Zhongjie He · Hua Li
Karl Erik Birgersson

Reduced Modelling of Planar Fuel Cells

Spatial Smoothing and Asymptotic Reduction

Springer

Reduced Modelling of Planar Fuel Cells

Zhongjie He · Hua Li · Karl Erik Birgersson

Reduced Modelling of Planar Fuel Cells

Spatial Smoothing and Asymptotic Reduction

Springer

Zhongjie He
Energy Research Institute at NTU
Nanyang Technological University
Singapore
Singapore

Hua Li
School of Mechanical and Aerospace Engineering
Nanyang Technological University
Singapore
Singapore

Karl Erik Birgersson
Department of Chemical and Biomolecular Engineering
National University of Singapore
Singapore
Singapore

ISBN 978-3-319-42645-7 ISBN 978-3-319-42646-4 (eBook)
DOI 10.1007/978-3-319-42646-4

Library of Congress Control Number: 2016956628

Printed on acid-free paper

This Springer imprint is published by Springer Nature
The registered company is Springer International Publishing AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

Dedicated to my parents and my wife, Mrs Qianpian Zhang, for their constant support

Zhongjie He

Dedicated first and foremost to my motherland, and to Duer, Anne and my parents

Hua Li

Dedicated to my family.

Karl Erik Birgersson

Foreword

It is my great pleasure to write the foreword to this monograph. Since the authors informed me that they planned to write a book about reduced modelling methods for planar fuel cells, I have looked forward to its completion with great anticipation. This summarizes their extraordinary contributions in the area of fuel cell modelling. I believe this book will be of great value to both experts and those with a casual interest in fuel cell modelling, model reduction, sensitivity analysis, and fuel cell design within academia and industry. The three authors are among the most outstanding scientists in the world in the area of fuel cell modelling.

Fuel cell is an electrochemical energy conversion device for environmentally friendly and sustainable energy production. The principle of the fuel cell was convincingly demonstrated by Sir William Robert Grove in 1839. Nowadays, the applications of fuel cells have spread into four major areas: small/big power stations, residential electricity, transport facilities, and portable electric products. The majority of the related studies in fuel cell modelling are dedicated to introducing or developing a full set of equations to describe the multiphysics in the fuel cell. However, three-dimensional (3D) modelling of fuel cells requires massive computational resources, especially for stacks, considering the highly coupled and nonlinear nature of the mathematical formulation as well as a large number of functional domains in the cell. This monograph focuses on development of reduced models for the fuel cells and stacks fabricated with a plate-type structure (namely planar fuel cells), primarily with the methods of spatial smoothing and asymptotic reduction. It provides a systematic and comprehensive study covering validation of full 3D models with experimental data, analysis of model reduction for single cells and stacks, numerical implementation of the mathematical formulation, verification of the reduced models, as well as sensitivity analysis. The research work is illustrated with the proton exchange membrane fuel cell and the planar solid oxide fuel cell, which are two typical kinds of the planar fuel cell. The reduced models can be solved without sacrificing leading-order physics in solutions while the computational demand is reduced by more than two orders of magnitude. Based on the fast and efficient reduced models, integrated stochastic and deterministic sensitivity

analysis is conducted to investigate both individual and simultaneous effects of design factors on the cell and stack performance. This provides important information for fuel cell design.

This book is written in a straightforward manner without losing depth, so that it makes informative reading for a researcher or graduate student who is working or intends to work in this field. It will without doubt serve as a rich reference source for experts in this area. I congratulate Dr. Zhongjie He, Prof. Hua Li, and Prof. Karl Erik Birgersson for their tremendous achievement. I also hope and expect that the readers will benefit greatly from this book.

Bengt Sundén
Professor & Head of Division
Energy Sciences, Lund University

Preface

Fuel cell is an electrochemical energy conversion device for environmentally friendly and sustainable energy production, and fuelled by hydrogen or hydrocarbon operating at a specific temperature ranging from 50 to 1,000 °C depending on the cell type. It is generally fabricated into a plate-type structure where the flow field consists of parallel plain flow channels separated by solid ribs, such as proton exchange membrane fuel cell (PEMFC) and planar solid oxide fuel cell (P-SOFC). The cell performance typically involves complicated multiphysical behaviours, such as transport phenomena and electrochemical performance. To understand the characteristics and mechanism of the fuel cell, mathematical modelling is an efficient approach, compared with repetitive and costly experimental techniques.

To date, about 12 books have been published in the literature on fuel cell modelling. The authors primarily reviewed the fundamental principles of fuel cells, and/or introduced the existing approaches for fuel cell modelling based on a full set of conservation equations. In general, however, detailed three-dimensional (3D) modelling of fuel cells is computationally expensive, especially for stacks, due to the highly coupled and nonlinear nature of the mathematical formulation as well as a large number of functional domains in the cell. Although some books have been published in the literature to develop mathematical models for fuel cells, none of them focused on reducing the 3D full models to efficient and accurate counterparts. There are simplified fuel cell models from 3D to 2D, but the assumptions on dimensionality tend to lower the fidelity of model prediction.

