

SUMMARY OF COMPUTER PROGRAMS

Several programs are furnished with the text to help you learn the material and to assist in repetitive and/or complex calculations. Programs are available for: TI and HP calculators, IBM PC-compatible computers, and Microsoft® Excel. There is some duplication of capabilities among the different operating platforms in the sense that programs for the personal computers may also be available for the calculators. To install the programs on your computer or calculator, see Sections A.6 and A.7. The software is periodically updated. Visit the website for the latest version of the software and appendix.

A.1 HP48GII CALCULATOR PROGRAMS

Several programs are available in the file THRMO within the HP directory. The programs are organized in directories grouped as: EQ.S, for several commonly applied equations (e.g., C_p^{ig} , P^{sat}) that use the solver function; PRI, for Peng-Robinson calculations with one component; VLK for vapor-liquid K-value calculations, including bubble point pressure of multicomponent mixtures by the Peng-Robinson equation (k_{ij} specified by user for up to 5 components). Specifics for each program are presented below in accordance with the appropriate directory. See Section A.10 if you are a first-time HP48gII user.

EQ.S (Push the key below this heading to enter this directory. These are referred to as “menu keys.”)

1. INTRP—simple linear interpolation

Push the menu key below **INTRP**, then **rightshift-NUM.SOLVE-ENTER** to start the equation solver. The menu provides input slots for y_1 , y_2 , x_1 , x_2 , and the desired value of x . Fill in as appropriate and move the cursor until the slot for y is highlighted. Press the menu key labeled **SOLVE**.

Verification of program: $Y_2 = 2$; $Y_2 = 7$; $X_1 = 1$; $X_2 = 6$; $X = 4$; $Y = 5$.

2. IG—this is a directory with ideal gas properties as a function of T and P.

Push the menu key below **IG**. The following variables are in the directory.

Heq, Seq—Equations for Solver to use to calculate ΔH , ΔS , T or P.

T2, T1, P2, P1—Temperature in K, and P for states 1 and 2. (Pressure units don't matter for ΔS as long as they are the same for both states, however see V1, V2).

V1, V2—molar volumes at state 1 and 2, using $R = 8.314$ J/mol-K. These menu keys give molar volume in cm^3/mol if T in K and P in MPa.

ΔH , ΔS —quick calculation of ΔH and ΔS from variables stored in T1, T2, P1, P2 and C_p .

CPA, CPB, CPC, CPD—heat capacity constants from the appendix.

CP2—calculated value of C_p at T2.

ΔH_{eq} , ΔS_{eq} —The last value of ΔH and ΔS found by Solver, *not necessarily* the values corresponding to the current state variables.

EQ—The last equation used by Solver.

To use Solver, press **rightshift-NUM.SOLVE-ENTER**, and use the **CHOOSE** menu key, followed by the arrow keys to select Heq or Seq. Fill in as appropriate and move the cursor until the slot for desired unknown is highlighted. Press the menu key labeled **SOLVE**.

Verification of program: T1 = 273.15; P1 = 0.101325; T2 = 500; P2 = 0.7; Data for methane: CPA = 19.25; CPB = 5.213E-2; CPC = 1.197E-5; CPD = -1.132E-8; Gives V1 = 22412.7; V2 = 5938.6; $\Delta H = 9194.7$; $\Delta S = 8.0501$

3. ANTOI—calculation of vapor pressure given Antoine coefficients

Push the menu key below **ANTOI**, then **rightshift-NUM.SOLVE-ENTER** to start the equation solver. Use the **CHOOSE** menu key to select the natural logarithm or common logarithm equation. The menu provides input slots for A , B , C , and the desired value of T . Fill in as appropriate and move the cursor until the slot for P^{sat} is highlighted. Press the menu key labeled **SOLVE**. Be a little careful about units on this one and especially careful about the limitations on the temperature range for the Antoine coefficients.

Verification of program: Water: A = 8.07131; B = 1730.68; C: 233.426; T = 100; PSAT = 760.09.

4. V.P—calculation of vapor pressure according to the shortcut vapor pressure equation.

Push the menu key below **V.P**, then **rightshift-NUM.SOLVE-ENTER** to start the equation solver. The menu provides input slots for T_c , P_c , ω , and the mole fraction value of T . Fill in as appropriate and move the cursor until the slot for P^{sat} is highlighted. Press the menu key labeled **SOLVE**. Enter P^{sat} and highlight T to solve for T^{sat} at a given pressure. This equation is accurate to within 10% when $0.5 < T_r < 1.0$.

Verification of program: PC = 3.797; TC = 425.2_K; $\omega = 0.193$; PSAT = 1.88; T = 383.18_K

5. WT%—calculation of weight fraction given mole fraction or vice versa.

Push the menu key below **WT%**, then **rightshift-NUM.SOLVE-ENTER** to start the equation solver. The menu provides input slots for M_1 , M_2 , and the mole fraction value of X_1 . Fill in as appropriate and move the cursor until the slot for weight fraction W_1 is highlighted. Press the menu key labeled **SOLVE**. Enter W_1 and highlight X_1 to solve for mole fraction given weight fraction.

