

Introduction to Chemical Engineering Computing, 2nd edition, Bruce A. Finlayson, Wiley (2012)

The following web sites can be used to obtain material from Wiley. It includes the keys to the problems (useful to your Teaching Assistant), and the figures in the book (useful to you when you go to class). Go here to learn what is in the book:

<http://www.wiley.com/WileyCDA/WileyTitle/productCd-1118888316.html>

and here to fill out the form

<http://www.wiley.com/WileyCDA/Section/id-821455.html>

Program Objectives. List of problems, which program they use, and what students can learn

Chapter 2

Programs used

Excel: example, 3, 4, 5

MATLAB: examples, 4, 5

Aspen: examples, 2, 9

Program not specified: 6, 7, 8

Problems illustrating specific physical results

Compare equations of state: 2, 4, 5, 7, 8, 9

Computer techniques

Compare Excel and MATLAB on same problem: 1

Compare those with Aspen Plus: 2

Program Newton-Raphson method: 10, 11

Chapter 3

Programs used

Mainly Aspen Plus; Excel and MATLAB are used in one example and 1

Any program: 2

Aspen Plus: example, 3, 5-13

Problems illustrating specific physical results

Compare predictions by different equations of state: example, 8-10, 13

Different equations of state:

 Peng-Robinson: 5, 6

 SRK: 5, 6, 13

 RKSWs: 7

NRTL: 9, 13
UNIQUAC: 10, 11, 13
Wilson: examples, 10, 12
Compare predictions with data: examples, 7, 10-13
Theory of equations: 4
Correlation in range of desired use: 14, 15

Computer techniques

Newton-Raphson: 16, 17

Chapter 4

Programs used

Excel: example, 1, 2, 7, 12
MATLAB: example, 1, 2, 7, 13, 14
Aspen Plus: example, 3-11
Compare Excel, MATLAB: 1, 2
Compare Aspen Plus with 1 and 2: 3, 4
Compare Excel, MATLAB, Aspen Plus: 7, (10, 12, and 13)
Compare Excel and Aspen Plus: (11, 14)

Problems illustrating specific physical results

Multiple reactions: examples, 5, 6, 10, 11

Computer techniques

Newton-Raphson: 15, 16

Chapter 5

Programs used

Problems 1-8 use either Excel or Aspen Plus or both, and involve iteration with recycle streams

Only Aspen Plus is used for Problem 9

Chapter 6

Programs used

All examples and problems use Aspen Plus.

Problems illustrating specific physical results

Multi-component distillation, short-cut: examples, 1, 3-5, 9, 10

Multi-component rigorous method: example, 2-5, 9, 11

Compare DSTWU & RadFrac (1,2), 3, 4, 5, 9

Packed bed: example, 7, 8

Sensitivity: example of equilibrium reactor

Design specs: example of equilibrium reactors

Thermodynamic choices

RKS – first example, short-cut distillation

Chao-Seader – second example, rigorous distillation; gas plant

Wilson: 9

Peng-Robinson: 10, 11

NRTL: 10, 11

Comparison to NIST database: 10

Economics of distillation column: 6

Chapter 7

Programs used

All problems are solved with Aspen Plus.

Problems illustrating specific physical results

Flowsheets, convergence, test convergence, 2-8, 10, 11

Test thermo from NIST database: 9

Costs, optimization, control: examples

IGCC: 9, 10

Biodiesel: 12

Corn stover to ethanol: 13-18

Derivation: 1

Chapter 8

Programs used

Study	MATLAB	Comsol	Aspen	Excel
Steady Plug flow	examples, 1, 2, 6, 7, 8, 11, 12, 16, 17, 19, 20	examples, 1, 2, 16	example	22
Steady CSTR	examples, 3, 4, 5, 10			example, 3, 4, 5
ODE	14, 18			
CSTR	examples, 13, 15, 21			

Problems illustrating specific physical results

Multiple steady states and transient CSTRs: examples, 10, 13, 15

Stiff problems as temperature increases: examples, 15, 17

Mole changes: example

Mass transfer: example and 9

Computer techniques

Newton-Raphson method for algebraic equations: 21

Integrate ODEs with Euler and Runge-Kutta methods: 19, 22

Chapter 9

Programs used

Comsol: examples, 1-19, 21-22, 24-29, 34

MATLAB: examples, 2, 10, 12, 15, 19, 20

Excel, using numerical methods: 30-32

Most of the problems in Chapter 9 use Comsol. There are some that are picked to specifically compare methods.

