

# Contents

<b>Preface</b>	<b>xi</b>
<b>Acknowledgments</b>	<b>xiii</b>
<b>List of Figures</b>	<b>xv</b>
<b>List of Tables</b>	<b>xxi</b>
<b>1 Introduction</b>	<b>1</b>
1.1 Overview of Fuel Cell Technology	1
1.1.1 <i>Types of Fuel Cells</i>	2
1.1.2 <i>Planar and Tubular Designs</i>	3
1.1.3 <i>Fuel Cell Systems</i>	4
1.1.4 <i>Pros and Cons of Fuel Cells</i>	5
1.2 Modelling, State Estimation and Control	5
1.3 Book Coverage	6
1.4 Book Outline	6
<b>Part I FUNDAMENTALS</b>	
<b>2 First Principle Modelling for Chemical Processes</b>	<b>11</b>
2.1 Thermodynamics	11
2.1.1 <i>Forms of Energy</i>	11
2.1.2 <i>First Law</i>	12
2.1.3 <i>Second Law</i>	13
2.2 Heat Transfer	13
2.2.1 <i>Conduction</i>	14
2.2.2 <i>Convection</i>	15
2.2.3 <i>Radiation</i>	17
2.3 Mass Transfer	18
2.4 Fluid Mechanics	20
2.4.1 <i>Viscous Flow</i>	21
2.4.2 <i>Velocity Distribution</i>	21
2.4.3 <i>Bernoulli Equation</i>	21

2.5	Equations of Change	22
2.5.1	<i>The Equation of Continuity</i>	23
2.5.2	<i>The Equation of Motion</i>	23
2.5.3	<i>The Equation of Energy</i>	24
2.5.4	<i>The Equations of Continuity of Species</i>	26
2.6	Chemical Reaction	26
2.6.1	<i>Reaction Rate</i>	26
2.6.2	<i>Reversible Reaction</i>	28
2.6.3	<i>Heat of Reaction</i>	29
2.7	Notes and References	29
<b>3</b>	<b>System Identification I</b>	<b>31</b>
3.1	Discrete-time Systems	31
3.2	Signals	36
3.2.1	<i>Input Signals</i>	36
3.2.2	<i>Spectral Characteristics of Signals</i>	41
3.2.3	<i>Persistent Excitation in Input Signals</i>	44
3.2.4	<i>Input Design</i>	49
3.3	Models	50
3.3.1	<i>Linear Models</i>	50
3.3.2	<i>Nonlinear Models</i>	54
3.4	Notes and References	56
<b>4</b>	<b>System Identification II</b>	<b>57</b>
4.1	Regression Analysis	57
4.1.1	<i>Autoregressive Moving Average with Exogenous Input Models</i>	57
4.1.2	<i>Linear Regression</i>	59
4.1.3	<i>Analysis of Linear Regression</i>	60
4.1.4	<i>Weighted Least Squares Method</i>	61
4.2	Prediction Error Method	64
4.2.1	<i>Optimal Prediction</i>	65
4.2.2	<i>Prediction Error Method</i>	70
4.2.3	<i>Prediction Error Method with Independent Parameterisation</i>	74
4.2.4	<i>Asymptotic Variance Property of PEM</i>	75
4.2.5	<i>Nonlinear Identification</i>	76
4.3	Model Validation	79
4.3.1	<i>Model Structure Selection</i>	79
4.3.2	<i>The Parsimony Principle</i>	80
4.3.3	<i>Comparison of Model Structures</i>	81
4.4	Practical Consideration	82
4.4.1	<i>Treating Non-zero Means</i>	82
4.4.2	<i>Treating Drifts in Disturbances</i>	83

