

ISOMORPHOUS PHASE DIAGRAMS IN MATHCAD A POWERFUL TOOL FOR INSTRUCTORS

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Introduction

An important topic in introductory materials science courses is the phase diagram. The simplest phase diagram is one in which the two solids can be mixed in any proportions as a single solid phase. These are called isomorphous diagrams. A common example of such a diagram is the copper/nickel system. This article describes a Mathcad worksheet that can create and analyze an isomorphous phase diagram. The user inputs a series of data points that map the solidus and liquidus lines. These data points can be hypothetical, or they can be picked off a real phase diagram. Once these lines have been mapped, the user chooses a state point (a composition and a temperature), and the worksheet calculates the corresponding liquidus temperature, solidus temperature, liquid composition, solid composition, and relative amount of solid phase present. I use this worksheet to create homework and test questions. It saves time, because the solution key is produced without further effort.

Cubic Spline Curve Fitting in Mathcad

The actual worksheet is displayed in Figure 1. Mathcad's cubic spline function is the key to this worksheet. It is used to generate continuous functions for the liquidus and solidus lines from a set of discrete data points. These two continuous functions are the basis for all calculations.

Creation of these continuous functions involves use of two Mathcad functions: cspline and interp. Cspline operates on two arrays: the array of x coordinates (the compositions in the case of a phase diagram), and the array of y coordinates. For an isomorphous phase diagram there are two y-coordinate arrays: one for the

liquidus temperatures and one for the solidus temperatures, so the cspline function is used twice. The interp function uses the output of the cspline function to produce a continuous function for each of the curves.

Solving and Back-Solving in Mathcad

Once the functions for the liquidus and solidus curves have been generated, there are two types of calculations to be performed for a given state point. Calculation of the liquidus and solidus temperatures corresponding to the sample composition involves straightforward application of the functions. A command like

Liquidus(Comp)

generates the liquidus temperature corresponding to the previously defined sample composition named "Comp." Calculation of the solidus temperature is similar.

Calculation of the solid and liquid phase compositions requires a Mathcad "solve block." The worksheet already contains guess values for the compositions. The solve block looks like this:

Given

Liquidus(Comp_L)=Temp

Solidus(Comp_S)=Temp

Comps:=Find(Comp_L,Comp_S)

By internal trial and error, Mathcad finds the value of Comp_L that causes the Liquidus(Comp) function to produce a temperature that equals the previously specified sample temperature "Temp." Likewise, Mathcad finds the value of Comp_S that causes the Solidus(Comp) function to produce a temperature equal to "Temp."

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Once the solid and liquid compositions are known, the tie line calculation is straightforward.

Error Traps

As discussed below, the only user interaction required to use this worksheet is the entry of the state point values. The danger here is that the user may enter a state point that is in a single phase region or a point that is higher than the highest liquidus temperature or lower than the lowest solidus temperature. In the absence of error traps, such a state point would produce erroneous results or no results at all. To eliminate the confusion that might ensue, the worksheet contains extensive error traps. These are clearly delineated in the actual worksheet shown in Figure 1. They are not discussed further here. Suffice it to say that all possible state point entries, including those in single phase regions, produce results that are valid. Any state point above the liquidus line results in a liquid composition equal to the sample composition and an amount of liquid of 100%. The result for solid composition will be "Single phase. All liquid." Any state point below the solidus line results in a solid composition equal to the sample composition, "Single Phase. All solid." for the liquid composition, and 100% for the amount of solid.

Using the Worksheet

The user may wish to create a different phase diagram than the one built into the worksheet. This simply involves entering new data into the arrays y_1 and y_2 for the solidus and liquidus temperatures respectively. One cautionary note here, the worksheet will not work correctly unless the freezing temperature along the right temperature axis is higher than the freezing temperature along the left temperature axis.

