Nov 11, 2024

# TCONTOUR - John Pilling

**Introduction**

Tcontour is designed to display scientific data obtained from ternary systems ie. a measured value is a function of three values not the usual two, subject to the constraint that the total combination of the three variables add to 100%.

Example:

*You have measured the resistivity of wires made from several mixtures of copper, silver and gold and you want to see how the resistivity varies with the changes in composition. -*

You need **Tcontour**.

In these cases, a normal x-y cartesian representation does not serve any useful purpose and the data is often better presented in the form of an equilateral triangle whose vertices represent one of each of the three components (variables) which define the system. Any mixture of any two of the components is then represented by a point on the perimeter of the triangle while any mixture of all three components can be represented by a point within the triangle. Points outside the triangle are not valid combinations of the three variables.

**Preparing your data**

There are two ways to prepare your data for input in to TContour

1. Use your favourite word processor to make a plain text file with the following format:

lines 1 to 4 (note string length should be 31 characters or less)
string identifying component A
string identifying component B
string identifying component C
string identifying the variable (z) being plotted.

lines 5 and onwards.

These take the form of three numbers separated by spaces. The first two numbers represent the percentage of A and the percentage of B in the mixture (don't worry about C as this must be the difference betweeen 100 and the sum of A+B). The third value on the line is the measured property Z ie.

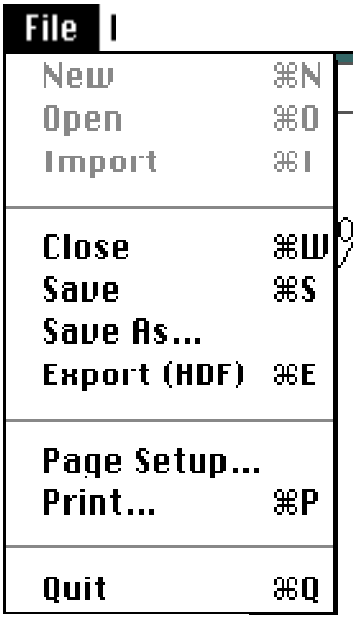
| | | |
|---|---|---|
| 10 | 20 | 5.3e4 |
| 50 | 30 | 6.8e3 |
| %A | %B | Z |

and so on!

2. Enter the numerical data only into a spreadsheet in row-column format as shown above. This data can then be copied from the spreadsheet into TContour via the normal cut and paste technique.

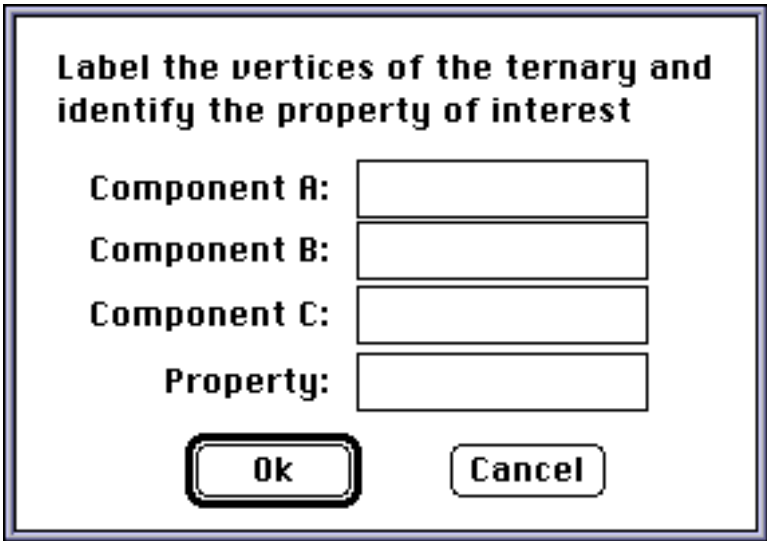
**File Menu**

When Tcontour is started from the finder there is no data and the file menu allows you to create a new ternary (this will have an empty data set ), open an existing TContour document or import a plain text file in the format set out in 1 above.




**New**

The dialog shown below will appear. You should enter the labels for your three components and the property of interest. Select cancel if you want to use one of the other methods of input.




Selecting Ok will draw the new system and present you with an empty data window. You should switch to your spreadsheet program, mark the block of data that you wish to bring into TContour and either cut or copy the block of n rows by 3 columns into the clipboard. Switch back to TContour - click in the data window and then use the Paste command to insert the data.

**Open**

A standard dialog is presented that allows you to choose which TContour file to load.

TContour 3.0

Nov 11, 2024

**Import**

You can select your plain text file using the standard file dialog and it will be loaded in.

Tcontour has three main windows, these are : **.data, .rom, .map**. The input data is displayed in the .**data** window. This allows you to check that everything loaded ok, you can scroll up and down, and check that the data is correct.