4.4.3	<i>Robustness</i>	83
4.4.4	<i>Additional Model Validation</i>	83
4.5	Closed-loop Identification	84
4.5.1	<i>Direct Closed-loop Identification</i>	85
4.5.2	<i>Indirect Closed-loop Identification</i>	87
4.6	Subspace Identification	92
4.6.1	<i>Notations</i>	92
4.6.2	<i>Subspace Identification via Regression Analysis Approach</i>	97
4.6.3	<i>Example</i>	100
4.7	Notes and References	102
<b>5</b>	<b>State Estimation</b>	<b>103</b>
5.1	Recent Developments in Filtering Techniques for Stochastic Dynamic Systems	103
5.2	Problem Formulation	105
5.3	Sequential Bayesian Inference for State Estimation	107
5.3.1	<i>Kalman Filter and Extended Kalman Filter</i>	110
5.3.2	<i>Unscented Kalman Filter</i>	112
5.4	Examples	116
5.5	Notes and References	120
<b>6</b>	<b>Model Predictive Control</b>	<b>121</b>
6.1	Model Predictive Control: State-of-the-Art	121
6.2	General Principle	122
6.2.1	<i>Models for MPC</i>	122
6.2.2	<i>Free and Forced Response</i>	125
6.2.3	<i>Objective Function</i>	125
6.2.4	<i>Constraints</i>	126
6.2.5	<i>MPC Law</i>	126
6.3	Dynamic Matrix Control	127
6.3.1	<i>Prediction</i>	127
6.3.2	<i>DMC without Penalising Control Moves</i>	129
6.3.3	<i>DMC with Penalising Control Moves</i>	130
6.3.4	<i>Feedback in DMC</i>	130
6.4	Nonlinear MPC	134
6.5	General Tuning Guideline of Nonlinear MPC	136
6.6	Discretisation of Models: Orthogonal Collocation Method	137
6.6.1	<i>Orthogonal Collocation Method with Prediction Horizon 1</i>	137
6.6.2	<i>Orthogonal Collocation Method with Prediction Horizon N</i>	140
6.7	Pros and Cons of MPC	142
6.8	Optimisation	142
6.9	Example: Chaotic System	144
6.10	Notes and References	145

**Part II TUBULAR SOFC**

<b>7</b>	<b>Dynamic Modelling of Tubular SOFC: First-Principle Approach</b>	<b>149</b>
7.1	SOFC Stack Design	149
7.2	Conversion Process	150
	7.2.1 <i>Electrochemical Reactions</i>	150
	7.2.2 <i>Electrical Dynamics</i>	153
7.3	Diffusion Dynamics	155
	7.3.1 <i>Transfer Function of Diffusion</i>	156
	7.3.2 <i>Simplified Transfer Function of Diffusion</i>	157
	7.3.3 <i>Dynamic Model of Diffusion</i>	158
	7.3.4 <i>Diffusion Coefficient</i>	159
7.4	Fuel Feeding Process	160
	7.4.1 <i>Reforming/Shift Reaction</i>	160
	7.4.2 <i>Mass Transport</i>	162
	7.4.3 <i>Momentum Transfer</i>	164
	7.4.4 <i>Energy Transfer and Heat Exchange</i>	165
7.5	Air Feeding Process	166
	7.5.1 <i>Mass Transport in the Cathode Channel</i>	166
	7.5.2 <i>Cathode Channel Momentum Transfer</i>	167
	7.5.3 <i>Energy Transfer in the Cathode Channel</i>	168
	7.5.4 <i>Air in Injection Channel</i>	168
7.6	SOFC Temperature	169
	7.6.1 <i>Dynamic Energy Exchange Process</i>	169
	7.6.2 <i>Conduction</i>	170
	7.6.3 <i>Convection</i>	171
	7.6.4 <i>Radiation</i>	172
	7.6.5 <i>Cell Temperature Model</i>	174
	7.6.6 <i>Injection Tube Temperature Model</i>	174
7.7	Final Dynamic Model	175
	7.7.1 <i>I/O Variables</i>	175
	7.7.2 <i>State Space Model</i>	176
	7.7.3 <i>Model Validation</i>	180
7.8	Investigation of Dynamic Properties through Simulations	181
	7.8.1 <i>Dynamics of Diffusion</i>	182
	7.8.2 <i>Dynamics of Fuel Feeding Process</i>	184
	7.8.3 <i>Dynamics of Air Feeding Process</i>	186
	7.8.4 <i>Dynamics due to External Load</i>	188
7.9	Notes and References	190
<b>8</b>	<b>Dynamic Modelling of Tubular SOFC: Simplified First-Principle Approach</b>	<b>193</b>
8.1	Preliminary	193
	8.1.1 <i>Relation of Process Variables</i>	194
	8.1.2 <i>Limits to Power Output</i>	194