This is the first monograph of its kind, which is dedicated to developing reduced models of planar fuel cells and stacks. The present model reduction is primarily based on the method of spatial smoothing and asymptotic reduction, such that the fuel cell models can be solved fast and efficiently without sacrificing leading-order physics in numerical solutions. In particular, when reducing a 3D fuel cell model to a spatially smoothed counterpart, correlation and variation factors are developed to account for the effects of solid ribs on the pathways of heat, mass and charge transports. Reduced PEMFC and P-SOFC models are developed and verified with their 3D counterparts that were developed and validated with some experimental data reported in the literature. As a result, both the average and variability

of dependent variables along the cell width in the 3D geometry are captured by a quasi-3D reduced model solved with respect to the directions along the flow and through the cell thickness. The computational cost for cell and stack modelling is reduced by two orders of magnitude or more with desired numerical accuracy. Moreover, based on the efficient reduced models, integrated stochastic and deterministic sensitivity analysis is carried out to investigate not only individual but also simultaneous effects of a group of design factors (including geometrical, material, and operational parameters) on the cell and stack performance, which provides important information for fuel cell design. For such sensitivity analysis, Monte Carlo simulation of the reduced model is conducted with a sample size in the order of 10^3 at both single-cell and stack levels without prohibitive computation requirement, which is illustrated with the P-SOFC. In addition, apart from the PEMFC and P-SOFC, the present work can be extended to other kinds of plate-type fuel cells.

This book can primarily meet the needs of scientists and R&D engineers in the broad fields of fuel cell modelling and design, especially the PEMFC and P-SOFC. It is not only useful for them as a research reference but also allow further studies to extend the present work to suit their practical applications. The primary readers also include postgraduates doing research in the area of fuel cells, in particular, whose work involves numerical simulation, model reduction, scaling and asymptotic analysis, as well as sensitivity analysis. Possible secondary readers are the third- and fouth-year undergraduate students taking courses of advanced mechanical and electrochemical engineering. As a good reference source for course lectures, the book sections introducing the fundamental of fuel cell modelling are especially helpful for the students to learn more about fluid dynamics, electrochemistry, and transport phenomena pertaining to mass, momentum, and heat transfer. In addition, apart from fuel cells, the present approach of model reduction can also be extended to other energy systems where multiphysical phenomena are studied.

The authors would like to thank Prof. Bengt Sundén for writing the foreword to this book. Special thanks also go to Drs. M. Vynnycky, H. Ly, A.K. Sharma, and S.H. Khor for their invaluable contributions to this research.

Singapore

Zhongjie He
Hua Li
Karl Erik Birgersson

Acknowledgment

The authors would like to sincerely acknowledge the use of figures reproduced from the following sources:

Zhongjie He, Hua Li, Birgersson E (2016) Correlating variability of modeling parameters with cell performance: Monte Carlo simulation of a quasi-3D planar solid oxide fuel cell. Renew Energy 85:1301–1315.
Zhongjie He, Hua Li, Birgersson E (2014) Correlating variability of modeling parameters with non-isothermal stack performance: Monte Carlo simulation of a portable 3D planar solid oxide fuel cell stack. Appl Energy 136:560–575.
Zhongjie He, Birgersson E, Hua Li (2014) Spatially smoothed fuel cell models: variability of dependent variables underneath flow fields. Int J Hydrogen Energy 39 (9):4566–4575.
Zhongjie He, Birgersson E, Hua Li (2014) Reduced non-isothermal model for the planar solid oxide fuel cell and stack. Energy 70:478–492.
Sharma AK, Birgersson E, Khor SH (2014) Computationally-efficient hybrid strategy for mechanistic modeling of fuel cell stacks. J Power Sources 247:481–488.
Zhongjie He, Hua Li, Birgersson E (2013) Reduced model for the planar solid oxide fuel cell. Comput Chem Eng 52:155–167.
Sharma AK, Birgersson E, Vynnycky M (2013) An aggregate measure for the local current density coupling in fuel cell stacks. J Electrochem Soc 160(11):F1237–F1240.
Ly H, Birgersson E, Vynnycky M (2012) Fuel cell model reduction through the spatial smoothing of flow channels. Int J Hydrogen Energy 37(9):7779–7795.
Ly H, Birgersson E, Vynnycky M (2011) Computationally efficient multi-phase models for a proton exchange membrane fuel cell: asymptotic reduction and thermal decoupling. Int J Hydrogen Energy 36(22):14573–14589.
Ly H, Birgersson E, Vynnycky M (2010) M., Asymptotically reduced model for a proton exchange membrane fuel cell stack: automated model generation and verification. J Electrochem Soc 157(7):B982–B992.

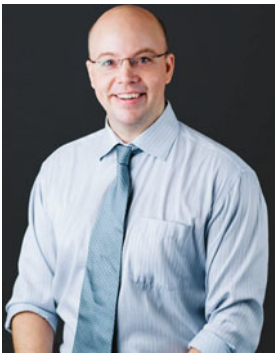
Contents

About the Authors

Dr. Zhongjie He received his B. Eng. degree in Mechanical Engineering (major in Industrial Design) and Ph.D. degree in Engineering Mechanics from Nanyang Technological University in Singapore in 2009 and 2014, respectively. Currently, Dr. He is a research fellow in Energy Research Institute at Nanyang Technological University (ERIAN). He is strong at multiphysics modelling and simulation, especially at developing fast and efficient models for fuel cells whose performance typically involves multiphysical behaviours such as transport phenomena, thermal dynamics, and electrochemical performance. His research interests also include electrostatic precipitation, cyclone design, steam soaking, and particle agglomeration to remove particulate matters from air.

Dr. Hua Li received his B.Sc and M.Eng. degrees in Engineering Mechanics from Wuhan University of Technology, P.R.C., in 1982 and 1987, respectively. He obtained his Ph.D. degree in Mechanical Engineering from the National University of Singapore in 1999. From 2000 to 2001, Dr. Li was a Postdoctoral Associate at the Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign. At the end of 2005, he was a Visiting Scientist (on invitation) at the Department of Chemical and Biomolecular Engineering of Johns Hopkins University. From 2001 to 2006, he was a Research Scientist in the A*STAR Institute of High Performance Computing. Dr. Li joined Nanyang Technological University (NTU) as Assistant Professor in June 2006 and he was promoted to Associate Professor in March 2013.