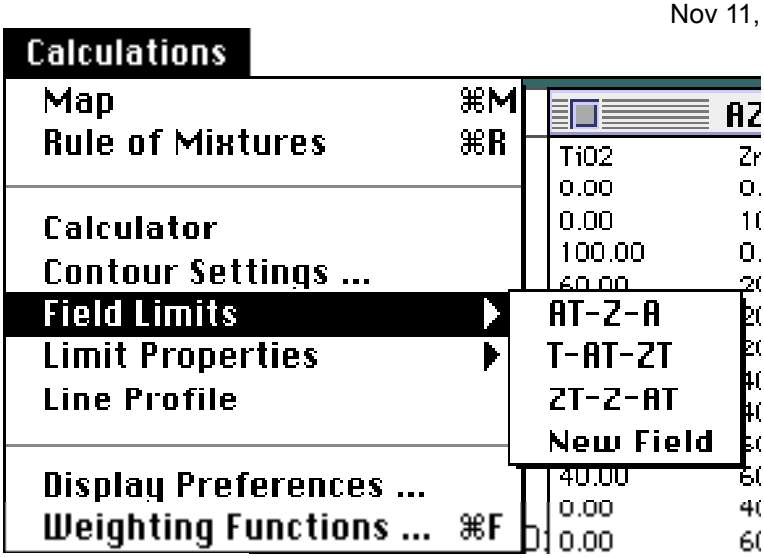
The input data is scanned and a tentative minimum and maximum assigned for the purpose of mapping Once data is loaded the calculations menu is enabled and you can proceed. The data window will scroll automatically and supports cut and paste of data points ie. (%A,%B,%C and Z sets). Possible operations are:

1. Mapping the data (contouring)
2. Rule of Mixtures modelling
3. Spot calculations.
4. Line Profiles.

AZT.data

| TiO2 | ZrO2 | Al2O3 | CTE (x10-6/C) |
|---|---|---|---|
| 0.00 | 0.00 | 100.0 | 8.60 |
| 0.00 | 100.00 | 0.0 | 10.60 |
| 100.00 | 0.00 | 0.0 | 9.40 |
| 60.00 | 20.00 | 20.0 | -4.18 |
| 40.00 | 20.00 | 40.0 | -2.39 |
| 20.00 | 20.00 | 60.0 | -0.05 |
| 20.00 | 40.00 | 40.0 | 0.30 |
| 40.00 | 40.00 | 20.0 | 0.48 |
| 20.00 | 60.00 | 20.0 | -0.60 |
| 40.00 | 60.00 | 0.0 | 3.58 |
| 0.00 | 40.00 | 60.0 | 7.55 |
| 0.00 | 60.00 | 40.0 | 6.82 |
| 60.00 | 0.00 | 40.0 | -2.64 |
| 60.00 | 40.00 | 0.0 | 7.65 |
| 0.00 | 20.00 | 80.0 | 7.06 |
| 80.00 | 20.00 | 0.0 | 8.76 |
| 80.00 | 0.00 | 20.0 | 10.39 |
| 20.00 | 0.00 | 80.0 | -2.00 |
| 50.00 | 50.00 | 0.0 | 7.26 |
| 10.00 | 70.00 | 20.0 | 3.73 |
| 0.00 | 70.00 | 30.0 | 7.13 |

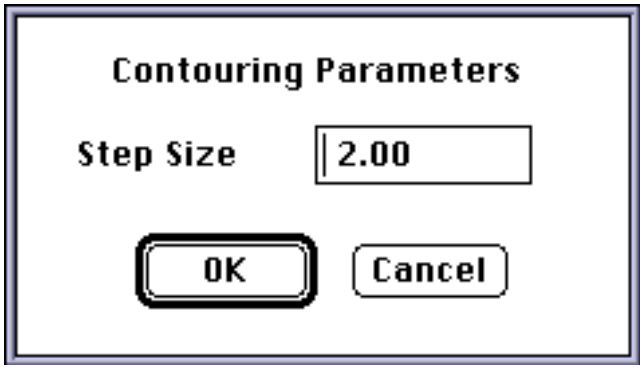
An Example of the Data Window




Calculations Menu showing a heirarchical phase fields menu.

