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            PRESSURE-VOLUME CURVE ANALYSIS PROGRAM

                      USER'S GUIDE


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*******************    INTRODUCTION    *********************

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This guide is a description of how to use the pressure
volume (PV) curve analysis program for the IBM-PC (DOS
environment) microcomputer.  It is intended to assist the
user in running the program as well as give some detail on
program function.

The progam was written almost 20 years ago and has not
received much in the way of updating.  Therefore the graph-
ics capabilities are fairly crude.  You might want to take
advantage of the option for saving the results of the
analysis and use some other graphics program for creating
nice graphs.

Pressure-volume analysis has been used extensively in
plant research for estimating the osmotic and pressure com-
ponents of water potential in various plant parts as well as
for providing information on bulk tissue elastic properties.
The theory and methods of PV analysis are described by Tyree
and Hammel (1972), Tyree and Richter (1981), Richter et al.
(1980), and Wilson et al. (1979) to name a few.

The traditional approach has involved graphing the data
points with the negative inverse water potential on the

y-axis, and either the volume of water expressed from the xylem or the relative water content at the measured water potential on the x-axis.  Generally a two-phase curve is produced, having a non-linear region at high water content and a linear region at low water content.  A straight-edge is then used to help judge which points belong in the linear region of the curve.  Thus determined, it is possible to obtained estimates of tissue osmotic potential at any water content.  By subtracting the osmotic potential from the water potential at that water content, the bulk turgor pressure in the tissue can also be estimated.

The development of computer programs by the author for analyzing PV-curves arose out of a project involving over 200 sets of data.  Aside form the obvious desire to reduce the time required for analysis, it was apparent that the traditional graphical approach involved a certain degree of subjectivity in determining the points to be included in the linear region.  See the paper by Schulte and Hinckley (1985) for a description of the various approaches that were tried.  All programs assumed that data were collected by the "weighing" method with saturated weight, dry weight, and the series of water potential/fresh weight pairs.

The earliest method involved applying simple linear regression to the linear region of the curve, but this method was quickly abandoned.  The program included on this disk applies a non-linear least squares analysis, using the equations referred to as "PVC" in the Schulte and Hinckley (1985) paper.

When the PV-curve analysis program (PV) is run, the file name of a data set will be requested.  The non-linear least squares fit uses the linearization or Taylor-series method (Draper and Smith, 1966).  When the least squares routine has completed, a menu will be presented to allow for the selection of various output forms or further calculations.

This program is written with the Microsoft QuickBASIC system, and provided as a compiled, executable (.EXE) file.  If you want to print any of the graphs on a dot matrix printer that is graphics-compatible (capable of using the "Prtsc" key), the DOS program called "GRAPHICS.COM" needs to be run (only once unless the computer is rebooted) before starting the PV program.

Math coprocessor support is provided automatically; the program will run with or without a coprocessor, although it will run several times faster if a coprocessor is present.

As a note to programmers, if the computer contains a math coprocessor and you wish for it to be ignored by this program, add the statement "NO87= " (one or more spaces after the equal sign) as a DOS environment variable.  This may be done by typing "SET NO87= " at the DOS prompt.  Coprocessor use may be restored by

typing "SET NO87=" without a space after the equal
sign.  This DOS environment variable only affects cop-
rocessor use by this program and has no hardware
affect.


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****************    DATA ENTRY    *************************

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     The program reads data from a file that you may create
with any editor or even a word processor if you make sure to
safe the file as a simple ASCII text file without word pro-
cessor formatting.  Follow the format shown below.  The
intended units are grams for all masses and megapascals
(MPa) for all potentials.

"data set name"
saturated mass
dry mass
number of data points to follow
fresh mass,water potential
fresh mass,water potential
(and so forth)

Here's a sample data set...