He is currently in the School of Mechanical & Aerospace Engineering at NTU. His research interests include the multiphysics modelling of soft matters (smart hydrogel in bioMEMS and biological cell in microscale fields); development of highly efficient numerical computational methodology (meshless & multiscale algorithms); simulation of sustainable energy (building energy efficiency and fuel cell system); and dynamics (high-speed rotating shell and composite materials structure). He has sole-authored a monograph book entitled "Smart Hydrogel Modelling" published by Springer, co-authored two monograph books entitled "Meshless Methods and Their Numerical Properties" by CRC Press and "Rotating Shell Dynamics" by Elsevier, and 2 book chapters, one on MEMS simulation and the other on hydrogel drug delivery system modelling, and authored/co-authored over 140 articles published in peer-reviewed international journals. He received the Silver Award in HPC Quest 2003—The Blue Challenge presented by IBM & IHPC in 2003. He is also extensively funded by agencies, including the principal investigator of a computational BioMEMS project awarded under A*STAR's strategic research programme in MEMS, and by industries, including SUN Microsystems (Oracle), Sony, Philips, DSO and JTC.



Dr. Karl Erik Birgersson is Associate Professor at the Chemical and Biomolecular Department and an affiliate of the Engineering Science Programme at the National University of Singapore (NUS) and the Solar Energy Research Institute of Singapore. He was awarded his Ph.D. in Fluid Mechanics from the Royal Institute of Technology (KTH), Stockholm, in 2004. He also holds an MS degree in Chemical Engineering from KTH (1998) and a Licentiate degree (2003). He was a postdoctoral fellow (2004–2005) and research engineer (2005–2006) at the Institute of High Performance Computing, A*Star, Singapore. He specializes in mathematical modelling and transport phenomena; his current research focuses on electrochemical energy systems and organic solar cells. He has published around 150 papers (journal, conference and book chapters).

Symbols

a	Water activity
a_{ij}, c_{ij}	Constants for functional polynomials
$\mathfrak{a}_0, \mathfrak{a}_1, \mathfrak{a}_2$	Constants for the reverse function of water content
$\mathfrak{b}_0, \mathfrak{b}_1, \mathfrak{b}_2, \mathfrak{b}_3$	Constants for the reverse function of water content
$a^{(\mathrm{l})}$	Surface area of the agglomerate including water per unit volume (m^{-1})
$a^{(\mathrm{p})}$	Surface area of the agglomerate per unit volume of catalyst layer (m^{-1})
A	Area (m^2)
$\mathcal{A}$	Actual reactive surface area per unit volume of the reaction zone (m^{-1})
$\mathcal{A}^{g-s}$	Specific surface area of porous media for heat exchange (m^{-1})
$\langle \mathbf{B} \rangle$	Superficial volume average of quantity **B**
c_1, c_2, c_3, c_4	Constants for saturation pressure of water (K^{-1}, K^{-2}, K^{-3})
c_{F}	Form-drag constant
$c_{\mathrm{H_2}}^{\mathrm{ref}}$, $c_{\mathrm{O_2}}^{\mathrm{ref}}$	Reference concentration of hydrogen and oxygen (mol m^{-3})
c_i	Molar concentration of species i (mol m^{-3})
c_p	Specific heat capacity (J kg^{-1} K^{-1})
$c_{p,i}^{(\mathrm{g})}$	Specific heat capacity of gas species i(J mol^{-1} K^{-1})
c_v	Coefficient of variation
$\mathfrak{c}_{\mathrm{i},1}, \mathfrak{c}_{\mathrm{i},2}, \mathfrak{c}_{\mathrm{i},3}, \mathfrak{c}_{\mathrm{i},4}$	Constants for the specific heat capacity equations (J mol^{-1} K^{-1}, J mol^{-1} K^{-2}, J mol^{-1} K^{-3}, J mol^{-1} K^{-4})
d	Characteristic pore diameter (m)
d_{par}	Average particle diameter of porous media (m)
$D^{(\mathrm{c})}$	Capillary diffusion (m^2 s^{-1})
D_0	Constant (m^2 s^{-1})
D_h	Hydraulic diameter (m)