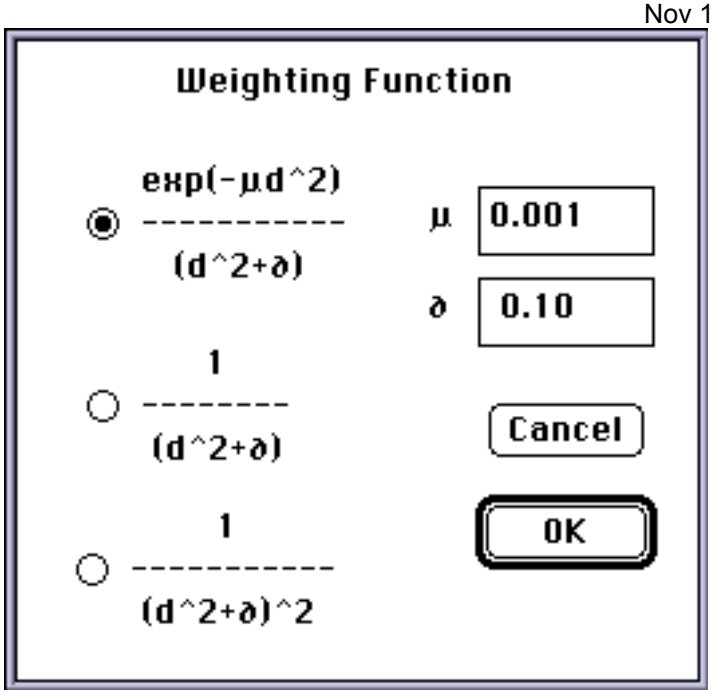
**Mapping.**

Before issuing the mapping command, you should use contour settings to set the step size over which you want the calculations to be carried out. The default is an increment of 2%. The smaller the number entered here the better your data will look but the gridding process will take longer. Going from 2% to 1% quadruples the calculation time. Values smaller than 0.5% do not give any improvement in the picture as this corresponds to 1pixel at normal screen resolutions. Its your choice - larger values give coarser more jagged displays but window update times are much much shorter.

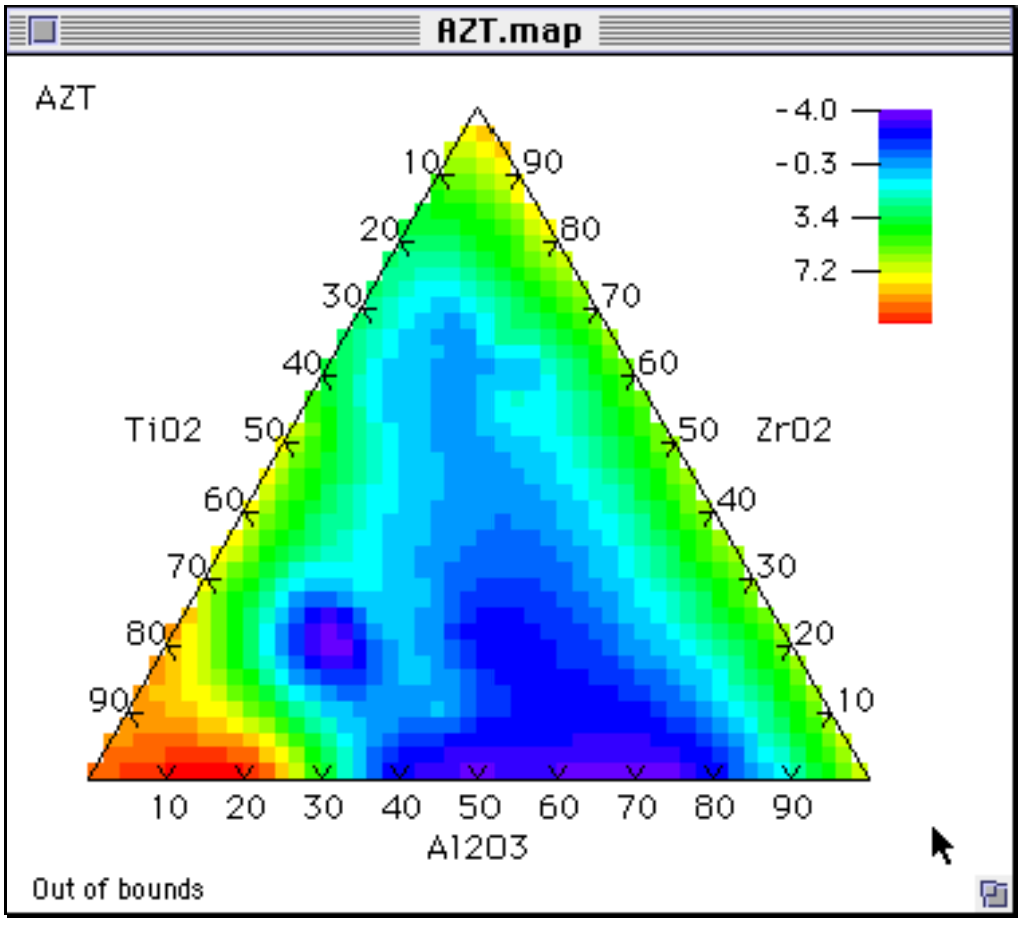



Setting the Step Size for Mapping

Data is mapped onto the ternary graph using a weighted least squares interpolation based on all the data. The program sets the weighting function and factors although you may select your own by using the weighting functions command in the EDIT menu. The contouring algorithm is based on '*Drawing Contours from Arbitrary Data Points*', D.H.M$^{c}$Lain, The Computer Journal, **17(4)** 1974 p318-324.




Default Weighting Function and Constants

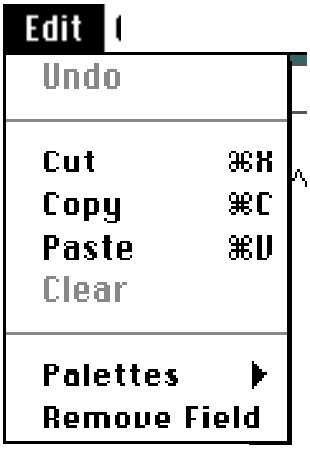



Example of the Contour Map Window

TContour 3.0

Nov 11, 2024

**Editing Commands**




**Palette**

Choosing the palette item in the EDIT menu will display a list of colour tables to change the appearance of the display.