Verification of program: (P_2O_5 is 43.66 wt% P and 28.57 mol% P). M1 = 31; M2 = 16; X1 = 0.2857; W1 = 0.4366.

PRI — PVT and departure properties by the Peng-Robinson equation

1. INCRT—run this first to enter critical constants and the acentric factor. Example: For water, $T_c = 647.3$, $P_c = 22.12$, $\omega = 0.344$ used in examples.
2. PVTF—gives volume(cm^3/mole) and fugacity(MPa). Prompts for P and T , then offers the user the cubic equation real root(s) for the compound's constants previously entered by INCRT or REF(see below). Example: for superheated steam at 0.01 MPa and 323 K, run INCRT (or REF), then press PVTF, enter $T = 323$, $P = 0.01$, choose the vapor root ($Z = 0.9987$), gives $V = 268,208 \text{ cm}^3/\text{mol}$, $f = 0.00999 \text{ MPa}$. Scroll up to review the Z value.
3. ZALT—allows selection of alternate roots and reruns PVTF without changing P, T . This program is not necessary if you know which root to use. For multiple roots, the center root is unstable, and among the others, the most stable root is the one with the lower fugacity.
4. DEPFUN—calculates U, H, S departures for the last root selected from PVTF. Example: following the PVTF example above, press DEPFU to find $U - U^{ig}/RT = -0.00196$, $H - H^{ig}/RT = -0.0032$, $S - S^{ig}/R = -0.00196$.

Property Programs

5. REFS—enters the critical properties, acentric factor, and heat capacity constants for the compound and the reference state temperature, pressure and state of aggregation (vapor or liquid root). After running this program, run PVTF to set the P and T of interest and select the root (optionally followed by ZALT). Example: For water, $T_c = 647.3$, $P_c = 22.12$, $\omega = 0.344$, $CPA = 32.24$, $CPB = 1.924\text{E-}3$, $CPC = 1.055\text{E-}5$, $CPD = -3.596\text{E-}9$, $T_{ref} = 273$, $P_{ref} = 0.0006$, choose liquid reference state ($Z = 5.5\text{E-}6$), departures at reference state are displayed (e.g. $U - U^{ig}/RT = -19.675$). Then run PVTF.
6. UHSG—calculates U, H, S, G using the last root selected from PVTF. This program uses the heat capacities and reference state entered by the REF program. Example: After running REF and PVTF as above, press UHSG to find: $U = 45918 \text{ J/mol}$, $H = 48600 \text{ J/mol}$, $S = 152.261 \text{ J/mol-K}$, $G = -580 \text{ J/mol}$. Scroll up to review P, T, V .

Comparing the calculations with the steam tables, at the last state, $S = 152.26 \text{ J/mole-K} = 8.4589 \text{ J/g-K}$; at the same pressure and 100°C (373), we obtain $S = 8.7313 \text{ J/g-K}$. The value for ΔS is then 0.2724 J/g-K . This compares to a value of 0.2730 from a typical steam table. This may be a significant error for a design project situation, but accurate enough for many quick, order of magnitude calculations.

 γ —activity coefficients by the van Laar equations

1. VLA—van Laar A_{ij} calculation given activity coefficients of a binary solution at a single composition.
Hit the menu key labeled VLA to input the values of activity coefficients, γ_1 and γ_2 , and desired composition of component 1, x_1 , A_{12} and A_{21} are displayed on the screen.
2. VLAR—van Laar activity coefficient calculation given A_{12} and A_{21} of a binary solution.
Hit the menu key labeled VLAR to input the values of A_{12} and A_{21} and desired composition of component 1, x_1 , γ_1 and γ_2 are displayed on the screen.

PRMIX—vapor-liquid K-ratios, and bubble point pressure for mixtures by the Peng-Robinson equation. The number of components must be less than or equal to five.

1. INCRT—input critical properties of components for Peng-Robinson and bubble-point calculations.

Hit the menu key labeled **INCRT** to input the number of components, critical temperatures (type all critical temperatures in a row with a blank space between each), critical pressures, acentric factors, and binary interaction coefficients (k_{ij} 's). For critical pressures, temperatures, and acentric factors, type all values sequentially with a blank space between. For the k_{ij} 's, the first row gives values for interactions with component 1, the second row for component 2, and so forth. The value of 0 should be entered for the k_{ij} of each component with itself. To start a new row, hit the rightshift-(down & left arrow). **You must run this program before you can run BPIS, or KVAL, or BUBP.** Example: nitrogen + methane. Number of components = 2, Tc = [126.2 190.2, (note the space between the two values), Pc = [33.94 46, w = [.04 .011, K = [[0 0 0 0. (The matrix is entered row by row. You can type the 0's for the k_{ij} 's straight in or include the line-feed to help you keep it straight for a bigger matrix. The result is the same.)