If the user is content to use the phase diagram built into the worksheet, he or she need only enter a value for "Comp" and a value for "Temp" in the shaded areas near the end of the worksheet. On the actual worksheet the data entry fields are shaded with a green background,

but the color does not show in Figure 1. Note that Mathcad's *global equals sign*, \equiv , is used here. When this sign is used, the value applies everywhere on the worksheet rather than only below and to the right of the entry point. This facilitates placing the state point values adjacent to the calculated results and eliminates the need for extensive scrolling through the worksheet. The worksheet produces a table of results directly below the data entry fields. This table begins with the repetition of the input values for composition and temperature. Following that, the table displays the liquidus and solidus temperatures corresponding to the sample composition and the solid and liquid compositions corresponding to the system temperature. Finally, the table displays the relative amount of solid in percent. Directly below the table of results is the phase diagram itself. In addition to the solidus and liquidus lines, the diagram includes a diamond that shows the state point chosen by the user.

Conclusions

This worksheet simplifies the process of creating homework and test problems. I suppress the display of the state point diamond and print a phase diagram that I give to students. Then I reactivate the state point diamond and print a phase diagram for my solution key. Finally, I print the table of results, and the solution key is done.

Biographical Information

Edwin G. Wiggins holds BS, MS, and Ph.D. degrees in chemical, nuclear, and mechanical engineering respectively from Purdue University. He is the Mandell and Lester Rosenblatt Professor of Marine Engineering at Webb Institute in Glen Cove, NY. Ed is a past chairman of the New York Metropolitan Section of the Society of Naval Architects and Marine Engineers (SNAME) and a past regional vice president of SNAME. A Centennial Medallion and a Distinguished Service Award recognize his service to SNAME. As a representative of SNAME, Ed Wiggins serves on the Board of Directors of the Accreditation Board for Engineering and Technology (ABET).

Figure 1: Mathcad Worksheet

This worksheet generates a hypothetical isomorphous phase diagram. The diagram itself can be given to students and used by them to practice phase diagram calculations. Meanwhile, the instructor need only enter values of sample temperature and composition, and the worksheet will produce the following results: liquidus temperature, solidus temperature, liquid composition, solid composition, and amount of solid. Although state points outside the two phase envelope are not interesting, they are handled correctly.

The array x contains alloy compositions. The array y_1 contains the solidus temperatures. The array y_2 contains the liquidus temperatures. Although these values are hypothetical, values read from a real phase diagram may be entered.

$$\begin{array}{l}
 x := \begin{pmatrix} 0 \\ 10 \\ 20 \\ 30 \\ 40 \\ 50 \\ 60 \\ 70 \\ 80 \\ 90 \\ 100 \end{pmatrix}
 \end{array}
 \qquad
 \begin{array}{l}
 y_1 := \begin{pmatrix} 200 \\ 210 \\ 220 \\ 230 \\ 245 \\ 270 \\ 305 \\ 350 \\ 400 \\ 450 \\ 500 \end{pmatrix}
 \end{array}
 \qquad
 \begin{array}{l}
 y_2 := \begin{pmatrix} 200 \\ 253 \\ 308 \\ 363 \\ 412 \\ 448 \\ 473 \\ 485 \\ 490 \\ 495 \\ 500 \end{pmatrix}
 \end{array}$$

The *cspline* function produces an array, given the name vs , that contains the constants for a cubic spline that is fitted to the solidus line data above.

$$vs := \text{cspline}(x, y_1)$$

A continuous function for the solidus line is defined in terms of the spline constants by means of the *interp* function.

$$\text{Solidus}(z) := \text{interp}(vs, x, y_1, z)$$

$z := 0, 2..100$ A range variable of values for the x axis of the graph below

The *cspline* function is used again to produce a continuous function for the liquidus line.

$$vt := \text{cspline}(x, y_2)$$

$$\text{Liquidus}(z) := \text{interp}(vt, x, y_2, z)$$

The liquidus and solidus functions are used to find the liquidus and solidus temperatures corresponding to the sample composition specified below.

$$\text{Liquidus}(\text{Comp}) = 412$$

$$\text{Solidus}(\text{Comp}) = 245$$

The values of Comp_L and Comp_S are initial estimates.

$$\text{Comp}_L := 20 \quad \text{Comp}_S := 80$$

A solve block is used to determine the compositions of liquid and solid at the sample temperature.