**Copy**

You may copy the **.map , .rom** or **.profile** window into the clipboard and paste it to any macintosh graphics applications that supports PICT format files. Select the window then choose copy from the Edit menu.

You may copy any highlighted data sets in the **data** window into the clipboard and paste the information into any program that supports <tab> delimited text ie. a spreadsheet. Note: You do not have to highlight the entire row of data, highlighting a single value in a row will copy the entire row.

If you wish to copy the numerical values of the line profile displayed in the **profile** window select the TEXT export option in the preferences dialog first. This will export in a form suitable for pasting into spreadsheets ie.

1 x step size <tab> rom value at x <tab> mapped value at x <cr>
2 x step size <tab> rom value at x <tab> mapped value at x <cr>
3 x step size <tab> rom value at x <tab> mapped value at x <cr>
.....
n x step size <tab> rom value at x <tab> mapped value at x <cr>

where step size is the value chosen in the contour settings dialog.

**Cut**

The cut command enables data sets (%A,%B,%C and Z: ie. a row of data in the data window) to be cut from the data window. The data can be pasted into a text file or a spreadsheet, edited and pasted back into the data window or just discarded. Note: when pasting the data only 3 values will appear (%A,%B and Z) in the spreadsheet etc. since the %C value is redundant. This also maintains consistency with the text format input data.

**Paste**

The Paste command is only available when the data window is frontmost. This allows you to add new points to an existing set of data without having to re-enter all the field information. You should only import data cut from a spreadsheet or tab delimited text file. The data to be pasted should be in row - column format ie.

%A <tab> %B <tab> Z <cr>
%A <tab> %B <tab> Z <cr>
%A <tab> %B <tab> Z <cr>

**Modelling.... The Rule of Mixtures.**

In many cases the property of interest of each of the three components is known and the property of the mixture is given by what is known as a rule of mixtures. ie. if you have equal amounts of A and B the property of the mixture will be the average of that of A and B. Mathematically this is represented as

$$Z_{mix} = (\%A.Z_A + \%B.Z_B + \%C.Z_C)/100$$

where the phases are in series and

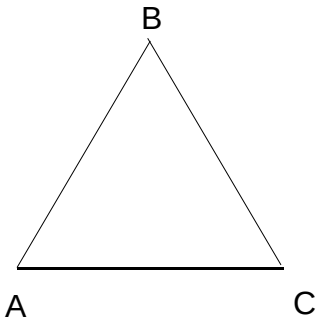
$$1/Z_{mix} = (\%A/Z_A + \%B/Z_B + \%C/Z_C)/100$$

where the phases are in parallel, given that

$$\%A+\%B+\%C=100$$

**Limits of Field**

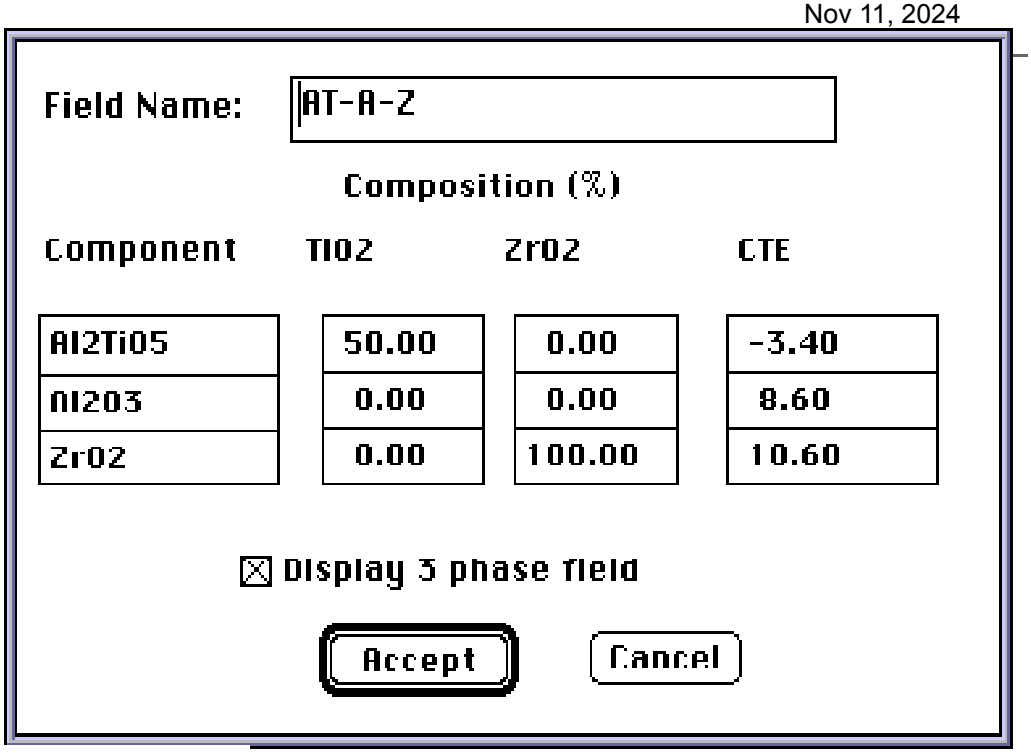
The program will let you define the values for the limiting properties of the base components so that this type of calculation can be carried out. This command lets you enter the property value of interest - in the example it was resistivity, for each of the components of interest - the three Z fields. The composition fields should not be adjusted unless you wish to define a new 3 component triangle as the basis of your calculations - more about that later. Values of 100 0 is A, 0 100 would be pure B and 0 0 (which gives 100 C by default) is pure C.