$\mathfrak{D}_{ij}$	Combined diffusivity of species i and j involving both ordinary and Knudsen diffusion ($m^2\ s^{-1}$)
$D_i^{(g)}$	Diffusivity of gas species i ($m^2\ s^{-1}$)
$D_{i,\text{eff}}^{(g)}$	Effective diffusivity of gas species i ($m^2\ s^{-1}$)
$D_{H_2O,\text{eff}}^{(m)}$	Effective diffusivity of water in the membrane ($m^2\ s^{-1}$)
$D_{O_2,\text{eff}}^{(agg)}$	Effective diffusivity of oxygen in ionomer inside the agglomerate for PEMFC ($m^2\ s^{-1}$)
$D_{O_2}^{(l)}$, $D_{O_2}^{(p)}$	Diffusivity of oxygen in the liquid water and polymer film ($m^2\ s^{-1}$)
D_{ij}	Ordinary binary diffusivity of species i and j ($m^2\ s^{-1}$)
D_{ij}^0	Binary diffusivity of species i and j at the reference temperature and 1 atm ($m^2\ s^{-1}$)
$D_{\text{Kn},i}$	Knudsen diffusivity of species i ($m^2\ s^{-1}$)
$\mathcal{D}_{ij}$	The ij component of the multicomponent Fick diffusivity matrix ($m^2\ s^{-1}$)
$\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$	Coordinate vector
E^{act}	Activation energy for electrochemical reactions ($J\ mol^{-1}$)
E^{rev}	Reversible potential (V)
E^{ocv}	Open circuit voltage (V)
E^0	Reversible potential at standard conditions (V)
$f(\lambda)$	Additional function
$\mathfrak{f}_1, \mathfrak{f}_2, \mathfrak{f}_3, \mathfrak{f}_4, \mathfrak{f}_5, \mathfrak{f}_6$	Constants
F	Faraday's constant ($A\ s\ mol^{-1}$)
h_j	Thickness of a layer j (m)
h_{ks}	Statistic indicating the result of the Kolmogorov–Smirnov test
h_{rel}	Relative humidity
h^{g-s}	Convective heat transfer coefficient ($W\ m^{-2}\ K^{-1}$)
$\mathcal{H}$	Dimensionless height
H_{vap}	Heat of evaporization ($J\ kg^{-1}$)
$H_{O_2}^{(l)}$, $H_{O_2}^{(p)}$	Henry's constant for air–water and air–polymer interfaces ($atm\ m^3\ mol^{-1}$)
$\mathbf{i}$, i	Current density ($A\ m^{-2}$)
i_0	Exchange current density ($A\ m^{-2}$)
$\mathbf{I}$	Unit matrix
j	Repeating unit in a stack
J	Volumetric current density ($A\ m^{-3}$)
J_0^{ref}	Reference volumetric exchange current density ($A\ m^{-3}$)
$\mathcal{J}$	Leverett function
k	Thermal conductivity ($W\ m^{-1}\ K^{-1}$)
k_c	Dimensionless rate constant
k_{cond}, k_{vap}	Condensation and evaporation rate constants ($kg\ m^{-3}\ s^{-1}$)
k_{dis}	Dissolved/vapour mass transfer coefficient (s^{-1})

K	Equilibrium constant of electrochemical reactions
L	Cell length (m)
$\mathfrak{m}$	Mobility of liquid phase
$\dot{m}_{H_2O}$	Interphase mass transfer of water (kg m^{-3} s^{-1})
$m^{(C)}$, $m^{(p)}$, $m^{(Pt)}$	Carbon, polymer, and platinum loading (kg m^{-2})
m, n	Numbers of terms in polynomials
$M^{(g)}$	Mean molecular mass of the gas phase (kg mol^{-1})
M_i	Molecular mass of species i (kg mol^{-1})
$M^{(m)}$	Equivalent weight of dry membrane (kg mol^{-1})
n	Number of cells in a stack
$n^{(agg)}$	Number of agglomerates per unit volume (m^{-3})
n_d	Electroosmotic drag coefficient
n_{fc}	Number of flow channels in a flow field
n_i	Molar number of species i (mol)
$\mathbf{n}$	Unit normal vector pointing out of the domain
$\mathbf{n}_i$	Mass flux of species i (kg m^{-2} s^{-1})
Nu	Nusselt number
p	Pressure (Pa)
$p^{(c)}$	Capillary pressure (Pa)
$p^{(g)}$	Pressure of gas phase (Pa)
$p_{H_2O}^{(sat)}$	Saturation pressure of water (Pa)
p_{ks}	Statistic of the Kolmogorov–Smirnov test
Pr	Prandtl number
$\mathbf{q}$	Heat flux (W m^{-2})
$r^{(agg)}$	Radius of agglomerate (m)
R	Gas constant (J mol^{-1} K^{-1})
$\mathcal{R}$	Electric resistance (Ω)
$\Re$	Asymmetry factor
Re	Reynolds number
r	Average pore radius (m)
S	Wetted perimeter of a rectangular duct (m)
s_{H_2O}	Water saturation
S_i	Mass source term of species i (kg m^{-3} s^{-1})
S_{mass}	Mass source term (kg m^{-3} s^{-1})
S_{pot}	Electric source term (A m^{-3})
S_{temp}	Heat source (W m^{-3})
$\Im_0$, $\Im_1$, $\Im_2$	Constant (K)
$\mathbf{t}$	Unit tangential vector to the boundary
$\mathfrak{t}$	Constant for reversible potential
T	Temperature (K)
$\mathcal{T}$	Coefficient for temperature scaling
$\mathbf{v}, u, v, w, U$	Velocities (m s^{-1})
V	Volume (m^3)

V_{cell}	Cell voltage (V)
w	Width (m)
$\mathcal{W}$	Dimensionless width
x, y, z	Coordinate (m)
x_i	Mole fraction of species i
X_i	Input parameter
$X_i^{'}$, $\mathrm{Y}_i^{'}$	Ranks of paired data (X_i, Y_i) in a sample
Y_i	Dependent variable
$z_{\alpha/2}$	Upper $100(1-\alpha/2)^{\text{th}}$ percentile of the standard normal distribution at a confidence level of α
$\vert$	At a certain height in the cell

