modelling of Low Temperature Proton Exchange Membrane Fuel Cell Power Systems for Clean Aviation

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I. Introduction

Immediate action is required if we are to limit anthropogenic warming to 2 °C by the year 2100 [1]. As of 2021, aviation contributed an estimated 4% of total warming, but projected growth in demand is expected to increase this to between 6 and 17% by 2050 [2]. Despite consistent incremental improvements in conventional aeroengine technology, there remain challenges with respect to the emission of carbon dioxide, nitrogen oxides, water, hydrocarbons, carbon monoxide, sulphur oxides, particulates, and other pollutants when relying on the combustion of hydrocarbon fuels. Consequently, there is interest in developing and adopting alternative energy vectors and power systems to facilitate transition away from fossil fuels towards clean aviation. Hydrogen fuel cells (FCs) offer a potential route to clean aviation at scale. Fuel cell systems generate electrical energy from hydrogen and oxygen emitting only water as a by-product, thus enabling electric aviation and zero emissions at the point of use. Low temperature proton exchange membrane (LT-PEM) fuel cells are a mature branch of current hydrogen fuel cell technology. They have been the focus of significant development since the early 2000s for automotive and civil applications due to their reliability and preferable dynamic characteristics relative to temperature (HT)-PEMFCs, and solid oxide fuel cells (SOFCs).

There is currently a global effort to scale LT-PEMFC systems to meet the power requirements of large transport aircraft [3–6]. This follows from a period in which academic institutions [7], industrial bodies [8], and governmental organisations [9] worked to demonstrate fuel cell powered Unmanned Aerial Vehicles (UAVs) and General Aviation (GA) aircraft. Despite the considerable knowledge gained from the application of LT-PEMFCs to small aircraft, and the existing wealth of experience in the automotive and civil sectors, there are design, operation, and integration challenges unique to large aircraft that must be addressed before wider adoption becomes possible. For example, LT-PEMFC systems are complex and dynamical. Their multi-scale nature means that small-scale multi-physics effects can govern top level system performance. LT-PEMFC systems for large aircraft will be subject to extreme safety constraints and conflicting design objectives of minimal mass and maximal power and efficiency are expected to force high current density operation under take-off conditions and simultaneously reduce the ability of the thermal management and water management systems to mitigate against flooding, drying, and steep transient temperature gradients which threaten the ability of the cell to provide the required power at take-off. Careful study of these effects in proposed systems are necessary to ensure safe, efficient, and reliable operation, but is not present in existing preliminary design studies of LT-PEMFC aircraft. As such there are number of open questions that must be addressed to facilitate future design and certification of future LT-PEMFC aircraft.

1) Which, if any, dynamic effects threaten the safe operation of future LT-PEMFC power systems under take-off conditions.
2) How should LT-PEMFC stack and balance of plant systems be designed and scaled to efficiently provide the required power.
3) How do top level integration and architectural decisions impact the optimal LT-PEMFC power system design and vice versa.

To address these questions the authors are currently developing models and methods to efficiently leverage multi-scale and multi-physics effects on the dynamic performance of LT-PEMFC power systems. The following sections will aim to

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outline the relevant background to, and proposed methodology of, these models and methods. Section II will provide a background for fuel cell stack design and operation, providing detail on the physical effects limiting LT-PEMFC performance at high current densities. Then, section III will introduce the proposed cell models, surrogate modelling approach, and existing dynamic system modelling framework.

II. Background

This section aims to outline the design of design LT-PEM cellss and stack, discuss mechanisms governing performance limiting water and thermal effects, and outline approaches previously used in the preliminary design of LT-PEMFC aircraft. The objective is to make clear the impact of capturing physical processes relevant at high current density operation of the fuel cell power system at take-off.

A. Cell

Hydrogen fuel cells utilise a reaction between oxygen and hydrogen. At the cathode, gaseous oxygen is reduced to water, and at the anode gaseous hydrogen is oxidised to form H+ ions as per the half reactions given in equations 1 and 2. An ionomer membrane facilitates the transport of protons between cathode and anode via an acidic electrolyte.

$$2H_2 \rightarrow 4H^+ + 4e^- \tag{1}$$

$$O_2 + 4e^- \rightarrow 2H_2O \tag{2}$$

To allow gaseous fuel to reach reaction sites, the electrodes are porous. The pores are infused with catalyst nanoparticles, typically platinum, often supported on carbon particles, and dispersed throughout the ionomer matrix. This structure increases the surface area available for reactions to occur, and facilitates the interaction of gaseous fuel, solid catalyst, and dissolved ion, known as three phase contact.