The default orientation of the components A,B and C.

Don't forget to give the field a name so that you may select it from the menus and to click the visible button so that the field is displayed and added into the fields sub-menu. You should also give a label to each vertx of the 3 phase field you are defining.

Unfortunately, it is not certain whether the property of interest depends on the % of each component as measured by weight, by volume or (for the chemists) by moles. Whatever value you entered for the % in the datafile was probably the case you were interested in but should you need to convert between types you can.




Tcontour 2.2
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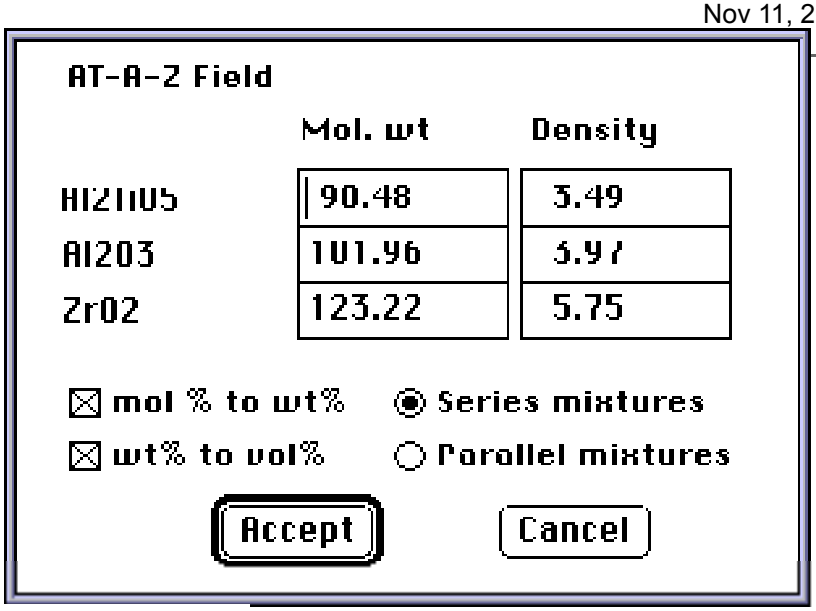
**Properties of Limits**

This command lets you enter the molecular weights of the components so that you can convert from mol% to wt% (check the mol to wt button to activate this choice) and/or from wt% to vol% if you enter the densities of each of the components (check the wt to vol button to activate this option). Don't forget to select which rule of mixtures is operative for the particular property you are plotting.

Use the Rule of Mixtures (R) command to plot out the ROM calculated property within the triangle of interest. The results of the calculation are displayed in the ROM window. You can size both the **data** and **rom** windows alike and place them next to each other to compare your data (and interpolations) with the ROM calculations.

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Dialog used for setting up % switching

**Deleting Fields**

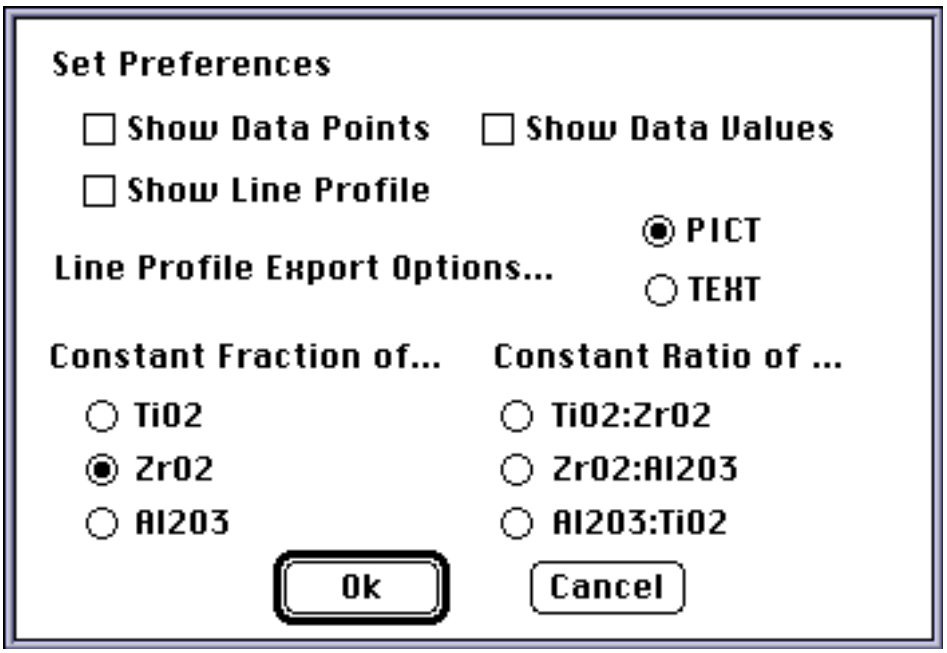
First select the field you wish to delete using the Field Limits command (the current field is checked). Use the Delete Field command in the edit menu. Note: You cannot delete the 'New Field ' field.

