Teach Yourself the Basics of Aspen Plus

RALPH SCHEFFLAN
TEACH YOURSELF
THE BASICS OF
ASPEN PLUS™
TEACH YOURSELF
THE BASICS OF
ASPEN PLUS™

RALPH SCHEFFLAN
Chemical Engineering and Materials Science Department
Stevens Institute of Technology
To Ruth
CONTENTS

PREFACE xiii

1 INTRODUCTION TO ASPEN PLUS 1

1.1 Starting Aspen Plus / 2
1.2 Graphic Users Interface / 3
1.3 Next Button / 4
1.4 Setup Specifications Display / 5
1.5 Simulation Options / 6
1.6 Units / 6
1.7 Components / 8
1.8 Properties / 10
1.9 Streams / 12
1.10 Blocks / 14
1.11 Viewing Results / 14
1.12 Object Manager / 16
1.13 Plotting Results / 17
References / 19

2 PROPERTIES 21

2.1 Pure Component Data Banks / 21
2.2 Property Analysis / 24
2.3 Property Estimation / 25
CONTENTS

2.4 Workshops / 34
References / 35

3 THE SIMPLE BLOCKS 37

3.1 Mixer/Splitter Blocks / 37
3.1.1 Mixer Block / 37
3.1.2 Fsplit Block / 38
3.2 Simple Separator Blocks / 39
3.2.1 Sep Block / 40
3.2.2 Sep2 Block / 41
3.3 Some Manipulator Blocks / 42
3.3.1 Dupl Block / 42
3.3.2 Mult Block / 44
3.4 Workshops / 45

4 PROCESSES WITH RECYCLE 49

4.1 Blocks with Recycle / 50
4.2 Heuristics / 53
4.3 Workshops / 54
References / 58

5 FLOWSHEETING AND MODEL ANALYSIS TOOLS 59

5.1 Introduction to Fortran in Aspen Plus / 59
5.2 Basic Interpreted Fortran Capabilities / 60
5.2.1 Primary Fortran Operators / 61
5.2.2 Precedence of Calculations / 61
5.2.3 Statement Format / 62
5.2.4 Program Logic Control / 62
5.3 Sensitivity Function / 63
5.4 Design Specification / 65
5.5 Calculator Function / 67
5.6 Transfer Function / 69
5.7 Workshops / 71
References / 72

6 THE DATA REGRESSION SYSTEM 73

6.1 Parameters of Equations of State / 74
6.2 Parameters of Activity Coefficient Equations / 76
6.3 Basic Ideas of Regression / 77
6.4 Mathematics of Regression / 80
6.4.1 Newton–Raphson Method for Solution of Nonlinear Equations / 80
6.4.2 Direct Optimization of an Objective Function / 81
6.5 Practical Aspects of Regression of VLE or LLE Data / 82
   6.5.1 Regression of VLE Data / 82
   6.5.2 Regression of LLE Data / 85
6.6 Workshops / 87
References / 90

7 FLASHES AND DECANTER 93
   7.1 Flash2 Block / 93
   7.2 Flash3 Block / 96
   7.3 Decanter Block / 99
   7.4 Workshops / 101
References / 103

8 PRESSURE CHANGERS 105
   8.1 Pump Block / 105
   8.2 Compr Block / 105
   8.3 MCompr Block / 107
   8.4 Pipelines and Fittings / 107
   8.5 Workshops / 109
Reference / 110

9 HEAT EXCHANGERS 111
   9.1 Heater Block / 112
   9.2 Heatx Block / 115
   9.3 Mheatx Block / 118
   9.4 Workshops / 118
References / 121

10 REACTORS 123
    10.1 RStoic Block / 123
    10.2 RYield Block / 125
    10.3 REquil Block / 126
    10.4 RGibbs Block / 128
    10.5 Reactions for the Rigorous Models / 129
        10.5.1 Equilibrium Class / 130
        10.5.2 Powerlaw Class / 130
        10.5.3 Langmuir–Hinshelwood–Hougen–Watson Class / 133
## CONTENTS

10.6 RCSTR Block / 134
10.7 RPlug Block / 135
10.8 RBatch Block / 138
10.9 Workshops / 139
References / 144

### 11 MULTISTAGE EQUILIBRIUM SEPARATORS

11.1 Basic Equations / 145
11.2 The Design Problem / 148
11.3 A Three-Product Distillation Example / 150
11.4 Preliminary Design and Rating Models / 154
   11.4.1 DSTWU / 154
   11.4.2 Distl / 156
11.5 Rigorous Models / 157
   11.5.1 RadFrac / 158
   11.5.2 Extract / 164
11.6 BatchSep / 167
11.7 Workshops / 170
References / 173

### 12 PROCESS FLOWSHEET DEVELOPMENT

12.1 Heuristics / 175
12.2 Example: The Production of Styrene / 176
12.3 A Model with Basic Blocks / 177
12.4 Properties / 177
12.5 Rigorous Flash and Decanter / 178
12.6 Analyzing the Rigorous Distillation / 181
12.7 Integrating the Rigorous Distillation Into the Flowsheet / 181
   12.7.1 Selection of a Tear Stream / 183
   12.7.2 Sequence of Calculations / 183
12.8 Reactor Feed / 183
12.9 Miscellaneous Considerations / 185
12.10 Workshops / 185
Reference / 189

### 13 OPTIMIZATION

13.1 Optimization Example / 192
13.2 Workshops / 195
References / 198
14  COMPLEX EQUILIBRIUM STAGE SEPARATIONS  199
   14.1  Energy Integration Applications / 199
   14.2  Homogeneous Azeotropic Distillation / 202
   14.3  Extractive Distillation / 203
   14.4  Heterogeneous Operations / 205
   14.5  Workshops / 207
References / 211

INDEX  213
PREFACE

During my years working as a chemical engineer in development laboratories, process engineering groups, and plant startup and support operations, the most frequently referenced documents were process flow diagrams (PFDs), which contain the material and energy balances and the basic process design information. Equally important were process and instrument diagrams (P&IDs), which contain details of all equipment, all controls, all instruments, and all lines (i.e., process, instrument, and utilities). Process simulation software is an excellent tool for producing high-quality PFDs, and when integrated with computer-aided design software, facilitates the production of P&IDs. There are several process simulation software systems available to the chemical engineering community, and Aspen Plus is arguably the most popular.

Teach Yourself the Basics of Aspen Plus™ evolved from two graduate courses that I taught at Stevens Institute of Technology over the past 20-odd years. The first course, ChE662, is an introduction to steady-state chemical process simulation, which is usually taken by graduate students and is organized around a series of workshops that introduce Aspen Plus functionality. Occasionally, undergraduates are enrolled and typically experience difficulties in the thermodynamics of phase equilibrium and parameter estimation, due to limitations in their undergraduate courses. The second course, ChE612, deals with the analysis and design of complex equilibrium stage processes and with difficult multicomponent problems such as, extractive distillation systems. Over time, the course evolved from the use of stand-alone two- and three-phase flashes, decantation, and two-phase distillation software, to their equivalent blocks in Flowtran and later, Aspen Plus.

The idea for this book originated from my observations of students in these courses. I noted that after an initial period dedicated to learning the basics of how to navigate, locate material, and enter data into Aspen Plus, students could proceed through the exercises, within the workshops, mostly on their own. I would give an introductory lecture for each subject studied, show examples, and provide individual help on the