B. Stack

LT-PEM cells are connected in series to increase operating voltage and power. This is achieved using bipolar plate to "sandwich" cell assemblies. Bipolar plates serve a number of functions:

- Conducting current from anode to cathode between cells.
- Evenly distributing reactant gasses across the cell.
- Removing heat via gas supply and internal cooling channels.
- Transferring and resisting mechanical loads.
- Providing structural support to the flexible cell assembly.

The design of the bipolar plate determines the performance of a wide range of systems. Larger gas channels aid feed flow convection and limit pressure losses, easing performance requirements on fluid supply systems, whilst simultaneously reducing the area available to conduct charge and thickening the plate which increases Ohmic losses, cell mass, and rigidity. Small gas channels provide the inverse benefits and limitations. For any proposed bipolar plate design solution there is therefore a multi-objective trade off between gas supply, structural, mass, water, thermal, and electrical objectives. For these reasons, bipolar plate design is a common area of study in fuel cell design optimisation, and a range of strategies have been applied to investigate their design.

C. Water & Thermal Effects

In a LTPEMFC, there exists opposing needs to hydrate the membrane and avoid flooding pores, which may be controlled by varying the humidification of the reactant flows. Under high humidification, water may condense and flood pores in the electrodes, even at low current densities. This is exacerbated at the cathode, where the Oxygen Reduction Reaction

Table 1 A listing of the key features from the discussed preliminary LT-PEMFC aircraft design studies.

Author(s)	Massaro *et al.*	Nicolay *et al.*	Datta	Kasim *et al.*	Schmelcher
Dimension	Quasi-One	Quasi-One	Zero	Zero	Zero
TMS	Yes	No	Yes	No	Yes
WMS	No	No	No	Yes	No
Isothermal	Yes	Yes			
Dynamic	No	No	No	No	No
Aircraft Class	Regional	General	General	Commuter	Many

(ORR) forms water. The resulting impedance of oxygen transport to the cathode causes in a reduction of the cell voltage due to low local oxygen availability.

Under low humidification there is the potential for membrane drying, which prevents the transport of protons across the membrane, and limits reaction rates at the electrodes. High temperatures in the electrode result in an increased reactant gas saturation pressure, driving greater evaporation and increasing the mass of water removed. This can mitigate against flooding or accelerate drying depending on the operating conditions of the cell. High temperature gradients in the cathode and the adjacent GDL can induce flooding as the saturation pressure of the reactant decreases as the gas cools. In this case simultaneous flooding and drying is possible, as water is removed from the membrane and deposited elsewhere.

These transient effects may significantly impact cell power output when operating at high current densities. They are hyper-relevant in the design of PEMFC systems for aircraft as they threaten the ability to provide sufficient power at take-off where the highest power demand is traditionally imposed, and the lowest temperature difference is available to the Thermal Management System (TMS) for heat rejection. The ability of the TMS and Water Management Systems (WMS) to enable predictable high current density operation will be key to safe and reliable operation of LT-PEMFC aircraft. Challenges arise when considering traditional aircraft design objectives such as lightweighting and fuel consumption, which will incentivise smaller stacks, smaller TMS and WMS, and higher current densities.

D. Aircraft Design

Preliminary design studies of LT-PEMFC aircraft have been presented in literature. Massaro *et al.* [10] and Nicolay *et al.* [11] present studies of regional and general aviation aircraft respectively . Their works use a semi-empirical, quasi-one-dimensional, steady-state, isothermal model presented by Kulikovsky [12, 13]. Datta [14] and Kasim *et al.* . [15] present studies on eVTOL and commuter aircraft respectively, whilst Schemer et al. [] considers GA, commuter, regional, and short to medium range aircraft [16]. All use semi-empirical, zero-dimensional, steady-state, isothermal models. The models these studies rely on calibration against representative data to capture multi-scale effects. In the cases of Massaro, Nicolay, Datta, and [check others], calibration is conducted against experiments on 25cm^2 Membrane Electrode Assemblies (MEAs) with ideal stoichiometry and fuel excesses, while the studies consider designs with active areas of $O(1000)$ cm^2. This prepresents ideal fuel cell operating conditions, suggesting that the calibrated models may overestimate system performance.

III. Methodology

To address the identified gaps and support the goal of designing efficient, reliable, and safe LT-PEMFC systems for aircraft, the authors are developing:

1) Dynamic multi-scale and multi-physics LT-PEM cell models.
2) Parametric stack, TMS, WMS, fuel supply, and air supply models.
3) Advanced physics-aware machine learning LT-PEMFC stack surrogates.
4) A computational framework for dynamic fuel cell system modelling.
5) Advanced computational methods to efficiently explore optimal system design.