Greek Symbols

$\alpha_{1,2}$	Charge transfer coefficient
β	Pre-exponential factor of exchange current density (A m^{-2})
$\beta^{(\text{m})}$	Modification factor
ΔG^0	Standard Gibbs free energy change (J mol^{-1})
Δp	Gauge pressure (Pa)
Δs	Molar entropy change (J mol^{-1} K^{-1})
Φ	Place holder for dependent variables
γ	Reaction order of the electrochemical reaction
$\gamma^{(\text{agg})}$, γ_{cl}, $\gamma^{(\text{p})}$, $\gamma^{(\text{PtC})}$	Volume fraction for the agglomerate model
δ	Thickness of film (m)
ε	Porosity
ϵ	Relative convergence error for the nonlinear solver in COMSOL
η	Polarization (V)
θ_{c}	Wetting angle
μ	Mean of a population
$\mu^{(\text{g})}$	Dynamic viscosity of gas phase (kg m^{-1} s^{-1})
μ_i	Dynamic viscosity of species i (kg m^{-1} s^{-1})
μ_{mix}	Dynamic viscosity of gas mixture (kg m^{-1} s^{-1})
κ	Permeability (m^2)
κ_{rel}	Relative permeability
λ	Water content
λ_{m}	Mean free path length in the gas (m)
Ω	Placeholder for dependent variables
ρ	Density (kg m^{-3})
σ	Standard deviation
σ_{elc}	Electrical conductivity (Ω^{-1} m^{-1})
σ_{ion}	Ionic conductivity (Ω^{-1} m^{-1})
$\widetilde{\sigma}$	Variation factor
$\sigma^{(\text{m})}$	Protonic conductivity (S m^{-1})

$\sigma^{(s)}$	Electric conductivity (S m^{-1})
σ_{st}	Surface tension (N m^{-1})
ϕ	Potential (V)
Φ	Thiele modulus or volume fraction of the electron conducting particles in electrodes
$\Phi_{\alpha\beta}$	Dimensionless quantities for calculating thermal conductivity
ς	Switch for interphase mass transfer
τ	Tortuosity
ω	Mass fraction
$\omega^{(p)}$	Mass fraction of polymer loading
$\omega^{(Pt)}$	Mass fraction of platinum loading on carbon
ς	Stoichometry
ς	Switch of interphase transfer
ξ, ζ	Correlation factors for the pathways of transport processes
ξ_1, ξ_2, ξ_3	Correction factors for agglomerate model

Subscripts

α, β, i, j	Index for the species: O_2, N_2, H_2, H_2O
a, c	Anode, cathode
avg	Average
bl	Backing layer
el	Electrolyte
elc	Electronic
cc	Current collector
crit	Critical number
fc	Flow channel
ff	Flow field
g	Gas phase
H_2	Hydrogen
H_2O	Water
ic	Interconnect
ion	Ionic
j	Functional layer j
Kn	Knudsen diffusion
mass	Mass source term
max	Maximum
mix	Gas mixture
mom	Source term for the momentum conservation
N_2	Nitrogen
O_2	Oxygen
pot	Potential, or source term for the electric conservation
rib	Rib

rl	Reaction zone layer
s	Solid phase
/	Interface between layers
$\perp$	Surface perpendicular to the streamwise direction

Superscripts

(agg)	Agglomerate
act	Activation polarization
(c)	Capillary
(C)	Carbon
con	Concentration polarization
cool	Cooling
eff	Effective
(ff)	Flow field
(fc)	Flow channel
(g)	Gas phase
g-s	Heat exchange between the gas and solid phases
(ic)	Interconnect
in	Inlet
(l)	Liquid phase
leak	Leak polarization
(m)	Membrane
ohm	Ohmic polarization
oper	Operating condition
out	Outlet
(p)	Polymer
(Pt)	Platinum
(PtC)	Platinum and carbon
ref	Reference
(s)	Solid phase
sat	Saturation
†	Transpose of a tensor
0	Standard condition

Chapter 1
Introduction

1.1 Background

Sustainable energy development for a growing population is a critical issue in the 21st century. The energy report of the European Environment Agency (EEA) in 2008 anticipated that the global energy requirement would be higher in 2030 than that in 2005 by 55 %, if governments around the world continued with their current policies [1]. About 84 % of the increase in primary energy demand would come from fossil fuels [1]. This increase in energy demand was also reported by the International Energy Agency (IEA) in 2008, as depicted in Table 1.1 [2]. Excessive use of fossil fuels must pose a number of environmental impacts like oil supply insecurity, air pollution, greenhouse gas emissions, and adverse influences on ecosystems during energy production processes. Increasing energy demand, diminishing natural resources, and growing environmental concerns have invoked the continuous development of new energy conversion technologies to fulfill the sustainable development strategy and environmental friendliness while meeting the anticipated annual growth in energy demand presented in Table 1.1.

One of the promising new energy technologies is fuel cell [3, 4], which directly converts the free energy of chemical reactants to electrical energy and heat without combustion. It is widely accepted that the fuel cell was invented by Sir William Robert Grove, who convincingly demonstrated the principle of fuel cell in 1839 [3]. Nowadays, the fuel cell has grown up into a big family of many members operating at specific temperatures. The most common ones are the proton exchange membrane fuel cell (PEMFC), alkaline fuel cell (AFC), phosphoric-acid fuel cell (PAFC), molten-carbonate fuel cell (MCFC), and solid oxide fuel cell (SOFC) [5], as introduced in Table 1.2. In general, a number of cells are stacked together in electric-series to generate desired output voltage and power ranging from microwatt for micro-electromechanical systems to megawatt for power plants. Applications of the fuel cell spread to four major areas: small/big power stations, residential electricity, transport facilities (e.g., car and bus), and portable electric products (e.g.,

Z. He et al., *Reduced Modelling of Planar Fuel Cells*,
DOI 10.1007/978-3-319-42646-4_1

Table 1.1 World energy demand in cities reported by International Energy Agency [2]

Year	2006		2015		2030		2006–2030
	Mtoe	Cities as a % of world	Mtoe	Cities as a % of world	Mtoe	Cities as a % of world	Average annual growth rate (%)
Oil	2519	63	2873	63	3394	66	1.2
Coal	2330	76	3145	78	3964	81	2.2
Gas	1984	82	2418	83	3176	87	2.0
Hydro	195	75	245	76	330	79	2.2
Biomass and waste	280	24	358	26	520	31	2.6
Nuclear	551	76	630	77	726	81	1.2
Other renewable	48	72	115	73	264	75	7.4
Total	7908	67	9785	69	12374	73	1.9
Electricity	1019	76	1367	77	1912	79	2.7

laptop, digital camera, hand phone, and PDA) [6]. As an innovative source of energy, the fuel cell technology has gained a good reputation for high efficiency, environmental friendliness, and compatibility with renewable energy sources [3–5]. Many countries (U.S, China, European Union, Japan, etc.) and companies have invested plenty of human power and capital on the fuel cell technology for many years [7, 8].

