

# Object-Oriented Simulation of Chemical and Biochemical Processes



Damien Hocking

Department of Chemical Engineering  
University of Adelaide

Thesis submitted for the Degree of  
Doctor of Philosophy  
in  
The University of Adelaide  
Faculty of Engineering

February 1997

# CONTENTS

<b>Chapter 1: Introduction and literature review</b>	<b>1</b>
1.1 Simulation Techniques	1
1.1.1 Sequential-Modular	1
1.1.2 Equation-Oriented	2
1.1.3 Parallel-Modular	4
1.2 Object-Oriented Process Simulation	4
1.2.1 Object-Oriented Simulation	6
1.2.2 Languages	6
1.2.3 Object-Oriented Simulation Environments	14
1.2.4 Summary of Object-Oriented Simulation	18
1.3 Biochemical Process Simulation	19
1.3.1 Summary of Biochemical Process Simulation	21
1.4 Physical Property Calculation	22
1.5 Numerical Analysis Methods	24
1.5.1 Nonlinear Algebraic Equations	24
1.5.2 Integration Methods	27
1.6 Conclusions and Project Scope	29
<b>Chapter 2: Simulator Development and Data Structure</b>	<b>31</b>
2.1 Development Language	31
2.2 Data Structure	35
2.2.1 Physical Information	36
2.2.2 Simulator Executive	39
2.2.3 Mathematical Information	40
2.3 Functionality and Behaviour	48
2.3.1 Structural Analysis	48
2.3.2 Equation Evaluation	51
2.3.3 Model Evaluation	52
2.3.4 Behavioural Changes	54
2.3.5 Numerical Methods	56
2.3.6 Interchangeable Simulation Techniques	60

2.4 Chemical Components and Property Calculation	62
2.5 Summary	66
<b>Chapter 3: C++ Implementation</b>	68
3.1 C++ Constructors and Destructors	68
3.2 Vectors and Matrices	69
3.3 Process Class Structure	73
3.3.1 System Class and Descendants	73
3.3.2 Port Class and Descendants	77
3.3.3 Stream Class and Descendants	80
3.4 Mathematical Class Structure	81
3.4.1 Variable Class and Descendants	81
3.4.2 Equation_Set and Dynamic_Set classes	83
3.5 Component, General_Component_Mixture and Properties Classes	88
3.5.1 Component class and Descendants	89
3.5.2 General_Component_Mixture Class	90
3.5.3 Properties Class and Descendants	90
3.6 Numerical Method Classes	91
3.7 Summary	92
<b>Chapter 4: Modelling and Simulation</b>	93
4.1 Decomposition Techniques	93
4.1.1 Medium and Machine Decomposition	93
4.1.2 Primitive Behaviour Decomposition	94
4.1.3 Mathematical Decomposition	95
4.2 Modelling Examples	97
4.2.1 Mixing Tank	98
4.2.2 Bi-Directional Information Flow	105
4.2.3 Connected-System Modelling	112
4.2.4 Multiple-Inheritance Modelling	120
4.2.5 Modelling with Physical Properties	126
4.3 Simulation	130

4.3.1 Instruction Sequence	130
4.3.2 Steady-state example	131
4.4 Summary	135
<b>Chapter 5: Major Test Problems</b>	<b>136</b>
5.1 Cavett Problem	136
5.2 Tennessee Eastman Process	141
5.2.1 Control Systems	143
5.2.2 Simulation Results	150
5.3 Recombinant Fermentation Model	157
5.3.1 Model Description	158
5.3.2 Control System	161
5.3.3 Simulation Results	162
5.4 Discussion	165
5.5 Summary	167
<b>Chapter 6: Summary, Conclusions and Recommendations</b>	<b>168</b>
6.1 Summary	168
6.2 Class Description	168
6.3 Modelling	169
6.4 Simulation	170
6.5 Recommendations	171
<b>Bibliography</b>	<b>173</b>
<b>Nomenclature</b>	<b>180</b>
<b>Appendices</b>	<b>182</b>
<b>Appendix A: General member function descriptions</b>	<b>183</b>
A.1 <b>System-based classes</b>	<b>183</b>

A.1.1 <b>System</b> Connectivity and Mathematical interface functions	183
A.1.2 <b>System</b> Analysis	185
A.1.3 <b>Convergence_Block</b> class interfaces	185
A.2 <b>Port-based</b> classes	186
A.2.1 <b>Port</b> , <b>Input_Port</b> and <b>Output_Port</b> class interface functions	186
A.2.2 <b>Process_Output_Port</b> and <b>Process_Input_Port</b> class interface functions	187
A.2.3 <b>Signal_Input_Port</b> and <b>Signal_Output_Port</b> class interface functions	189
A.2.4 <b>Energy_Input_Port</b> and <b>Energy_Output_Port</b> class interface functions	190
A.3 <b>Stream</b> classes	190
A.3.1 <b>Stream</b> class interface functions	190
A.4 <b>Variable-based</b> classes	190
A.4.1 <b>Variable</b> class interface functions	190
A.4.2 <b>Derivative</b> class interface functions	192
A.4.3 <b>Equation</b> class interface functions	192
A.4.4 <b>Equation_Set</b> and <b>Dynamic_Set</b> class interface functions	193
A.5 <b>Physical Property</b> Classes	195
A.5.1 <b>Component</b> class interface functions	195
A.5.2 <b>User_Component</b> class interface functions	196
A.5.3 <b>Component_Set</b> class interface functions	196
A.5.4 <b>General_Component_Mixture</b> class interface functions	197
A.5.5 <b>Ideal_VLE</b> class interface functions	200
A.6 <b>Mathtool</b> class interface functions	200
<b>Appendix B: Flash Class Member Functions</b>	202
B.1 <b>Constructor</b>	202
B.2 <b>Port Setup</b>	205

B.3 Connection Functions	205
<b>Appendix C: Tennessee Eastman Unit Models</b>	<b>207</b>
C.1 Mixer Model	207
C.2 Reactor Model	208
C.3 Separator Model	210
C.4 Stripper Model	211
C.5 Nomenclature	212
<b>Appendix D: Tennessee Eastman Flowsheet Definition</b>	<b>214</b>
<b>Appendix E: Fermentation Model Parameters</b>	<b>221</b>