8.2	Low-order State Space Modelling of SOFC Stack	195
8.2.1	<i>Physical Processes</i>	195
8.2.2	<i>Modelling Assumptions</i>	197
8.2.3	<i>I/O Variables</i>	197
8.2.4	<i>Voltage</i>	198
8.2.5	<i>Partial Pressures</i>	199
8.2.6	<i>Flow Rates</i>	200
8.2.7	<i>Temperatures</i>	203
8.3	Nonlinear State Space Model	204
8.4	Simulation	205
8.4.1	<i>Validation</i>	205
8.4.2	<i>Step Response to the Inputs</i>	207
8.4.3	<i>Step Responses to the Disturbances</i>	209
8.5	Notes and References	211
<b>9</b>	<b>Dynamic Modelling and Control of Tubular SOFC: System Identification Approach</b>	<b>213</b>
9.1	Introduction	213
9.2	System Identification	213
9.2.1	<i>Selection of Variables</i>	213
9.2.2	<i>Step Response Test</i>	214
9.2.3	<i>Non-typical Step Response</i>	217
9.2.4	<i>Input Design</i>	218
9.2.5	<i>Linear System Identification</i>	220
9.2.6	<i>Nonlinear System Identification</i>	234
9.3	PI Control	241
9.3.1	<i>Set Point Tracking</i>	243
9.3.2	<i>Disturbance Rejection</i>	243
9.3.3	<i>Internal Model Control for Discrete-time Processes</i>	243
9.3.4	<i>Application of Discrete-time IMC to Multi-loop Control of SOFC</i>	254
9.4	Closed-loop Identification	257
9.5	Notes and References	263

### Part III PLANAR SOFC

<b>10</b>	<b>Dynamic Modelling of Planar SOFC: First-Principle Approach</b>	<b>267</b>
10.1	Introduction	267
10.2	Geometry	268
10.3	Stack Voltage	268
10.4	Mass Transport	270
10.5	Energy Balance	271
10.5.1	<i>Lumped Model</i>	272
10.5.2	<i>Detail Model</i>	273

10.6	Simulation	277
	10.6.1 <i>Steady-state Response</i>	277
	10.6.2 <i>Dynamic Response</i>	278
10.7	Notes and References	280
<b>11</b>	<b>Dynamic Modelling of Planar SOFC System</b>	<b>283</b>
11.1	Introduction	283
11.2	Fuel Cell System	283
	11.2.1 <i>Fuel and Air Heat Exchangers</i>	284
	11.2.2 <i>Reformer</i>	286
	11.2.3 <i>Burner</i>	287
11.3	SOFC along with a Capacitor	287
11.4	Simulation Result	289
	11.4.1 <i>Fuel Cell System Simulation</i>	290
	11.4.2 <i>SOFC Stack with Ultra-capacitor</i>	292
11.5	Notes and References	292
<b>12</b>	<b>Model Predictive Control of Planar SOFC System</b>	<b>295</b>
12.1	Introduction	295
12.2	Control Objective	296
12.3	State Estimation: UKF	297
12.4	Steady-state Economic Optimisation	298
12.5	Control and Simulation	301
	12.5.1 <i>Linear MPC</i>	301
	12.5.2 <i>Nonlinear MPC</i>	303
	12.5.3 <i>Optimisation</i>	305
12.6	Results and Discussions	306
12.7	Notes and References	307
<b>Appendix A</b>	<b>Properties and Parameters</b>	<b>309</b>
A.1	Parameters	309
A.2	Gas Properties	309
	<b>References</b>	<b>315</b>
	<b>Index</b>	<b>321</b>