2. BPIS—bubble point pressure of an ideal solution from the shortcut vapor pressure equation. (Run INCRT first.)

Hit the menu key labeled **BPIS** to input the value of T and desired composition of all components. P is displayed on the screen. You must run this before running BUBP the first time. Example: nitrogen + methane at 100K, $x = [.5 .5, P = 4.097$ bars.

3. KVAL—vapor-liquid K-ratios from the Peng-Robinson equation given estimated phase compositions. (Run INCRT first.)

Hit the menu key labeled **KVAL** to input the values of T and desired compositions of all components in the liquid, x , and all components in the vapor, y . This calculation actually assumes that all binary interaction coefficients are zero. It takes a few seconds.

4. BUBP—bubble point pressure from the Peng-Robinson equation.

You must run INCRT and then run BPIS at least once to get an initial estimate of the pressure before running this program. Further calculation, as for phase envelopes, can proceed without calling BPIS if the previous result for the pressure provides a reasonable guess for the pressure at the new conditions. Hit the menu key labeled **BUBP** to input the values of T and desired compositions of all components in liquid, x . This calculation treats all binary interaction coefficients as given. It may take a minute. By changing values of k_{ij} , azeotropes can be characterized and studied much like the van Laar equation. Example: nitrogen + methane at 100K and $x = [0.5 0.5, K1 = 1.89, K2 = 0.11, P = 4.250$ bars.

UNIFAC—Activity coefficients for mixtures of user-specified chemical structures by the UNIFAC group contribution method. The number of components must be less than or equal to five but components may have any number of functional groups each.

1. INIT—initial specification of number of components and their chemical structure.

Hit the menu key labeled **INIT** to input the number of components and the chemical structure of each component. After you enter the number of components you will be prompted for the chemical structure of component 1 ("COMP1"). Type the number of occurrences of a given functional group, then press the menu key for that functional group (e.g., for pentane, press **3 [CH2] 2 [CH3][INCPT]**). Some functional groups are listed on later windows that can be viewed by pressing the key **[NXT]**. When all functional groups have been specified for that component, press **[NXT]** to return to the first window and press **[INCPT]** to input that component. After a few seconds, you will be prompted for the next component. Continue until all components have been specified. (E.g., for methanol, press **[NXT] 1 [MEOH] [NXT] [NXT] [INCPT]**).

2. CONC—specification of concentration and output of activity coefficients. Run NEWT before this program to change the temperature.

Hit the menu key labeled **CONC** to input the mole fractions of components. At the x:[] prompt, type the mole fractions of the components, separated by spaces. (E.g., x:[0.5 0.5]) After about 20–60 seconds the activity coefficients are displayed (e.g., 1.822, 1.789 for the pentane + methanol system at 80°C).

3. **NEWT**—specification of a new temperature.

Hit the menu key labeled **NEWT** to change the value of temperature. At the TDEGC: prompt, type the new temperature in degrees Celsius. After about 25 seconds the initial menu will reappear. The activity coefficients are not strong functions of temperature, so it may be sufficient to perform several calculations with the same value of temperature. Press **CONC** to recalculate the activity coefficients, or **INIT** to enter new components.

4. **TDEGC**—Use **TDEGC** to display the current value of temperature.

A.2 TI-85 PROGRAMS

Program PENG is documented in the Word6 file DEPFU4TI.DOC in the TI directory. This program provides *Z* and departure functions for the TI-85. The code is also provided.

A.3 PC PROGRAMS FOR PURE COMPONENT PROPERTIES

See Section A.9 for an introduction to Excel.

PREOS.XLS—(Same capabilities as **PRPURE.EXE**, but superior user interface). An Excel 5.0 workbook for calculating roots to the Peng-Robinson equation at sub and supercritical conditions. Also calculates departure functions and thermodynamic properties. You need to have the following information available:

Critical Temperature (K), Critical Pressure (MPa), Acentric factor

In addition, if you wish to calculate departure functions, you will need ideal gas heat capacity coefficients from Appendix B or Reid, Prausnitz and Poling.

PRPURE.EXE—FORTRAN code for Peng-Robinson equation calculation of vapor pressure, compressibility factor, fugacity, and fugacity coefficients. See the recommendations in Section A.8 regarding execution in a Command Prompt Window. **PRPURE.FOR** is the source code. The program has the same capabilities as **PREOS.XLS**, but advantages for generating an output file for repetitive calculations. Requires same input information as **PREOS.XLS**. See section A.9 for instructions on importing the output files into Excel for plotting, etc. **PRPURE.EPS** is a flowsheet of the program in postscript printer format.

STEAM.XLS—Steam property calculator. Same formulation implemented in Harvey, A. P., Peskin, A. P., Klein, S. A., NIST/ASME Steam Properties, Version 2-1, NIST Standard Reference Data Program, December 1997.