1. The pipe flow example of Eq. (9.26) is solved in the text using Comsol; problem 9.31 uses Excel with the finite difference method.
2. The transient heat transfer problem of Eq. (9.28) is solved in the text using both Comsol and MATLAB. Problem 9.32 uses Excel with the finite difference method in space and the Euler method in time.
3. The Boltzmann equation is solved in Problem 9.17 using Comsol and in Problem 9.30 using Excel. In Excel this involves a circular reference.
4. Problems comparing Comsol and MATLAB are:
 - a. The example of Eq. (9.22) is solved with both Comsol and MATLAB.
 - b. 9.2 and 9.10, reaction-diffusion
 - c. 9.12, transient heat transfer
 - d. 9.15, electrical field
 - e. 9.19, including the shear stress

Problems illustrating specific physical results

Effect of a viscosity that depends on shear rate: examples and problems 20, 23, 25

Strong convection: chromatography example, 26

Effect of discretization: example of non-Newtonian flow

Effect of linearizing a non-linear function: 15, 17, 18, 27

Effect of inertia in spinning: 21, 22

Semiconductor: 16

Shear stress in flow: 19

Multiple solutions and stability: 4, 8, 9

Computer techniques

Parametric solutions: Example of reaction-diffusion, 20

Use of constraints in Comsol: 24

Circular references in Excel: 30

Finite difference methods: 30, 31, 33 and Euler method, 32

Chapter 10

Programs used

All the problems use Comsol

Problems illustrating specific physical results

Entry flow – Newtonian: example and 1; non-Newtonian: example and 2, 3

Microfluidic flows

T-sensor in 2D: example, 8 (2D), 16 (3D), 27 (2D)

Pressure drop in 2D: 17, 19 (contraction), 21 (H- and T-sensor), 23 (cross), 24 (bend)

Pressure drop in 3D: 18 (curved pipe), 20 (contraction), 23 (cross), 24 (bend), 25 (H-sensor), 26 (serpentine)

Turbulent flow: example and 15

Transient flow: example and 5, 6

Orifice flow: example and 7

Serpentine: example, 26

Coupling variable, 2D ->3D: example

Viscosity comparisons: 4

Boundary layer flow: 9

Drag on sphere: 10 ($Re = 0$), 11 ($Re = 1$ to 100), 12 (in tube), 13 (compare with data)

Drag on cylinder: 14

Microscopic porous media: 22

Hole pressure: 28 in 2D, 29 in 3D

Compare 2D and 3D: T-sensor (8, 16); H-sensor (21, 25); cross (23); bend (24); hole pressure (28,29)

Linear coupling – example, 20, 24, 25, 26

Chapter 11

Programs used

All problems use Comsol except for 30 and 31 (Excel) and 32 (MATLAB).

Problems illustrating specific physical results

Heat transfer in two dimensions: examples (2), 1, 6, 30, 31

Heat transfer with flow: 7-11

Microfluidics, convection and diffusion: 2D: T-sensor example, 16-18, 28, 29; 26 (bend),
3D: 22 (pipe), 23 (H-sensor), 24 (serpentine), 25 (T-sensor), 27 (scale-up)

Use of the material browser to get fluid properties: 6

Viscosity depending upon concentration: example

Flow with viscous dissipation, 19

Chemical reaction: 4, 5, 14

Reaction with flow: 12, 13

Transient reaction 15

Wall reaction: example

Electrochemical: 2

Scale-up: 27

Difference in 2D and 3D flow: channel, 20,21; T-sensor: 16,25; bend: 26; H-sensor: 17

Computer techniques

Linear coupling example, 20-21, 23, 24, 25, 26, 27

Mathematical singularity: 3

Finite difference method in 2D, using Excel: 30 and 31

Finite difference method in space and ODE solver in time using MATLAB: 32

Appendix E

Mathematical Derivations

Prove stability: 1, 2 (cylindrical and spherical), 3 (2D and 3D)

Prove truncation error: 4

Evaluate solution accuracy using the residual: 5