Together these actions aim to help the community understand the impact of LT-PEMFC power system transients at take-off, and begin tackling challenges surrounding the integration of these systems on board future large transport aircraft.

A. Cell Modelling

The physical processes necessary for the operation of LT-PEMFCs occur across a wide range of length scales. The catalysed ORR at a three-phase boundary and transport of water across the ionomer are governed by molecular level physics. Simultaneously the convective transport of reactants occurs first over the cell width, and second, through pores of diameter smaller than the mean free path of the gas molecules. These multi-scale mass, momentum, species, charge, and energy transfers are tightly coupled, resolving them fully is infeasible with current computational capability.

$$\frac{\partial(\epsilon C_k)}{\partial t} + \nabla(\vec{u} + C_k) = \nabla(D_k^{\mathrm{eff}} \nabla C_k) + S_k \qquad \frac{\partial(\rho c_p)_m T}{\partial t} + \nabla(\rho c_p \vec{u} T) = \nabla(k_{\mathrm{eff}} \nabla T) + S_T \tag{3a, 3b}$$

$$\frac{1}{\frac{\partial(\epsilon\rho\vec{u})}{\partial t} + \frac{1}{\nabla(\rho\vec{u}\vec{u})}} = -\nabla p + \nabla\tau + S_u \qquad \frac{\partial(\epsilon\rho)}{\partial t} + \nabla(\rho\vec{u}) = S_m \tag{4a, 4b}$$

$$\nabla(\kappa^{\mathrm{eff}} \nabla \Phi_e) = -S_\Phi \qquad \nabla(\sigma^{\mathrm{eff}} \nabla \Phi_s) = S_\Phi \tag{5a, 5b}$$

Table 2 Source terms for the single-phase fuel cell model presented by [wang]

	Gas Diffusion Layer	Catalyst Layer	Membrane
Mass (4b)		$S_m = \sum_k M_k S_k + M_{\mathrm{H_2O}} \nabla(D_{w,m} \nabla C_{\mathrm{H_2O}})$	
Momentum (4a)	$S_u = -\vec{u}(\frac{\mu}{K})$	$S_u = -\vec{u}(\frac{\mu}{K})$	$\vec{u} = 0$
Species (3a)		$S_k = -\nabla\left(\frac{n_d}{F} i_e\right) - \left(\frac{s_k j}{nF}\right)$	$-\nabla\left(\frac{n_d}{F} i_e\right)$
Charge (5a, 5b)		$S_\Phi = j$	
Energy (3b)		$S_T = j\left(\eta + T\frac{dU_0}{dT}\right) + \frac{i_e^2}{\kappa^{\mathrm{eff}}}$	$S_T = \frac{i_e^2}{\kappa^{\mathrm{eff}}}$

Commonly, when investigating cell and stack polarisation, assumptions of continuity allow diffusive processes to be modelled without resolving pore scale effects. This allows for the derivation of Partial Differential Equations (PDEs) commonly solved via finite element methods and finite volume methods. Often, a single set of equations is applied over the full domain of a cell, with the response of different subdomains governed by their source terms. One such set of PDEs, presented by [wang], is given in table 2. A wide range of PDEs of differing fidelities are presented throughout literature, trading computational cost against physics complexity.

Open-source fuel cell models are of interest in this work as they provide an efficient approach to incorporating multiple model fidelities. A non-exhaustive list of open-source models are presented in table [].

Table 3 Do This

Authors	Vetter & Schumacher	Secanell *et al.*	Zhang *et al.*	Kone *et al.*	Gass *et al.*
Dimension	One	Up to three	Three	Three	One
Isothermal					
Water Phase	Multi	Multi	Multi	Single	Multi

B. Surrogate Modelling

[Autoregressive Multi-fidelity GPs]

[Active learning, and Bayesian Optimisation]

[Non-myopic Bayesian optimisation]

[Proposed Fuel Cell Stack Surrogate]

C. Dynamic Fuel Cell System Model

A computational framework for dynamic fuel cell system modelling has been developed by the authors to allow modular development and simple composition of fuel cell system component models. This has been accompanied by implementation of the following sub-models from the work of Pukrushpan et al [17].

- Electric Motor
- Compressor
- Manifold
- Humidifer
- Cathode
- Anode
- Membrane Hydration
- Stack Voltage

The resulting LT-PEMFC power system model has been validated against the work of Pukrushpan et al, as demonstrated in Figures **??** and **??**.