**Preferences**

The preferences dialog will be displayed. This allows you to activate /deactivate the display of the data points or the property values on the ternary diagram.

You can elect to display the line along which the line profile is made on both the **map** and **rom** ternary plots and specify the format in which the **profile** data is exported into the clipboard as either PICT ie. the graph or TEXT for pasting into a spreadsheet etc.

You can select the type of line profile by selecting a fixed amount of component A, B or C or a fixed ratio of components A:B, B:C or C:A.



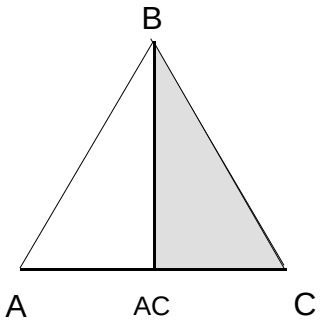

Preferences Dialog

**Advanced Use - Defining a new Three Phase Field.**

Many ternary systems often contain sub-ternaries, the ABC equilateral triangle being made up of many sub-triangles of non-regular shape. This is common when A, B or C react to form intermediate compounds with distinct properties of their own. For the ROM calculations, the property of a mixture may depend on the relative proportions of the intermediate compounds not on the pure components. You can use the Field Limits command to define the extent of any three component triangle within the ABC ternary.

For example say A and C react to form an equimolar compound AC but A and B do not react neither do B and C nor does AC and B. The reaction effectively divides the equilateral triangle into two 30-60 right angle triangles by drawing a line from AC to B. If you want to calculate the properties of a mixture of AC, B and C then use the field limits to set these values.

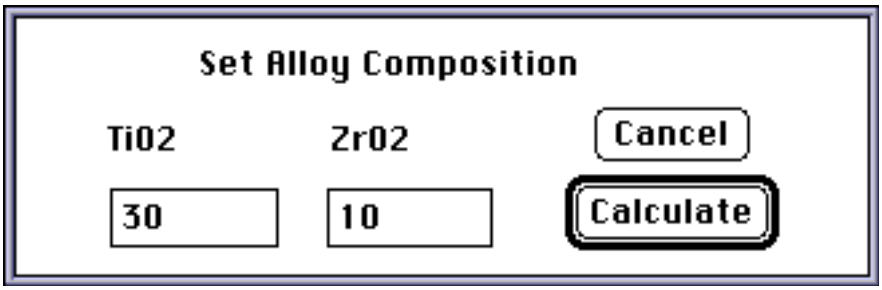
For 'A' enter 50 and 0 ie. 50% A and 0%B (and 50%C by difference)
For 'B' enter 0 100 ie. 0% A, 100%B (and 0%C by difference)
For C enter 0 0 ie. 0% A, 0%B (and 100%C by difference)



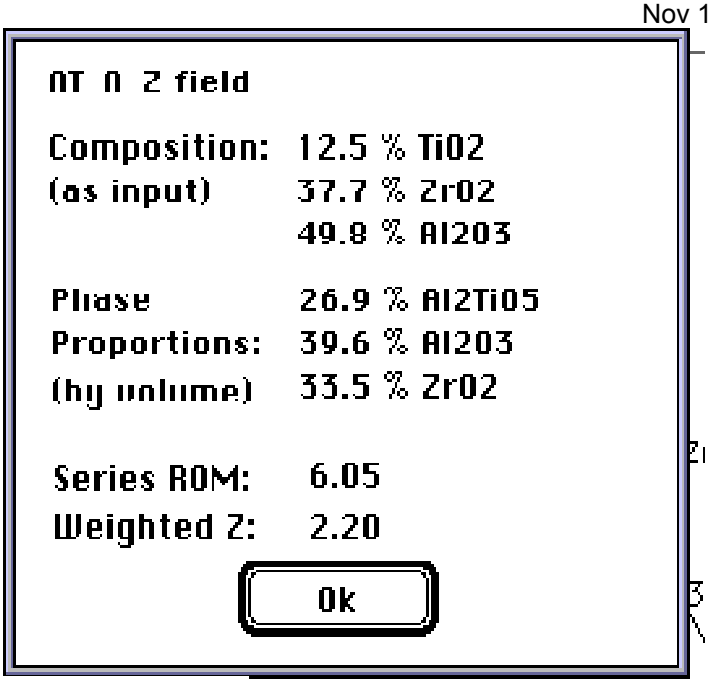

An example of a ternary system containing two sub-ternaries A-AC-B and AC-B-C.