Given

$$\text{Liquidus}(\text{Comp}_L) = \text{Temp}$$

$$\text{Solidus}(\text{Comp}_S) = \text{Temp}$$

$$\text{Comps} := \text{Find}(\text{Comp}_L, \text{Comp}_S)$$

$$\text{Comps} = \begin{pmatrix} 29.44 \\ 72.04 \end{pmatrix}$$

The solve block will fail to find a solution if the temperature is too high or too low. The conditional statements just below take care of those situations. In the first one, the liquid composition is set to 0 if the temperature is below the solidus temperature and set to the sample composition if the temperature is above the liquidus temperature.

$$\text{Comps}_0 := \begin{cases} \text{Comp} & \text{if } \text{Temp} > \text{Liquidus}(\text{Comp}) \\ 0 & \text{if } \text{Temp} < \text{Solidus}(\text{Comp}) \\ \text{Comps}_0 & \text{otherwise} \end{cases}$$

In the next conditional statement, the solid composition is set to the sample composition if the temperature is below the solidus temperature and set to 0 if the temperature is above the liquidus temperature.

$$\text{Comps}_1 := \begin{cases} \text{Comp} & \text{if Temp} < \text{Solidus}(\text{Comp}) \\ 0 & \text{if Temp} > \text{Liquidus}(\text{Comp}) \\ \text{Comps}_1 & \text{otherwise} \end{cases}$$

And here are the results

The liquid %B is $\text{Comps}_0 = 29.4$

The solid %B is $\text{Comps}_1 = 72.0$

Finally, a tie line calculation to find the amount of solid. There is an error trap in the event the user attempts to perform a tie line calculation in a single phase region.

$$\text{SOLID} := \begin{cases} 1 & \text{if Temp} \leq \text{Solidus}(\text{Comp}) \vee \text{Comp} > \text{Comps}_1 \\ 0 & \text{if Temp} \geq \text{Liquidus}(\text{Comp}) \vee \text{Comp} < \text{Comps}_0 \\ \frac{\text{Comp} - \text{Comps}_0}{\text{Comps}_1 - \text{Comps}_0} & \text{otherwise} \end{cases}$$

$$\text{Comps}_0 := \begin{cases} \text{"Single phase. All solid"} & \text{if SOLID} = 1 \\ \text{Comps}_0 & \text{otherwise} \end{cases}$$

$$\text{Comps}_1 := \begin{cases} \text{"Single phase. All liquid"} & \text{if SOLID} = 0 \\ \text{Comps}_1 & \text{otherwise} \end{cases}$$

The % of the sample that is solid is $\text{SOLID} = 24.8\%$

An array is created to contain the results of interest.

$$\text{Results} := \begin{pmatrix} \text{"Composition"} & \% & \text{Comp} \\ \text{"Temperature"} & \text{"C"} & \text{Temp} \\ \text{"Liquidus Temp"} & \text{"C"} & \text{Liquidus}(\text{Comp}) \\ \text{"Solidus Temp"} & \text{"C"} & \text{Solidus}(\text{Comp}) \\ \text{"Liquid Comp"} & \% \text{B} & \text{Comps}_0 \\ \text{"Solid Comp"} & \% \text{B} & \text{Comps}_1 \\ \text{"Amount Solid"} & \% & \text{SOLID} \cdot 100 \end{pmatrix}$$

Now specify a state point. That is specify the sample composition and temperature. Note the use of the global equals sign in these definitions. This causes the given values to be used above as well as below the definition.

Enter state point values here ==>>>
 Comp = 40
 Temp = 360

All results are generated automatically. If the state is in a single phase region, the reported composition of the phase that does not exist will be "NA".

Table of Results

Results =	"Composition"	"%"	40.0
	"Temperature"	"C"	360.0
	"Liquidus Temp"	"C"	412.0
	"Solidus Temp"	"C"	245.0
	"Liquid Comp"	"%B"	29.4
	"Solid Comp"	"%B"	72.0
	"Amount Solid"	"%"	24.8