A.4 PC PROGRAMS FOR MIXTURE PHASE EQUILIBRIA

PRMIX.EXE—Compiled program which performs bubble, dew, vapor-liquid flash, and liquid-liquid flash calculations for a multicomponent mixture using the Peng-Robinson EOS. Double-

click the file's icon on file manager or explorer. Components are specified using the index numbers in the endflap. A list is also available on screen during runtime. See the readme file to add more compounds to the database. See the recommendations in Section A.8 regarding execution in a Command Prompt Window.

ESD.EXE—Compiled program analogous to PRMIX.EXE using the ESD (1990) EOS for associating mixtures. See the recommendations in Section A.8 regarding execution in a Command Prompt Window.

ACTCOEFF.XLS—A workbook to calculate activity coefficients as a function of composition for the Margules, van Laar, Regular Solution, UNIQUAC, or UNIFAC models. These spreadsheets may be modified to calculate excess Gibbs energy, fugacities, and P - x - y diagrams.

1. MARGULES—A spreadsheet to use with the MARGULES activity coefficient model.
2. REGULAR—A spreadsheet to calculate VLE for methanol + benzene using van Laar and Scatchard-Hildebrand Theory.
3. UNIQUAC—A spreadsheet to use with the binary UNIQUAC activity coefficient model.
4. UNIQUAC5—A spreadsheet to use UNIQUAC with up to five components and can model LLE.
5. UNIFAC(VLE)—A spreadsheet to use with the UNIFAC activity coefficient model for up to five components to model VLE.
6. UNIFAC(LLE)—Two spreadsheets to use with the UNIFAC activity coefficient model to up to five components to model LLE.
7. ANTOINE—A table of Antoine parameters.

DEWCALC.XLS—Performs a dew temperature or dew pressure calculation for a binary system using activity coefficients and ideal gas phase. This spreadsheet demonstrates how to set up an iterative calculation on a spreadsheet.

GAMMAFIT.XLS—A spreadsheet for fitting activity coefficient parameters. Currently set up for the two-parameter Margules equation. A non-linear least squares technique is used via the Excel solver utility (make sure this has been installed in your PC's version of the Excel program). The spreadsheet can be converted to other activity coefficient models by editing the activity coefficient formulas.

FLSHR.XLS—A spreadsheet to calculate two-phase isothermal flash using Raoult's law. Currently set for a binary system.

IChemT.exe—A chemical theory program for calculating the true mole fractions at a given superficial mole fraction. The equilibrium constants need to be known before using the program. The equilibrium constants for input are the concentration equilibrium constants, which for a vapor phase would be K_y of Eqn. 14.21, which is $K_y = (K_a P^{-\sum v})/K_\phi$.

PRFUG.XLS—Worksheet to calculate component fugacities via the Peng-Robinson equation for up to three components. Useful for understanding mixing rules, and for manually following iterative steps for phase equilibria calculations.

RESIDUE.XLS—spreadsheet with macro for calculating residue curves for homogeneous systems using UNIQUAC for up to three components.

VIRIALMX.XLS—This spreadsheet calculates the second virial coefficient for a binary mixture using the critical temperature, pressure, and volume.

WAX.XLS—A spreadsheet to calculate wax solubilities.

A.5 REACTION EQUILIBRIA

RXNADIA.XLS—Adiabatic reaction temperature calculation for ammonia formation corresponding to the Example in the textbook. Instructions are given as a worksheet in the workbook.

RXNS.XLS—Workbook with spreadsheets used for multiple reaction equilibria in the text. Includes Gibbs energy minimization and simultaneous reaction and phase equilibria. Instructions are given as a worksheet in the workbook.

KCALC.XLS—Workbook to calculate equilibrium constants as a function of temperature.

CL2H2O.XLS—Worked electrolyte example.

A.6 HOW TO LOAD PROGRAMS

Download through the Internet from the website <http://www.egr.msu.edu/~lira/thermtxt.htm>, and follow the posted instructions.

A.7 TRANSFERRING HP PROGRAMS

To transfer programs to an HP48gII you will need either: 1) a classmate who has the programs on their calculator, or; 2) the communications cable that comes with the calculator. If you are transferring from the PC, the textbook software includes the communication program Kermit in the HP subdirectory. If you transfer from a classmate using the built in IR communications in the calculator, see the HP manual instructions. To transfer from the PC to your calculator:

1. Install the cable. It attaches to a serial COM port. You must enter the port number later in the procedure.
2. Change to the PC directory HP containing Kermit and THRMO.
3. Execute Kermit.
Type: set port com2 (or whatever COM port you're using).
Then type: set baud 115200.
4. Turn on your calculator, navigate to the **HOME** directory using **UPDIR** or the **FILES** application.
5. Then press **APPS** and choose "Transfer..." Set "PORT:" to "Wire," "XLAT" to "→255," "CHK" to "3" and set the baud to 115200.
6. Go back to the computer and give the command: SEND thrmo.
7. Quickly press the menu key on the HP48 that corresponds to RECV.
8. You should get a computer screen that notes the number of packets sent, the % delivered, and other vital statistics. The THRMO file takes a couple minutes to transfer.