In order to investigate the characteristics and mechanism of the fuel cells, mathematical modelling is a widely applied approach in comparison with repetitive and costly experimental approaches. There are three main reasons why mathematical modelling plays an important role as part of the overall research and development efforts on fuel cells in the last two decades. First, a properly constructed and validated mathematical model can provide an understanding and insight into the intrinsic phenomena on a local level in the various functional layers of a fuel cell, which is next to impossible from an experimental point of view because of the small length scales that can be found in the cell. Second, well-developed mathematical formalism and techniques from various mathematical branches (like calculus and algebra) can not only be employed as building blocks for the models themselves, but also provide the means towards cell performance improvements, such as optimization of designs and operating conditions. Third, modelling can aid in the troubleshooting of designs, experiments, and failures. The derivation of a large number of rich and diverse models for different types of fuel cell can be referred to the literature:

- References [9–13] for the proton exchange membrane fuel cell (PEMFC);
- References [14–17] for the alkaline fuel cell (AFC);
- References [18–20] for the direct ethanol fuel cell (DEFC);
- References [21–24] for the direct methanol fuel cell (DMFC);

Table 1.2 Operational characteristics and technological status of various fuel cells

Properties	PEMFC	AFC	PAFC	MCFC	SOFC	Refs.
Operating temperature	50–100 °C	60–220 °C	160–200 °C	600–700 °C	500–1000 °C	[3, 5, 36–38]
Prime cell components	Carbon-based	Carbon-based	Graphite-based	Stainless-based	Ceramic	[38, 54]
Electrolyte	Hydrated polymeric ion exchange membranes	Mobilized or immobilized potassium hydroxide (KOH) in asbestos matrix	Immobilized liquid phosphoric acid (H_3PO_4) in SiC	Immobilized liquid molten carbonate in $LiAlO_2$	Perovskites (ceramics)	[38, 54]
Electrodes	Carbon	Transition metals	Carbon	Nickel and nickel oxide	Perovskite and perovskite/metal cermet	[38, 54]
Catalyst	Platinum	Platinum	Platinum	Electrode material	Electrode material	[38, 54]
Interconnect	Carbon or metal	Metal	Graphite	Stainless steel or nickel	Nickel ceramic or steel	[38, 54]
Fuel	H_2, methanol	H_2	H_2	H_2, CH_4	H_2, CH_4, CO, other hydrocarbons	[37]
Charge carrier	H^+	OH^-	H^+	CO_3^{2-}	O^{2-}	[37, 54]
External reforming for hydrocarbon fuels	Yes	Yes	Yes	No, for some fuels	No, for some fuels and cell designs	[38, 54]
External shift conversion of CO to H_2	Yes, plus purification to remove trace CO	Yes, plus purification to remove CO and CO_2	Yes	No	No	[38, 54]

(continued)

Table 1.2 (continued)

Properties	PEMFC	AFC	PAFC	MCFC	SOFC	Refs.
Produce water management	Evaporative	Evaporative	Evaporative	Gaseous product	Gaseous product	[54]
Product heat management	Process gas + liquid cooling medium	Process gas + electrolyte circulation	Process gas + liquid cooling medium or steam generation	Internal reforming + process gas	Internal reforming + process gas	[54]
System output	<1–250 kW	10–100 kW	50 kW–1 MW	<1 kW–1 MW	<1 kW–3 MW	[3, 38]
Electrical efficiency	53–58 % (transport), 35 % (stationary)	60 %	32–38 %	45–47 %	50–60 %	[59, 111]
Energy efficiency	40–50 %	40–70 %	70 %	60 %	70 %	[38]
Lifetime projected 4(h)	>40,000	> 10,000	>40,000	>40,000	>40,000	[5]
Capital cost projected (U.S. $/kW)	>200	>200	3000	1000	1500	[5]
Applications	1. Backup power 2. Portable power 3. Small distributed generator 4. Transportation 5. Specialty vehicles	1. Military 2. Space	Distributed generator	1. Electric utility 2. Large distributed generator	1. Auxiliary power 2. Electric utility 3. Large distributed generator	[3]

- References [25–32] for the molten carbonate fuel cell (MCFC);
- References [33–35] for the planar and tubular solid oxide fuel cell (SOFC).

In view of the configuration of the above fuel cells (except the tubular SOFC), there is a common feature that they have a planar geometry where a plate-type electrolyte is sandwiched between a cathode and an anode. The fuel cells of this type of geometry are named as planar fuel cells. This book will focus on the PEMFC and the planar SOFC (P-SOFC) to elaborate and illustrate the present methodologies of model reduction for the planar fuel cells.