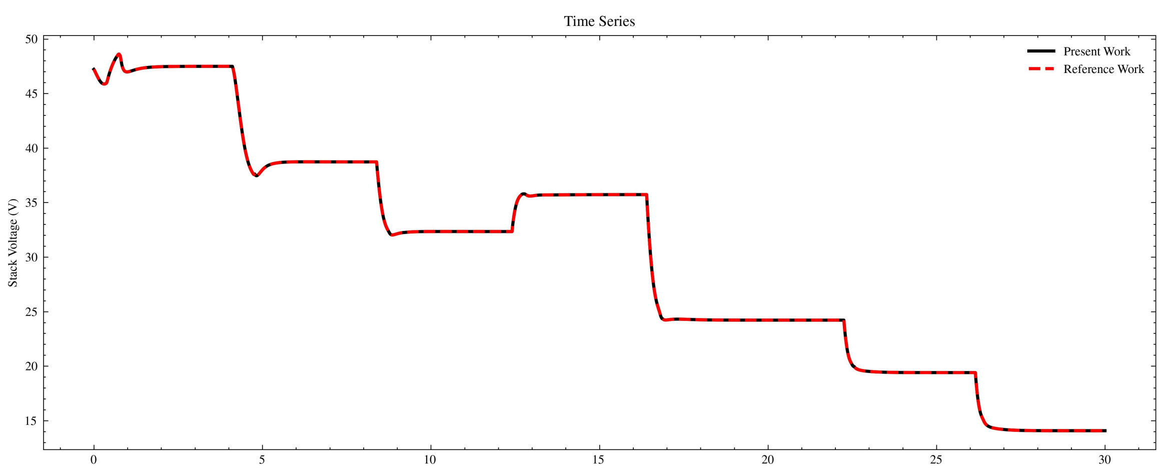

Fig. 1 Some caption

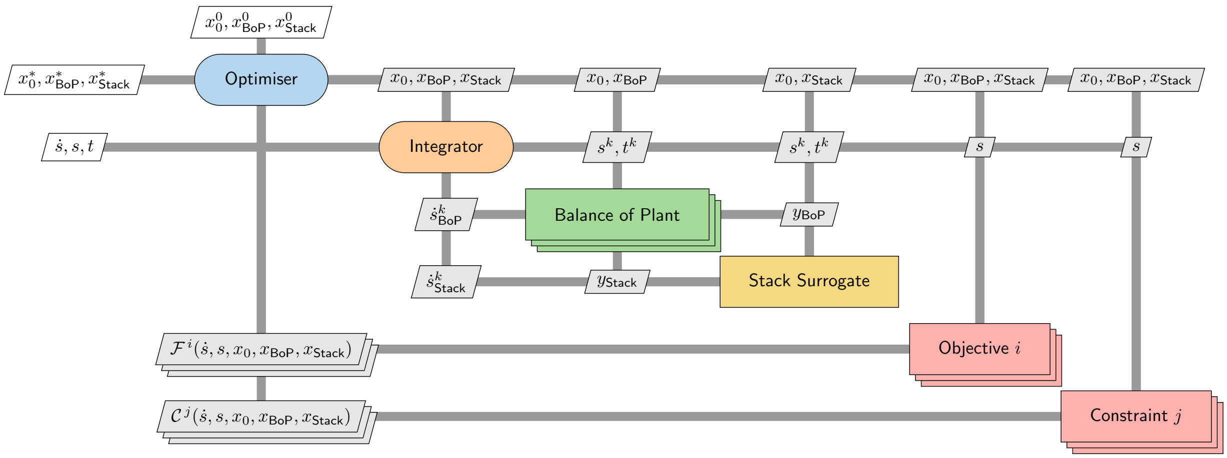

Fig. 3 XDSM Diagram of the proposed fuel cell system model

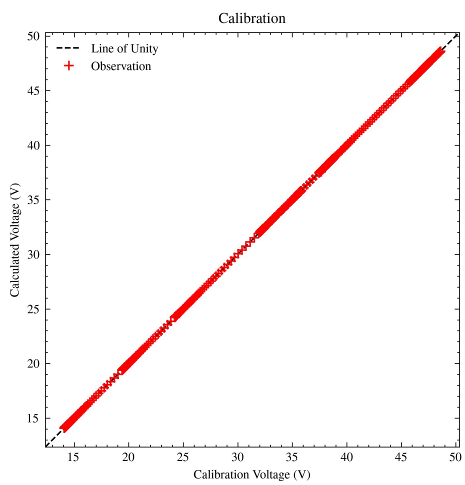

Fig. 2 Some caption

Future work is planned to implement sub-models for future LT-PEMFC aircraft systems. This will include water management, thermal management, air supply, and fuel supply systems. The response of a given stack design evaluated using the stack surrogate model described in section []. The system dynamic response is evaluated using an implicit adaptive Runge-Kutta integrator. An XDSM diagram of the proposed study is presented in figure 3.

D. Design Optimisation

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