"A"
.3462
.167
9
.346,-.18
.342,-.63
.333,-1.79
.328,-2.37
.319,-2.98
.317,-3.05
.312,-3.24
.298,-3.73
.285,-4.42


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****************    ANALYSIS OF PV-CURVE DATA    *************

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     To start the PV-curve analysis program from the DOS
prompt, simply type "PV".  After a title banner and some
other activities, the default parameter error tolerance is

displayed and there is an opportunity to change it.  A
simple carriage return indicates acceptance of the displayed
value.  This error tolerance indicates to the non-linear
least squares routine a maximum value that all parameter
corrections may have before the iterations will cease.  For
a description of this iterative procedure, see any text on
non-linear least squares analysis or Draper and Smith
(1966).  Decreasing the tolerance value below the default
may provide slightly greater accuracy, but longer program
running times will be required.  Experience has suggested
that tolerance values less than 0.01 generally will not
provide greater accuracy in the results, given the limits in
accuracy of the PV-curve data points themselves.  Tolerance
values of 0.1 may even be acceptable.

     Next enter a file name or "?" for a directory of the
disk.  If the file is found, the data will be read into
memory.  The program will allow you to enter multiple data
files in case you want to combine data sets.  So after
reading the data from a file, the program will keep asking
for another file name until you just enter a carriage return
(press enter) all by itself.

     As the non-linear least squares procedure involves suc-
cessive iterations to determine final values of the model
parameters, initial values or guesses are requested.  The
displayed default values may be adequate, or in cases where
convergence does not occur, these initial values may be
changed.

     When the initial values have been entered, the nonlinear
estimation begins and the corrections to these parameter
values will be indicated after each iteration.
When all corrections become less than the parameter error
tolerance value, the program will display a main menu.  From
this menu, the various outputs may be selected or the
analysis may be re-run.

     If convergence is not obtained...

     Ideally, the displayed parameter corrections will
rapidly approach zero, although some oscillation may be
apparent.  If this does not occur, the values may continue
to oscillate forever (more than a dozen or so iterations).
If the corrections are only slightly greater than the error
tolerance value, re-running the analysis with a larger tol-
erance may prove helpful (press ESC to get out of the
iterations, see below).  The most exciting failures-
to-converge, however, occur with wild oscillations of the
parameter corrections, a parameter such as the relative
water content for turgor loss becoming negative, or a
parameter approaching infinity!

     First of all, it is important to realize that non-linear
least squares algorithms are not like simple linear regres-
sion methods that quickly produce a clear, unambiguous
response.  Non-linear least squares involves an iterative,

successive approximation procedure.  As in simple linear
regression, a minimum error fit is the goal, but the diffi-
culty may be more apparent if you try to visualize an error
surface like a topographic map, and you are searching for
the minimum point.  For some functions and data sets,
the surface may have a single well-defined low point that is
easy to find.  Other situations may be complicated by mul-
tiple low points where you get lost in a "false minimum" or
wander back and forth over a narrow ridge.  In addition,
consider that the surface really involves four dimensions in
this program.

     With that in mind, the most common reason for noncon-
vergence is that the data set does not have a linear region
- either because of measurement errors or because the data
collection was not carried out to a low enough water poten-
tial.  Generally three points are required from water
contents lower than the turgor loss point (TLP).  In some
cases, the plant tissue may have lost turgor at a relative
water content (R) much higher than suggested by the default
initial value (0.85).  Sometimes increasing this value to
0.90 or even 0.95 will allow convergence to occur because a
linear region will be more "apparent" below the TLP esti-
mate.

     In general, either try changing the initial values from
the default settings or plot the data.  The data can be
plotted from within this program (from the main menu, select
"DISPLAY GRAPH", and then "PV curve"), although if the
iterative analysis has not completed, the fitted curve may
not be meaningful.  Occasionally a mis-entered or mismea-
sured data point is found in this way.

     At any point in the program when input is not being
requested from the keyboard, such as when a graph is being
drawn on the screen or when the least squares iterations are
running, pressing the ESC key stops the execution and
returns the program to the main menu.  This feature is not
completely tested, so I'd like to know if it causes
problems.  If the program is requesting input, the carriage
return must be pressed after the ESC key in order for it to
work.

Error Messages

     In order to minimize program length, the only error
messages that this program generates are the "FILE NOT
FOUND" message when a requested file name is not found on
the disk, and the "DISK ERROR" message indicating that some
type of disk reading error, such as the disk drive door
being left open, has occurred.  All other errors will cause
the program to generate an error number that a programmer
might find useful.