1.1.1 Proton Exchange Membrane Fuel Cell (PEMFC)

The first PEMFC was developed in 1960s by General Electric in the United States for the first manned space vehicles of NASA [36]. The PEMFC is generally operated at low temperatures ranging from 50 to 100 °C [3, 5, 36–38], which is advantageous over other types of fuel cells and thus allow the development of the PEMFC to start quickly, especially for portable and transport applications [39]. The core components of the PEMFC are a cathode and an anode separated by a polymer membrane, which form a membrane-electrode assembly (MEA) as shown schematically in Fig. 1.1. In a single fuel cell, a single-side flow field plate is located on top of the electrode to distribute the fuel or oxidant, collect the current to power the electric device, carry water away from the cell, and humidify the gases. In a stack, instead of the single-side plate, bipolar plates are placed between the cells. Some common designs for the flow field plates are schematically shown in Fig. 1.2, such as parallel straight channels, single or multiple serpentine channels,

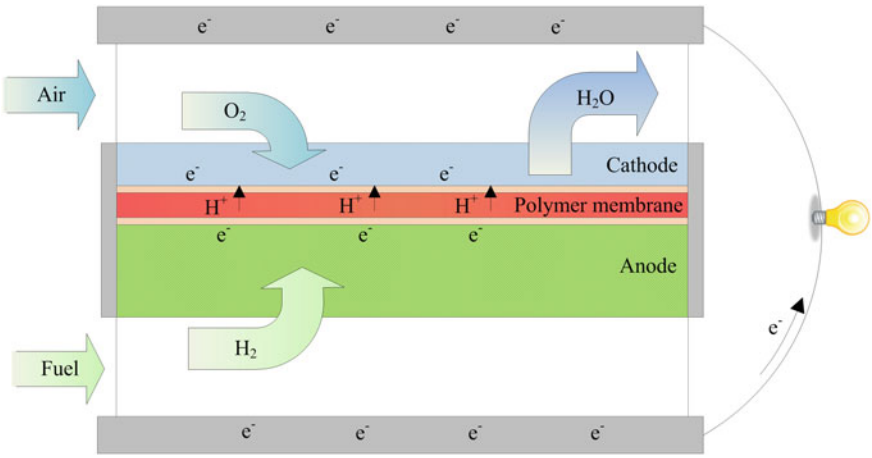


Fig. 1.1 Schematic of the working principle of the PEMFC

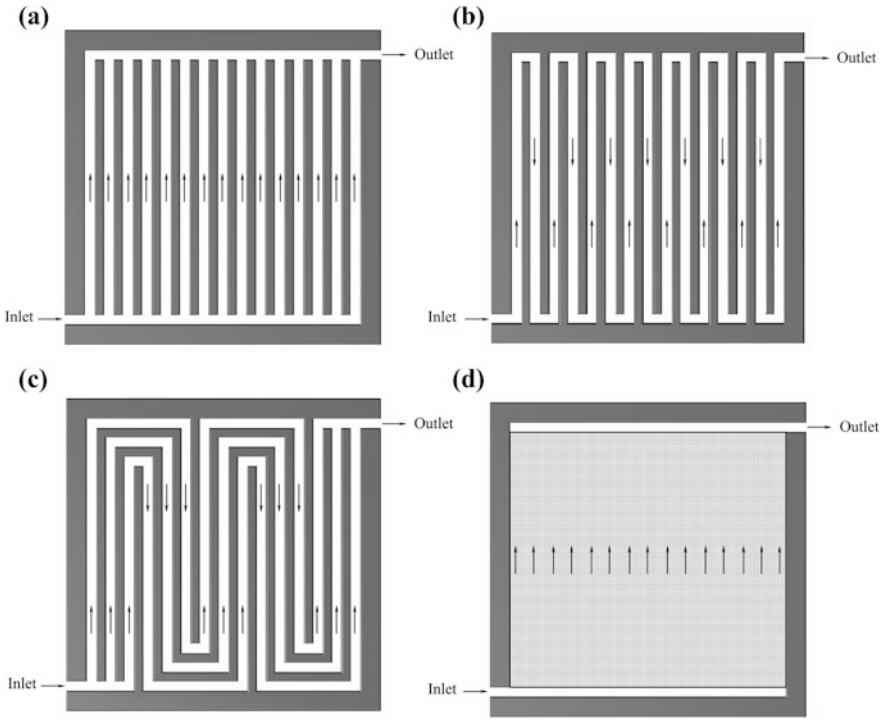


Fig. 1.2 Typical flow field design for planar fuel cells: **a** parallel straight channels; **b** single serpentine channels; **c** multiple serpentine channels; **d** porous [39–41, 110]

where the flow field consists plain channels surrounded by solid ribs [39–41]. Other types of flow channel designs were also suggested in the literature, such as interdigitated, pin, and bio-mimetic flow fields, which can be referred to Ref. [41] reviewing the flow field designs for the bipolar plate of the PEMFC. Apart from the plain flow channels separated by ribs, the flow field can also consist of a porous medium [42], as shown in Fig. 1.2d. In addition, coolant flow field layers may be needed for the overall PEMFC stack depending on the type of thermal management such as liquid water cooling, cooling via phase-change materials, forced or natural air-convection cooling.

The materials used for the MEA has maintained the same since the early 1990s [43]. The membrane is generally made of a perfluorinated polymer backbone with sulfonic acid side chains, which can become a good protonic conductor when fully humidified and thus has been used for decades [43, 44]. The latest development on the polymer membranes lies on improvement of their chemical stability and thinner membranes reduced from 175 to 25 mm [43]. For the electrodes, cloth with platinum on supported carbon or teflonated porous carbon paper have been used in both the anode and cathode [43, 44]. For the flow field plates of single cells, the most common materials are graphite and stainless steel, and other materials like

aluminium, steel, titanium, nickel, and polymer composites are also applicable. Most bipolar plates in the PEMFC stack are made of resin-impregnated graphite because of high conductivity, chemically inertness, and resistance to corrosion, although it is expensive and costly to manufacture [40].