- 9. Navigate to the **HOME** directory on the HP. If you started Kermit from windows, type “exit” to close the DOS window.

A.8 USING COMPILED FORTRAN PROGRAMS

The programs can be run from Windows by double clicking on them from the File Manager (or Explorer). However, some programs must be able to find input files in the same directory. It is recommended to run them from the Command Prompt Window to prevent the window from closing if execution errors cause the program to terminate. The error messages will remain in the Command Window to help the user trouble-shoot. If the program is started by ‘double-clicking’ the file name, the window will close upon execution errors too quickly for the errors to be displayed.

Running from a Command Window prompt

To keep the window from disappearing upon normal or error termination, the programs should be started from a Command Prompt Window (in WinME or older versions of windows, it is called the MS-DOS window). In WinXP or Win2000, the Command Prompt Window is found by "Start>All Programs>Accessories>Command Prompt". Once this started, move to the folder where the program is stored by using the change directory command "`cd <folder>\<subfolder>`" where the folder names are inserted. Additional subfolders can be appended using additional backslashes. Use "`cd ..`" to move 'up' folders. Once the correct directory is displayed at the command prompt, initiate the program by typing the program name. If you wish to view the folder contents, use the line command '`dir`'.

Depending on the program, there may be a large number of lines that are output to the console window but are not written to an output file. If they scroll off the top of the screen buffer, you may wish to increase the buffer. To increase the number of lines held in the window buffer in Win2000 or WinXP, click the icon in the upper left of the console window title bar, and select 'Properties'. In WinXP, select the 'Layout' tab, and adjust the Screen Buffer Size Height. Restart the program. It is not possible to change the number of lines in older versions of windows that use the MS-DOS window.

Some FORTRAN programs must be run with the drive containing data and output files as the default drive. Before you run the programs, type “dir” at the DOS prompt to be sure the input data files you need are on the default drive. If the directory does not contain the files you need, use “`cd <directoryname>`” to move to the desired directory. Some the output files from PRPURE.EXE are wide. It is recommended that you import wide files into Excel if you wish to print or manipulate them.

A.9 NOTES ON EXCEL SPREADSHEETS

Using Excel spreadsheets

- Start Excel. To open a data file, click on “File” on the menu bar, then choose “Open...” In the resulting dialog box, you can specify the drive for your data files. To print output, you can choose “Printer Setup...” to specify a printer, “Page Setup...” to specify margins, automatic scaling, etc., and “Print preview...” to preview output. To quit Excel and return to Windows, choose “File...”, “Exit.” To exit Windows, repeat the same commands from the File Manager screen.

*.XLS files

These workbooks are a starting point for homework problems. You may need to modify the existing spreadsheet to work a homework problem. The *.XLS files are provided in “document protected” format so that inadvertent modification will not occur. Only the unlocked cells which appear blue on the screen may be modified without turning the document protection off. (To change the document protection, select ‘Protection....’ from the ‘Tools’ menu. No passwords are used on the distributed spreadsheets. To change the protection status of individual cells, choose ‘Cell Protection’ from the ‘Format’ menu when document protection is turned off.) If you have access to other spreadsheet programs (like Lotus or Quattro) which can import Excel files, you may be able to use the Excel spreadsheets on your spreadsheet program. You may lose document or cell protection if you import the spreadsheet into a different spreadsheet program. Excel works like other spreadsheets. To enter a mathematical formula in a cell, start the formula with “=.” Excel enables you to point, click and drag to modify your spreadsheet and produce plots.

HELP! What cells use a calculation? To find out the interdependencies of cells, first unprotect the sheet, then use Tools... Auditing.....

Importing to Excel

Data files from PRPURE, ZCHEM or other programs may be easily imported into Excel 5.0. Output from PRPURE has specifically been delimited with commas to facilitate importing. Excel will recognize it as a Windows ANSI file. Import it as *delimited*, using *commas* to identify fields, *text qualifier* set to “ (double quote), and *treat consecutive delimiters as one* turned off. When prompted, accept the *General* format for importing. If desired, the cell widths can be adjusted after importing, although the default works well for most files. The data can be sorted easily in Excel and nice plots can be generated easily from sorted files. Output from ZCHEM is delimited by spaces, except text is identified with “.

Plotting

To create a graph, place the mouse in a corner of the cell range which you want to plot, hold the left mouse button down and drag the mouse over the cell ranges to be plotted. Release the mouse button to leave the area shaded. To use data in multiple areas that are not contiguous, press Ctrl while you drag the mouse over the second area. The wizards will help you create your plot. Generally the “x-y scatter plot” is the desired plot type. It is recommended that you add the plots on a second spreadsheet when prompted. Click on the portions of the graph to edit. If you get stuck, select ‘Help’ from any menu. Double click on the graph to edit and print.

You can turn on or off lines and/or data markers by *right* clicking on the data set on a plot. Select Format data series...., and follow the menus. To switch the x and y coordinates for a set of data, click the data set, then switch the cell ranges that appear in the formula bar. To add multiple data sets to an existing plot, highlight the data, then Copy...switch to the plot and choose Paste Special...Add cells as new series....and check the “Categories (X values in First Column)” checkbox.