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     *********************   PROGRAM OUTPUT   ******************

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     When the non-linear least squares routine has completed
successfully, a main menu appears from which various output
options are available,  Selecting "DISPLAY OUTPUT" gives
final estimates of the parameter values along with some
statistical information concerning model fit: R-squared, the
sum of squares regression (SSR), and the sum of squares
total (SST).  Subsequently, the data points are displayed
along with estimates based on the fitted equation and final
values of the parameters.

     Selecting "PRINT OUTPUT" also provides the information
described above, together with original data points, to a
printer.

     Selecting "SAVE OUTPUT TO FILE" allows you to save all
of the analysis results to a file.  My intent was for this
file to be a complete record of the analysis, and so it
includes all the original data points, the fitted model
parameters, and a table of variables that may be used by
another program for creating graphs of the various water
potential components, the elastic modulus and capacitance.
A sample output file (actually, the one generated by running
the analysis of the sample data set named "A" shown above)
is shown below.  The first section shows the input data
file.  Next comes a line with the fitted model parameters.
Lastly a table is included with data that may be useful for
making graphs.

Output file format:

Output file from PV (Version C) for: data set name
Input data file was:
saturated mass  dry mass  number of data points
point no.  fresh mass  1-R  water pot  -1/water pot
     -- repeat for all data points --
p-function coeff  (1-R)tlp  tlp Osm pot  sat Osm pot  sym-
plastic fraction
1-R  -1/water pot  water pot  osm pot  pressure  elas  capac
     -- repeat for (1-R) from 0.0 to 0.4 --

Abbreviations:
    R - relative water content
    pot - potential
    tlp - tutgor loss point
    sat - saturated
    osm - osmotic
    elas - modulus of elasticity (MPa)
    capac - hydraulic capacitance as change in volume
       divided by change in water potential (m^3/MPa).
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Sample output file:

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Output file from PV (Version C) for: A
Input data file was:
 .3462  .167  9
 1  0.3460 0.001 -0.180  5.556
 2  0.3420 0.023 -0.630  1.587
 3  0.3330 0.074 -1.790  0.559
 4  0.3280 0.102 -2.370  0.422
 5  0.3190 0.152 -2.980  0.336
 6  0.3170 0.163 -3.050  0.328
 7  0.3120 0.191 -3.240  0.309
 8  0.2980 0.269 -3.730  0.268
 9  0.2850 0.342 -4.420  0.226
 8.040  0.149 -2.983 -2.386  0.742
0.000 12.487 -0.080 -2.386  2.305 26.578  6.015E-09
0.004  5.060 -0.198 -2.398  2.201 25.634  6.182E-09
0.008  3.205 -0.312 -2.412  2.100 24.715  6.355E-09
0.012  2.362 -0.423 -2.425  2.001 23.837  6.529E-09
0.016  1.881 -0.532 -2.438  1.906 22.990  6.706E-09
     -- continues for another 94 lines --
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Selecting "DISPLAY GRAPH" will allow various plots to be
displayed on the screen.  A menu of choices will appear
including the standard PV-curve plot and other plots of
pressure potential and the modulus of elasticity.  After a
particular plot is selected, the user is given the choice of
manually selecting graph parameters (axis ranges and so
forth) or letting the program automatically select
reasonable values.  The "manual" option also allows you to
magnify small regions of plots.  For example, selecting a
narrow range for the x- and y-axis around the turgor loss
point of the PV-curve will fill the graph with this portion
of the curve.  Some care should be used in selecting graph
parameters; for example if the y-axis is to be numbered with
whole numbers (decimals = 0) and the range is 0 to 8,
selecting 5 for the number of tic marks will produce an
incorrect numbering of the axis.

The selection "PRINT GRAPH" should dump the last dis-
played graph to a graphics-compatible printer.  This
selection calls a DOS interrupt (5) similar to the "print
screen" on the keyboard.  In order for this routine to work,
the DOS-supplied program, "GRAPHICS.COM" must be run before
starting the PV programs.  The effects of this program will
be maintained until the computer is rebooted, so it need
only be run once.  The "GRAPHICS.COM" program is not much of
a talker, and nothing appears on the screen when it is run.

The selection "WATER POTENTIAL COMPONENTS" will give
estimates of water potential, osmotic potential, and
pressure potential for any relative water content.

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