The working principle of the PEMFC is demonstrated schematically in Fig. 1.1. The mobile ion through the polymer membrane is H^+ ions or protons. Apart from conducting ions from the anode to the cathode, the membrane also serves as an electronic insulator and a gas separator. On each electrode of the cell, a catalytically active region, namely catalyst layer or reaction zone, is attached to the membrane and thus form the membrane-electrode-assembly (MEA). During operation, the supplied hydrogen (H_2) diffuses from the fuel flow channel through the porous anode and then becomes oxidized in the catalyst layer to form protons, such that free electrons (e^-) are released:

$$\mathrm{H_2(g)} = 2H^+ + 2e^-. \tag{1.1}$$

The free electrons go through the electrically conducting solid phase of the anode to the current collector (top part of the flow field plate), and finally back to the cathode via an external circuit to perform useful work. Meanwhile, on the cathode, the protons through the membrane react with the oxygen (O_2) diffusing from the air flow channel and the free electrons conducted from the current collector, resulting in liquid water (H_2O) as the product:

$$\frac{1}{2}\mathrm{O_2(g)} + 2H^+ + 2e^- = \mathrm{H_2O(l)}. \tag{1.2}$$

The produced water diffuses back to the air flow channel through the pores in the cathode by capillary driven [45]. The overall cell reaction in the PEMFC is

$$\mathrm{H_2(g)} + \frac{1}{2}\mathrm{O_2(g)} = \mathrm{H_2O(l)}. \tag{1.3}$$

The theoretical open circuit voltage of a hydrogen-oxygen fuel cell is 1.23 V at 298 K. Under practical load conditions, the cell voltage is between 0.5 and 1.0 V, which corresponds to a current density up to 1.5 A cm^{-2} depending on real applications [43].

Furthermore, if the produced water is not removed properly, the accumulating liquid water may lead to serious issues for the PEMFC which is operated at low temperatures and hence low-saturation pressure [39]. Excess liquid water can cause flooding of the catalyst layer and backing layer [46–48] as well as clogging of the flow channel [39, 49, 50], although water is essential for the ion conduction in the membrane. As such, two-phase transport phenomena plays an important role in the simulation of the PEMFC [39, 45, 46, 51–53].

1.1.2 Planar Solid Oxide Fuel Cell (P-SOFC)

The high-temperature fuel cell, namely the SOFC, has attracted much interest in its potential applications to stationary power station, mobile power, auxiliary power for vehicles, and specialty applications [37]. The SOFC technology provides advantages over other types of fuel cells, such as fuel variety, relatively high sulphur resistance, and high electrical efficiency [54, 55]. Nevertheless, the SOFC technology is still away from commercialization due to some critical issues like long start-up transient time, thermal stresses and expansion mismatches, and sealing problems between cells in a SOFC stack.

In general, the SOFC is fabricated at temperatures between 1200 and 1300 °C and operates at temperatures ranging from 500 to 1000 °C. It produces electricity and heat directly from gaseous hydrogen or hydrocarbon fuels, such as natural gas, via electrochemical reactions with ambient air as an oxidant. The first SOFC was proposed by Schottky using the Nernst mass as the solid electrolyte, and then it was constructed by Baur and Preis in 1937 [56, 57]. The core components of a SOFC are two porous electrodes (i.e., anode and cathode) separated by a thin and dense ion-conducting ceramic electrolyte layer, as shown in Fig. 1.3. The gastight electrolyte is conventionally made of yttria (Y_2O_3)-stabilized zirconia (ZrO_2) (YSZ), in which yttrium is used within a range of 3−10 mol% to stabilize the zirconia lattice [58]. Conventionally, the YSZ can be named according to the contained amount of yttria, such as 3YSZ, 8YSZ, and 10YSZ refer to the YSZ with 3, 8, and 10 mol% of yttria, respectively. YSZ provides high ionic conductivity but negligible electric conductivity at temperatures above 700 °C. The solid electrolyte enables the SOFC to be free from many of the management issues in other types of fuel cells, such as electrode flooding, electrolyte migration, and catalyst wetting [5]. The cathode is commonly composed of strontium (Sr)-doped lanthanum manganite ($LaMnO_2$)

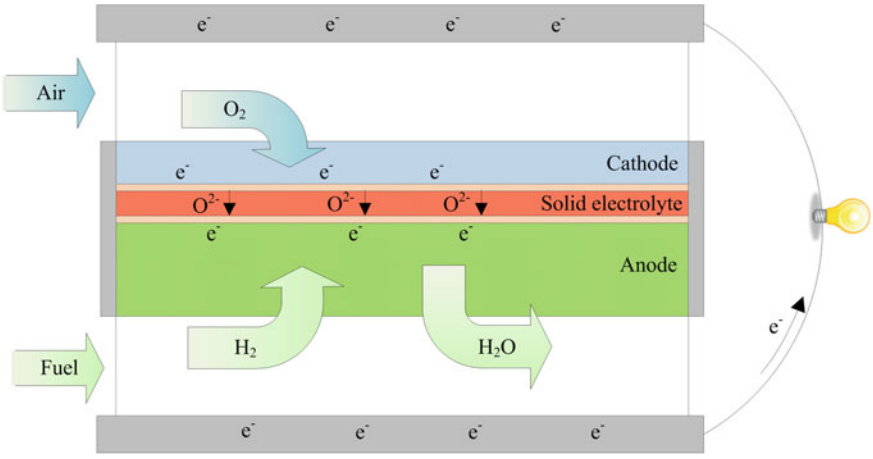


Fig. 1.3 Schematic of the working principle of the planar SOFC