

# MODELING AND SIMULATION IN CHEMICAL ENGINEERING

ROGER G. E. FRANKS

SENIOR CONSULTANT: ENGINEERING COMPUTATION AND ANALYSIS  
ENGINEERING DEPARTMENT

E. I. DU PONT DE NEMOURS & CO., INC.

1972

---

WILEY-INTERSCIENCE,

A DIVISION OF JOHN WILEY & SONS, INC.

NEW YORK | LONDON | SYDNEY | TORONTO

TECHNISCHE HOCHSCHULE DARMSTADT	
Fachbereich 1	
<u>Gesamtbibliothek</u>	
<u>Betriebswirtschaftslehre</u>	
Inventar-Nr. :	37.560
Abstell-Nr. :	A14/781
Sachgebiete:	1.6.9.18
	1.6.9.2

# CONTENTS

CHAPTER I	INTRODUCTION	1
	1-1 Equations, 6	
	1-2 Continuous System Simulations, 14	
	1-3 Dynamic Process Simulations, 15	
CHAPTER II	NUMERICAL SOLUTION OF ALGEBRAIC EQUATIONS	18
	2-1 Explicit and Implicit Equations, 18	
	2-2 Partial Substitution, 24	
	2-3 Wegstein Method for Algebraic Convergence, 26	
	2-4 Example: Beattie-Bridgeman Equation, 28	
	2-5 Newton-Raphson Convergence, 29	
	2-6 Example: Newton-Raphson Method, 31	
	2-7 Implicit Systems of Higher Order, 33	
	2-8 Arbitrary Function Generation (FUN1), 34	
	2-9 Use of FUN1 Subroutine, 37	
	2-10 Two-Dimensional Function (FUN2), 38	
CHAPTER III	NUMERICAL SOLUTION OF DIFFERENTIAL EQUATIONS	45
	3-1 Ordinary Differential Equations, 45	
	3-2 First-Order Method (Simple Euler), 47	
	3-3 Relationship Between Error and Increment Size, 49	
	3-4 FORTRAN Program, 52	
	3-5 Second-Order Integration, 55	

- 3-6 Subroutine INT, 56
- 3-7 Subroutine INTI, 58
- 3-8 Fourth-Order Runge-Kutta Method, 59
- 3-9 General Arrangement of Main Program, 61
- 3-10 Subroutine PRNTF, 63
- 3-11 Subroutine PRNTRS, 65
- 3-12 Programming Example Using INT System, 65
- 3-13 Accuracy of Integration, 67
- 3-14 Stability of Numerical Integration, 70
- 3-15 Variable Step-Size Methods, 73
- 3-16 Algebraic Solution of Derivative Equations, 76
- 3-17 Subroutine DER, 78

CHAPTER IV BASIC MODELING 82

- Case 4-1 Simple Hydraulic Tank, 84*
- Case 4-2 Variable Flow Hydraulic Tank, 86*
- Case 4-3 Enclosed Tank, 88*
- Case 4-4 Adiabatic Compression in Gas Space, 90*
- Case 4-5 Mixing Vessel, 93*
- Case 4-6 Mixing with Reaction, 94*
- Case 4-7 Reversible Reaction, 96*
- 4-8 Simultaneous Mass and Energy Balances, 96
- Case 4-8 Example: Steam Jacketed Vessel, 96*
- Case 4-9 Multiple Feeds to Jacketed Vessel 99*
- 4-10 Boiling, 101
- Case 4-10 Continuous-Flow Boiling System and Program, 105*

CHAPTER V MULTICOMPONENT VAPOR LIQUID EQUILIBRIUM 114

- 5-1 General Structure for DYFLO, 114
- 5-2 Subroutines ENTHL(I) and ENTHV(I), 116
- 5-3 Subroutine TEMP(I, L), 117
- 5-4 Vapor Liquid Equilibrium, 119
- 5-5 Dew-Point Calculation, 124
- 5-6 Generalized Phase Transformation, 125
- 5-7 Subroutine FLASH, 127
- 5-8 Adiabatic Flash, 131
- 5-9 Boiling Operations, 131
- 5-10 Partial Condenser (PCON), 132
- 5-11 Single-Phase Holdup (HLDP), 135