Use the ROM command to remap the calculations. The ROM calculations will be shown only in the selected triangle. Don't forget to use the Properties command to set up the new molecular weights and densities of the intermediate compounds before doing the rom calculation.

You can use the calculator command to enter specific compositions. As long as the composition lies within the A-B-C triangle a weighted least squares interpolation will be carried out and the property value displayed. If the point chosen also lay within the selected sub-triangle then the ROM calculated value will also be displayed. If the point lies outside the sub-triangle then an 'INVALID POINT' message will be displayed. Use the Limits of Field menu to select the field in which you want to make the calculation.




An alternative method of initiating calculations is by clicking the mouse in the triangle at the point where you wish a calculation to be made. The current composition is displayed in the bottom left of the window. As long as a valid point is clicked the calculation will be made and the result displayed. You can click in either the **.rom** or .**map** window. The program will attempt to work out which field you selected and will display this in the results window. If the point was not within a valid field then an 'INAVLID POINT' message will be displayed.




Tcontour 2.2
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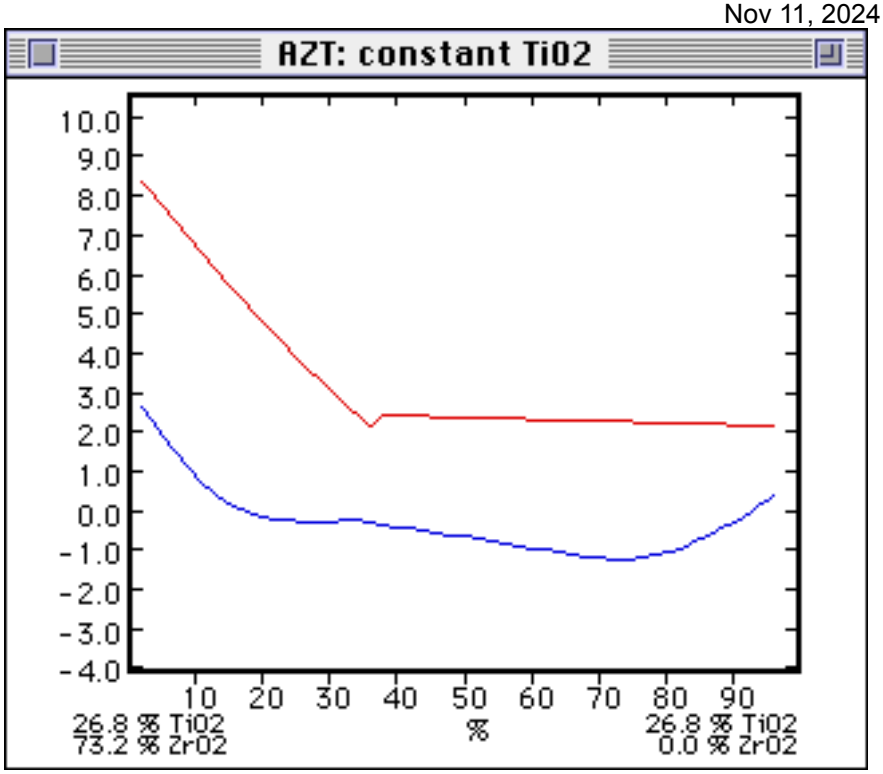
**Line Profiles**

Selecting the Line Profile Option from the Calculations menu will bring up a new window to display the profile and present the contour settings dialog to enable you to chose the stepping interval. The default is 2% steps, the line joining the two end points of the profile being divided into 50 steps.

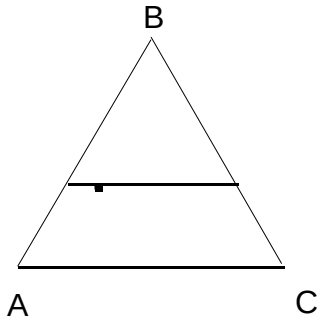
To get a line profile you must click the mouse on the diagram at a composition where you want the profile to be drawn. A line (selected in the preferences dialog) is then projected from this point and both the calculated contour height (blue) and the rule of mixtures (red) values are displayed. If no data is available on which to make the calculations no profile is displayed.

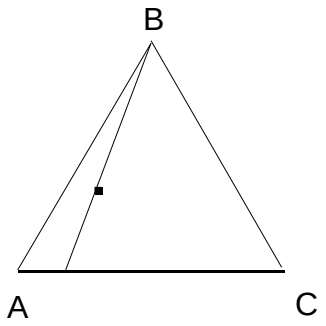



Example of line profile taken for a constant amount of one component

You may select one of 2 basic types of profiles either a constant amount of one of the three components or a constant ratio of any two of the three base components.

1. In the first case, constant amount of one component a line will be constructed parallel to the side of the triangle opposite the apex representing that component through the selected point. In the example this would be a constant amount of B.