Using Solver with Excel

Excel includes an “add-in” feature called Solver which can be used to solve single or multiple equations. The installation of the feature is optional. If it is installed, it will be listed under the **T**ools... drop down menu. A related feature is called **G**oal Seek..., but it is less powerful since it can

only solve a single objective function. If Solver is not installed, select **A**dd ins... from the **T**ools... menu and follow the on-line instructions for installation. To solve an equation for a single variable, Goal Seek or Solver can be used. We will use Solver since it is the more general tool, and use of Goal Seek is simple if desired, once Solve has been used. **If you are using Solver with a spreadsheet that has been protected, it must first be unprotected using Tools...Protection...**

Suppose we wish to solve

$$x^2 + 2x = 1$$

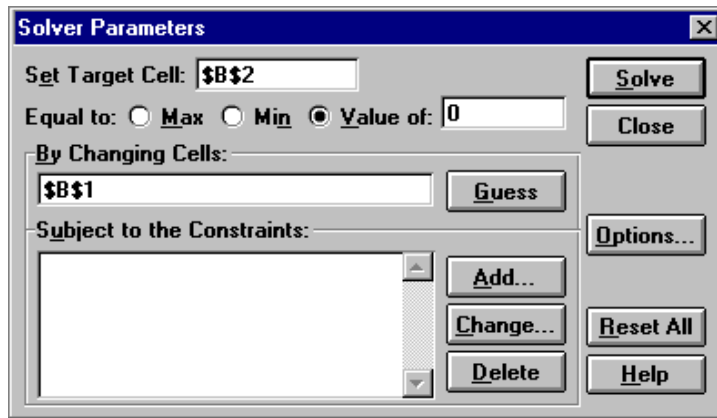
Although the solution may be quickly found by the quadratic formula, a spreadsheet will be created to illustrate the technique that can be applied to more complex problems.

1. Create the following table, entering the labels in column *A* and the initial guess of 0 for *x* in cell *B1*.

	A	B
1	x	0
2	F(x)	

2. Enter the following formula in cell B2: = B1^2 + 2·B1 – 1. (Note that you may click on B1 rather than typing the name as you enter the formula.)
3. Start Solver from the **T**ools... drop down menu. The Solver window will pop up as shown below. The objective function (Target cell) is entered in the top entry box. For this example, enter B2 (or click in the entry box, then click in B2). The radio buttons permit the objective cell to be maximized, minimized, or set to a specific value. In this example, select “Equal to: Value of:” and put the number 0 in the entry box. The **O**ptions... button controls the type of numerical technique that is applied, but we won’t use that now. (For more information on the options, click the Help button from the “Options” subwindow). The next entry box specifies the cells to adjust in the search for the objective function. For this example, enter B1. (For multiple cells you can drag the mouse over the cell ranges.)
4. Click on **S**olve. Look closely at the information box that pops up when Solver has finished. Since numerical techniques are used, Solver may have difficulty finding a solution for poor initial guesses or poorly defined objective functions, and the box notifies of problems in this event. However, we are solving a simple example here, and the answer is quickly found. The answer should be 0.414.
5. If the other root is desired, a different initial guess should be entered in cell B1. Enter the value –2 and re-solve the equation. The answer –2.414 should result.

Excel may also be used to solve multiple equations. Consider the set of equations



$$x^2 + 2y = 10$$

$$x + y = 4$$

Create the spreadsheet

	A	B	C	D
1	x	1	F1	
2	y	3	F2	

The initial values in the second column satisfy the second equation. Let's call the first function F1. In cell D1 enter the formula = B1^2 + 2*B2 - 10 and in cell D2 enter = B1 + B2 - 4. At this point some trial and error adjustment of the variable in column B can help create a good initial guess, while judging the quality of the guess by watching column D. When you are ready, start Solver. Instruct Solver to Set D1 to a value of 0 by varying B1:B2 subject to the constraint D2 = 0. (Click the **Add...** button to specify the constraint.) One solution is $x = -0.732$, $y = 4.732$. Another solution is $x = 2.732$ and $y = 1.268$.

Solving by Successive Substitution

Occasionally, solutions are needed to complex equations. For example, the equation $2.5x - \exp(0.75x) = 0$ has two solutions. The solutions can be found by successive substitution. The technique works by rearranging the function in the form $x = f(x)$. For the example, there are two possibilities:

$$x = \frac{\exp(0.75x)}{2.5} \quad (\text{A})$$

or

$$x = \frac{\ln(2.5x)}{0.75} \quad (\text{B})$$

Successive substitution works by using $f(x)$ to generate a new value of x and then substituting back into $f(x)$. The technique will converge only if $|f'(x)| < 1$ at the value of x guessed. For the present example, there are two solutions: $x = \{0.652536, 2.37512\}$. To begin, enter the table into Excel.

