



Three-dimensional computational fluid dynamics modelling and experimental validation of the Jülich Mark-F solid oxide fuel cell stack



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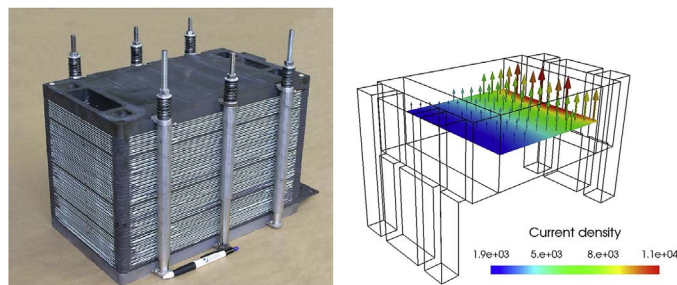
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HIGHLIGHTS

- Present solid oxide fuel cell stack model with coupled transport and electrochemistry.
- Demonstrate agreement between model and experimental 18-cell Jülich Mark-F stack.
- Predict stack performance in conditions of in-field power generation vs test furnace.

GRAPHICAL ABSTRACT



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ABSTRACT

This work is among the first where the results of an extensive experimental research programme are compared to performance calculations of a comprehensive computational fluid dynamics model for a solid oxide fuel cell stack. The model, which combines electrochemical reactions with momentum, heat, and mass transport, is used to obtain results for an established industrial-scale fuel cell stack design with complex manifolds. To validate the model, comparisons with experimentally gathered voltage and temperature data are made for the Jülich Mark-F, 18-cell stack operating in a test furnace. Good agreement is obtained between the model and experiment results for cell voltages and temperature distributions, confirming the validity of the computational methodology for stack design. The transient effects during ramp up of current in the experiment may explain a lower average voltage than model predictions for the power curve.

1. Introduction

The performance of solid oxide fuel cell (SOFC) stacks has improved substantially in recent years due to developments in materials and stack design through experimental analysis and modelling. For stationary applications, the design of large, powerful and durable stacks is desirable. However, in large stacks, operating concerns such as the uniform distribution of reactant species between cells and the efficient removal

of excess heat and reaction products become more apparent.

Experimental advances are limited, particularly at the stack scale due to the required time and expense of investigating a range of designs and operating conditions, and monitoring localised effects. Therefore it is necessary to employ models with proper experimental validation to address the unique design considerations at that scale and contribute to the development of fuel cells [1–3].

Solid oxide fuel models with little or no experimental validation can

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Nomenclature

A	area, m ²
c_p	specific heat, J kg ⁻¹ K ⁻¹
D	diffusion coefficient, m ² s ⁻¹
D_h	hydraulic diameter, m
E	Nernst potential, V
E_T	Reference potential, V
F	distributed resistance, kg m ⁻³ s ⁻¹
\mathcal{F}	Faraday's constant, C mol ⁻¹
f	friction factor
h	heat transfer coefficient, W m ⁻² K ⁻¹
H_e	thickness of electrolyte, m
ΔH_f	enthalpy of formation, J mol ⁻¹
i	current, A
k	thermal conductivity, W m ⁻¹ K ⁻¹
M	molecular weight, kg mol ⁻¹
m	mass, kg
p	pressure, Pa
q	heat source, W
R	gas constant, JK ⁻¹ mol ⁻¹
T	temperature, K
U	overall heat transfer coefficient, W m ⁻² K ⁻¹
u	velocity, m s ⁻¹
V	voltage, V
x	mole fraction
y	mass fraction

Non-dimensional numbers

Re	Reynolds number
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Greek letters

α	transfer coefficient, heat transfer coefficient, W m ⁻³ K ⁻¹
ε	volume fraction, emittance
μ	dynamic viscosity, kg m ⁻¹ s ⁻¹
ν	charge number
ρ	gaseous mixture density, kg m ⁻³
σ	Stefan-Boltzmann constant, Wm ⁻² K

Subscripts

i	domain phase general index
j	region index
n	neighbouring region index
w	wall
∞	free stream value

Superscripts

\cdot	per unit time
$''$	per unit area
$'''$	per unit volume

Abbreviations

ASR	area specific resistance
CFD	computational fluid dynamics
MEA	membrane electrode assembly
SOFC	solid oxide fuel cell

serve to misrepresent the characteristics of real operation. At the cell scale, some computational fluid dynamics (CFD) models including heat/mass transfer and electrochemical calculations have been compared with experimental results for simple configurations [1,4–8]. For fuel cell stacks, hydrodynamic models, with no heat transfer or electrochemistry, are commonly used to study the flow distribution with a variety of methods [9–16], some with experimental validation [17–23], often using particle image velocimetry. However, purely hydrodynamic models neglect the effects of the reaction on species and temperature distributions, and therefore transport and other properties due to composition and temperature changes. Results from hydrodynamic models can significantly misrepresent flow distributions in realistic operating conditions and it could be misleading to attempt to design or optimise manifold configurations based on such models [24]. Researchers have developed models capable of investigating the effects of flow paths on temperature and reaction distributions at the stack scale [2,16,24–33], each with key assumptions, but few with direct experimental validation. Others have studied the thermomechanical response of operating SOFC stacks [33–35] as well as the effects of furnace vs. insulated surroundings [36]. While the work focuses mainly on thermal stress analysis, it shows promise for advanced SOFC stack models with complex multiphysics.

In this work, the results of calculations for the voltage and temperature distributions for a three-dimensional computational fluid dynamics model are compared with results from an experimental programme with data for an 18-cell stack. In the model, solutions to the equations of conservation of mass, momentum, energy, and species transport coupled with electrochemical reactions, are obtained for the Jülich Mark-F geometry, corresponding to the experimental setup in a test furnace. This work is among the first to consider a comparison of physical experiments with a comprehensive solid oxide fuel cell stack model. Following a description of the model and experimental set-up, a comparison of voltage and temperature results are presented and

discussed.

2. Method*2.1. Model description*

Flow geometry and thermo-fluid interactions impact the electrochemical performance of solid oxide fuel cells. In this work, the governing equations of mass, momentum, species and heat transport are coupled with electrochemistry and solved using the open-source CFD platform, OpenFOAM [37]. To address limitations in computer memory and speed, a methodology is employed in which the diffusion terms in certain regions of the stack are replaced with inter-phase transfer (rate) terms. Nishida et al. [24] compare the present method with results from a previously verified cell-level model [38].

2.1.1. Governing equations

The basic methodology, and governing equations were discussed in detail in Refs. [24,26] and will therefore be dealt with only briefly, here. Four distinct computational domains are used to represent each of the four individual air, fuel, interconnect (defined here to include all metallic zones such as frames and baseplates), and membrane-electrode assembly (MEA) ‘phases’, which are to be considered as volume-averaged equations. In the fluid domains, the mass, momentum, species, and energy equations are applied in three dimensions as follows

$$\nabla \cdot (\varepsilon \rho \vec{u}) = \varepsilon \dot{m}''' \quad (1)$$

$$\nabla \cdot (\varepsilon \rho \vec{u} \vec{u}) = -\varepsilon \nabla p - \varepsilon F \vec{u} + \nabla \cdot (\varepsilon \mu \nabla \vec{u}) \quad (2)$$

$$\nabla \cdot (\varepsilon \rho \vec{u} y_i) = \nabla \cdot (\varepsilon \rho D \nabla y_i) + \varepsilon \dot{m}'''_i \quad (3)$$

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