2. In the second case, constant ratio, a line will be drawn from the apex of the triangle representing the unidentified component, through the selected point to the side of the triangle opposite the apex. In the example above this would be a constant ratio of A:C

**Printing**

Each of the **map, rom** and **profile** windows can be printed using the print command in the file menu. The printing process has been optimised for black and white output devices - I don't know anyone who has access to a colour postscript printer! So make sure you select black and white from the print dialog not colour! If you need colour then enlarge the window and take a photograph of the screen!. You can of course use the copy command to copy the colour map into any drawing program that supports PICT format images via the clipboard and use that program to do the colour printing.

The printed output uses the standard postscript halftones representing 8 grey levels. I tried more but the print time approaches 40minutes! Similarly using the greyscale/colour option in the print dialog gives print times around 40 minutes so make sure you set the printing to BLACK and WHITE !!

If you do not like the default colour mapping then use the palettes menu (located at the bottom of the edit menu) to change the colour look up table CLUT. More information about how to add your own custom clut's is given in the appendix.

**Saving Results and Data.**

There are two methods of saving the calculations SAVE and EXPORT

TContour 3.0

Nov 11, 2024

**SAVE**


*Finder Icon of Binary Files Saved by TContour*


*Finder Icons of ASCII HDF compatible files for use with the NCSA applications*

This will save the data and all the defined fields in a binary form which can be re-opened using the OPEN command in the file menu.

You can double click the Bin format documents in the finder to launch Tcontour and automatically open the document. Alternatively you can drop either the Bin format files or a correctly formatted text file onto TContour to launch and open the document.

IMPORTANT: System 7.0: TContour will not work with alias' as yet.

**EXPORT**

This will save the gridded (interpolated) data in a TEXT file in a format that can be read by the NCSA HDF import program for conversion to HDF format. This will allow your data to be ported between many computer platforms and analysis programs. More details on HDF format are available by ftp from zaphod.ncsa.uiuc.edu along with their analysis software for the MAC. (Future versions will export HDF binaries directly).

**More about custom clut's**

The colour palettes used by Tcontour are held as clut resources. These were created using NCSA PALedit (see above) and saved in CANVAS format . This format is a memory image of the 256 colour hardware lookup table - see inside macintosh V. The file created has a single clut resource with ID=999. which can be cut using **ResEdit** and pasted into Tcontours resource fork. Here's how:-

Use ResEdit to alter the clut ID from 999 to the next available number (cluts are numbered from 1 upwards) using the Get Resource Info command. Next open the STR# resource and add a new string item with the name of the new palette. For example, you paste a new clut into Tcontour and give it the next available ID say 6. Add string number 6 to the STR# resource - lets call it AMAZING COLOURS. Save the resource fork and quit ResEdit. When you restart Tcontour the STR# resources are read in. The number of strings determines the number of palettes that are available and the names are used to make the palette menu. The palettes are then read in from the resource file whenever you request a change of palette.

To avoid conflicts with the desktop and other open windows the CLUT resources are loaded by the palette manager as "tolerant" colours (actually a tolerance value of $1000) So some subtle colour palettes may not be displayed in their full glory. (Later versions may support adjustable tolerances )

**Hardware Requirements**

This program was written in Think Pascal 4.0 using the 68030/68882 options. It will only run on systems supporting 32 bit colour quickdraw ie. MACSE/30 and MAC II's. You really need a colour monitor.

John Pilling email via internet drjohn@mtu.edu
download program via ftp from austenite.my.mtu.edu ftp/pub directory

Dept. of Metallurgical and Materials Engineering

TContour 3.0

Nov 11, 2024

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TContour 3.0

Nov 11, 2024

Update Information

1. A bug in the window update routine has been fixed so that the whole contour map is drawn
2. A bug in the FIELDS menu has been fixed. The fields associated with a given ternary are now deleted from the FIELDS menu when the map is closed.

Update for version 2.1

3. Scientific Data Sets now write properly when the export option is selected.
4. Supports System 7 Apple Events.
5. Supports Cut and Paste of Colour Maps and Data.
6. The Data Window is now in the format of a spreadsheet, the data being arranged in cells and supports full cut/copy and paste.
7.. Desk Accessories\Applications etc. can now be launched from the apple menu.
8. Displays Data Points/Property Values on the ternary sections.

Update for version 3.0, Nov 11, 2024

Note: **The internal format of the binary data files has changed. Files created by version 2.2 and below cannot be open properly by version 3.0 . An attached updater can be used to convert the files to version 3.0 format. The change has been necessitated by an increase in the information content stored in FIELD objects.**

9. A bug in the copy ing of the colour contour data to the clipboard has been expunged.
10. Line profiling has been incorporated and supports the copy operation in either TEXT or PICT format.
11. User definable weighting functions (thedefaults are usually the best choice!).
12. Tcontour now supports ballon help for menus and dialogs.
13. Imported files which are saved with the same name as their plain text file originals were not recognised by the finder as Tcontour formatted binaries. This has been fixed.
14. Resizing of the datalist now only occurs when the data window is zoomed - unfortunately zooming <u>any</u> window used to do this without you asking!
15. Both Serial and Parallel rules of mixtures are now supported.
16. The user may now define labels to identify the limiting points in a 3 phase field. Hence the caveat above!