5-12	Boiler with Holdup, 138	
5-13	Output Editing: Subroutines PRL and RPRL, 141	
5-14	Case 5-1: Batch Distillation Example, 142	
5-15	Case 5-2: Two-Stage Batch Distillation, 146	
<b>CHAPTER VI</b>	<b>REACTION KINETICS</b>	<b>152</b>
6-1	General Modeling Scheme, 152	
6-2	Liquid Phase CSTR, 154	
6-3	Radical Kinetics, 160	
6-4	Heterogeneous Kinetics, 164	
6-5	Semibatch Solution Copolymerization, 173	
6-6	Particle Age Distribution in CSTR, 185	
<b>CHAPTER VII</b>	<b>FLUID FLOW</b>	<b>195</b>
7-1	Gas Flow Systems, 195	
	<i>Example 7-1</i> 197	
7-2	Hydraulic Transients, 197	
	<i>Example 7-2</i> 198	
	<i>Example 7-3</i> 200	
	<i>Example 7-4</i> 205	
<b>CHAPTER VIII</b>	<b>STAGED OPERATIONS</b>	<b>212</b>
8-1	Subroutine SPLIT (J, K, M, RKJ), 212	
8-2	Subroutine SUM (I, J, K, L), 213	
8-3	Example: Countercurrent Extraction, 214	
8-4	Computer Program, 219	
8-5	Distillation Columns, 223	
8-6	Multicomponent Separations, 225	
8-7	Generalized Column Program, 229	
8-8	Stiffness Aspects of Column Simulation, 229	
8-9	Subroutine STAGE, 231	
8-10	Feed Stage Subroutine STGF, 233	
8-11	Sidestream Stage Subroutine STGS, 236	
8-12	Column Bottoms Subroutine BOT, 237	
8-13	Subroutine STGH, 240	
8-14	Reboiler, 244	
8-15	Subroutine REB (A, H, CV, WC, JF, JB), 247	
8-16	DYFLO Simulation of a Distillation Column, 249	

CHAPTER IX	DISTRIBUTED SYSTEMS	260
	<i>Example 9-1</i> Countercurrent Heat Exchanger, 260	
	<i>Example 9-2</i> Pipeline Gas Flow, 263	
	<i>Example 9-3</i> 266	
	<i>Example 9-4</i> Flasher Design, 271	
	<i>Example 9-5</i> Tubular Reactor, 277	
	9-6 Condensation, 282	
	<i>Example 9-6</i> Condensation of a Pure Vapor, 282	
	<i>Example 9-7</i> Condensation of Multicomponent Vapors, 287	
	<i>Example 9-8</i> Multicomponent Condensation, 291	
	<i>Example 9-9</i> 294	
	<i>Example 9-10</i> Split Boundaries, 297	
	9-10 Steady-State Heat Exchanger for DYFLO Library, 299	
	<i>Example 9-11</i> Tubular Reactor, 302	
	<i>Example 9-12</i> Serial Integration, 306	
CHAPTER X	PARTIAL DIFFERENTIAL EQUATIONS	317
	<i>Example 10-1</i> Insulated Metal Bar, 318	
	<i>Example 10-2</i> Shell and Tube Heat Exchanger, 324	
	<i>Example 10-3</i> Underground Thermal Transients, 331	
	<i>Example 10-4</i> Laminar Flow Velocity Distribution, 336	
	<i>Example 10-5</i> Dynamic Simulation of a Fixed Bed Reactor, 339	
	<i>Example 10-6</i> Polymer Kinetics, 346	
CHAPTER XI	PROCESS CONTROL	356
	11-1 Basic Control Configuration, 356	
	11-2 Sensing Element: First-Order Transfer Function TFN1, 357	
	11-3 Second-Order Transfer Function, 359	
	11-4 Controllers, 361	
	11-5 Control Elements, 369	
	<i>Example 11-6</i> Batch Kettle Reactor Control, 372	
	<i>Example 11-7</i> Centrifugal Compressor Surge Control, 376	
	11-8 Distillation Column Control, 391	

APPENDIX A	Summary of INT and DYFLO Subroutines	399
APPENDIX B-1	Listing for Print Subroutine PRL	403
APPENDIX B-2	Listing for Repeat Print Subroutine RPRL	404
APPENDIX B-3	Listing for Subroutine INT	405
APPENDIX B-4	Listing for Subroutine INTI	405
APPENDIX B-5	Listing for Subroutine NRCT	406
APPENDIX B-6	Listing for Subroutine START	406
APPENDIX C	Implementation of INT and DYFLO	407
Index		409