	A	B
1	xnew = f(x)	
2	xold	1

Then for Eqn. A, enter into B1, = exp(0.75*B2)/2.5. For the substitution, the following strategy is used:¹

1. Copy cell B1.
2. Past the *value* into cell B2 by right-clicking on B2, selecting **Paste Special...** and then selecting the radio button for Paste **Values**. *A macro can easily be created to repeat these steps as described below.*

By repeating the substitution about 15 times, the iterations converge on $x = 0.6525$. Try to converge on 2.37 by starting from 2.2 or 2.6 in cell B2—you will find it impossible because the value of $f'(x) > 1$ at $x = 2.37$. Reprogram cell B1 to the right-hand side of Eqn. B. This time the successive substitution will converge to $x = 2.375$, but convergence to $x = 0.6524$ will be impossible.

Macros for Successive Substitution

Successive substitution can be tedious, but a macro can be quickly written to perform the task. Suppose the following spreadsheet is available for the above example, solving for Eqn. A, where cell B1 is calculated from cell B2.

	A	B
1	xnew = f(x)	0.8468
2	xold	1

From the menu bar select **Tools... Record new Macro...** Click **Options>>** and give your macro a name and a shortcut keystroke. When you are ready to record, click **OK**. A Stop box may pop onto your screen. Every key stroke or mouse click that is now entered will be recorded.

1. Copy cell B1.
2. Paste the *value* into cell B2 by right-clicking on B2, selecting **Paste Special...** and then selecting Paste **Values**.
3. Click the **Stop** button, *or* select **Stop Recording** from the **Tools... Record Macro...** menu.

If all the steps went as planned, just press your shortcut key repeatedly. If you want to record over your macro, simply create a new macro with the same name.

¹ Circular references can sometimes be created by entering =B1 into cell B2, after enabling iterations on the Tools... Options...Calculations.... window; however, the convergence or divergence can be unpredictable.

Naming Variables

Variables may be named for use in formulas. Select the cell range to be named (for an array, highlight the entire array range), then select the name box in the left-most edge of the formula bar. Type in the desired name. Default cell names cannot be used, e.g., X1 is invalid, but _X1 is acceptable. See “named ranges” in online help for more information.

Array Operations

See Appendix B for an overview of matrices. To use a particular array element from an array, use the function INDEX(array,row_num,col_num). If the following named matrices exist in Excel:

$$B = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{bmatrix}, \text{INDEX}(B,1,3) = 3, \text{INDEX}(B,2,3) = 6 \quad X = [0.4 \ 0.6], \text{INDEX}(X,1) = 0.4,$$

$$\text{INDEX}(X,2) = 0.6$$

When entering a formula for a matrix operation that will involve matrix multiplication or results in an array, select the entire array output range (with the correct number of rows and columns) before entering the formula, then press CNTL+SHIFT+ENTER (or COMMAND+RETURN on a Macintosh) to tell Excel that this is a matrix formula. Excel inserts braces around the formula after it is entered. Failure to select the correct number of output rows or columns, or failure to press CNTL+SHIFT+ENTER, or failure to observe the requirements of matching the number of rows and columns in multiplicands can result in unexpected results or errors. Some common operations are shown below. See SUM and MMULT in online help for more details.

One-dimensional arrays:

- (a) If both arrays appear as columns or both arrays appear as rows, use SUM(array1*array2);
- (b) If array1 is a row and array2 is a column, use MMULT(array1,array2);
- (c) If array1 is a column and array2 is a row, use MMULT(array2,array1).

Multidimensional arrays (select the entire output range before entering the formula):

(a) For $c_{ij} = \sum_k a_{ik}b_{kj}$, use MMULT(A,B);

(b) For $c_{ij} = \sum_k a_{ik}b_{jk}$, use MMULT(A,TRANSPOSE(B)).

A.10 NOTES ON HP CALCULATOR

Directory Structure

Moving about the HP is very similar to moving in the directories on a PC; however, the objects in a directory may be variables, equations, or other subdirectories. The objects in a directory can be quickly found by pressing the VAR key in the third row. The objects will be listed above the menu keys. Directories have an overbar above the object name. (If there are more objects than menu keys,

the next six objects can be found by pressing the **NXT** key in the third row.) The current directory will be displayed near the top of the display, and you can move down through the directory structure by using the menu keys.

Sometimes you will need to move up through the directory structure. The top directory is called the home directory. You can always get to the home directory using the **left shift-FILES**. To move up one directory at a time, press the **UPDIR** key in the third row.

Warm Restart

Occasionally the calculator processing flags are not reset properly. For example, if a program hangs or keys are pressed during execution when the hour-glass is present. If you notice that the calculator is slow when performing simple addition and subtraction, this is a symptom indicating the need to perform a warm restart. Another symptom is an “out of memory” message when running a program. To perform a warm restart, press **ON** and the **F3** key simultaneously. The screen will momentarily blank. The program memory will be preserved. In the rare event that this fails to reset your calculator, see the HP user guide to reset. After a warm restart, press **VAR** to list the directory objects.

Terminating a Program

If a program is executing, and you wish to terminate it, simply press **Cancel** at a prompt. You will want to perform a warm restart as described above, which ends up moving you back to the **HOME** directory.

Equation Solver

To access the equation solver, press **right-shift NUM.SOLVE**, and select **Solve equation**. Select the **EDIT** menu key. Type in the equation to be solved using variable names. For practice, enter the equation $x^2 + 2x = y$ by entering the calculator keystrokes. (To enter variable names, press the α key. For a power, use the y^x key.) Press **ENTER** when finished. The HP will automatically identify the variables x and y . Use the cursor keys to move among the variables, setting the values of the known variables. (In this case, set $y = 1$. Now this equation will be the same one that was solved above in the Excel example.) Move the cursor to the variable which you want to find, and enter an initial guess. (Your answer will depend on your initial guess if multiple solutions exist. For this example, use 0 as an initial guess for x .) Press the menu **SOLVE** key when the cursor is in the correct field. (In this case, move to the field for x .) Solve again using $x = -2$ as the initial guess. Press **CANCEL** to exit solver.

Using Variables

There are many ways to create and use variables. This section summarizes only one method for each task with the calculator set to operate in RPN mode. Consult the manual for more details.

- (a) For a list of objects (including variables) in the current directory, press the **VAR** key.
- (b) To create a new variable with a value: 1) enter the value in the stack; 2) press α and type the variable name; 3) press **STO**. The variable value is available by pressing the menu key. When a variable name is used in a program or equation, the current value will be automatically read from memory.
- (c) To recall a variable value (or to enter the variable into a program or equation), just press the variable's menu key.

- (d) To change the value of a variable in memory, enter the new value in the stack, then press **left-shift** followed by the variable's menu key.
- (e) To delete a variable, press ' followed by the variable's menu key, then **TOOL-PURGE**.
- (f) To create a new directory: 1) press **left-shift FILES** and move to the location where the new directory is to be placed; 2) press **NXT** and the menu key **NEW**; 3) enter the new directory name, and check the "directory" box, then press the **OK** menu key.
- (g) To purge a non-empty directory, follow the procedure given for purging THRMO in the updating procedure immediately below, but substitute the appropriate directory names in that procedure. Start the procedure in the parent directory where the directory variable that you wish to purge resides.

Updating THRMO

To update an existing THRMO directory, first make sure you move any of your programs you wish to save to a different directory. The calculator will not permit you to move directories; you will have to copy them, and then purge the old one. When you are ready to load the new THRMO, purge the old directory as outlined here. Follow the steps very carefully so that you do not purge something else accidentally. You will not be asked to confirm any step, and you cannot undo the purge. 1) move to {HOME}; 2) press ' followed by the THRMO menu key; 3) use the arrow keys, SPC and alpha keys to add the PGDIR command (PGDIR stands for *purge directory*)— your entry line should look like '**THRMO**' PGDIR; 4) Press enter. Now you can load the updated THRMO.

Programming the HP

First of all, do not use the THRMO directory for adding your programs. This is because the THRMO directory will need to be purged when it is updated, and *everything* in the directory will be deleted. Start a new directory with your programs.

Programming the HP can be quite powerful, and the manual is the best resource. However, simple programs are often the most useful, and don't require detailed reading of the manual. For example, a simple program to calculate area might be << 'H*W' →NUM >> where H is a variable for height and W is a variable for width. (You simply type the formula using the variables. The variable values will be read from memory when the program runs. The double angle brackets tell the HP that this is a program. The command →NUM is actually a key in the 3rd row, and to enter the command you just press the key—this command converts the result to a number when the program executes.)

Programming is easiest in RPN mode, and directions are summarized here for that mode. To create this program, first create the variables AREA, W, and H with any values initially stored in them. (AREA will end up being the menu key that will be used to run the program.) Then begin typing the program << 'H*W' →NUM >> (The angle brackets can be found on the minus key. The single quotes are important. You can enter variable names in the program by just pressing the menu keys for the variable that you created above.) After the program is typed, press the enter key to put the program in the stack. Then store the program in AREA the same way you would store a number. Before you run the program, enter the desired variable values for H and W, then press the menu key AREA, and the resulting number for the area will appear on the stack. Change the variable values for H and W and run the program again to confirm your success. To edit a program after it has been written, place the variable name in the stack, then press right-shift EDIT.

You may browse through the THRMO directory for other programs to see how they are constructed. Recognize that the calculator *is not write protected*, so any change you make will be writ-

ten to memory. Be very careful when using the left shift key that you don't accidentally over write a program by storing new contents in the memory location! Some of the programming features possible are subroutines, prompts, and directory changes. Notice that variables or subroutines can be shared between directories if they are placed in the directory *above* the directories which will share them.

A.11 DISCLAIMER

The programs provided with this text are for educational use only. They are provided AS IS, without any warranty. They must not be sold under any circumstances.