

THE IRON-IRON CARBIDE PHASE DIAGRAM IN MATHCAD

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INTRODUCTION

A previous article[1] in this journal presented a Mathcad worksheet that does calculations for a simple isomorphous phase diagram. This new article presents a Mathcad worksheet that performs similar calculations for steel in the vicinity of the eutectoid point. It determines the phases present, the relative amount of each phase, and the composition of each phase. Below the eutectoid temperature, the worksheet also calculates the amounts of pearlite and primary phase. Only two user inputs are required – the sample temperature and carbon content. The calculations are valid from 675°C to 900°C and from 0.0218% carbon to 1% carbon. Results are conveniently displayed in a table. The phase diagram, with the state point marked, is also displayed.

Curve Fits in the Phase Diagram

The entire Mathcad worksheet is contained in Figures 1 through 7, but only selected parts of the worksheet are discussed below. Details of the curve fitting are presented in Figure 1, parts (a) and (b). These figures depict the parts of the actual worksheet that do the curve fit calculations.

The A_3 and A_{cm} lines are modeled using Mathcad's cubic spline interpolation features described in the previous article. The boundaries of the all α region above and below the eutectoid temperature are modeled as straight lines. This representation is not as accurate as a cubic spline would be, but it is simpler, and little accuracy is lost, because the composition of the α phase has only a small effect on calculated results.

Cubic spline interpolation in Mathcad is described in detail in the earlier article. A brief

discussion of straight line interpolation is provided here. A typical section of the worksheet looks like this:

$$x_1 := \begin{pmatrix} 0 \\ 0.0218 \end{pmatrix} \% \quad y_1 := \begin{pmatrix} 900 \\ 727 \end{pmatrix}$$

The line function calculates the intercept and the slope.

| | Intercept | Slope |
|-------------------------------------|--------------------------|-------------------------------------|
| $\alpha_1 := \text{line}(x_1, y_1)$ | $\alpha_{1_0} = 900.000$ | $\alpha_{1_1} = -7.936 \times 10^5$ |

The function for the α boundary above 727C is simply:

$$a_1(x) := \begin{cases} \alpha_{1_0} + \alpha_{1_1} \cdot x & \text{if } x < 0.0218\% \\ 727 & \text{otherwise} \end{cases}$$

The two values in the array named x_1 are the x coordinates (carbon content) of the endpoints of the line, and the two values in the array named y_1 are the corresponding y coordinates (temperature). These two arrays are the arguments of the *line* function. Its outputs in array α_1 are the slope and the intercept of the line. From these values, the function $a(x)$ creates a straight line that approximates the boundary of the all α region above the eutectoid temperature. The second part of the definition of $a(x)$ draws a horizontal line at the eutectoid temperature. A similar procedure is used to approximate the boundary below the eutectoid temperature.

Brief Discussion of Figures 2 Through 5

Phase compositions are calculated by the equations shown in Figure 2, parts (a) and (b). Tie line analysis is performed by the equations shown in Figure 3, parts (a) and (b). The composition of the phases actually present at the

carbon content and temperature chosen by the user are calculated by the equations shown in Figure 4, and the relative amounts of these phases are calculated in Figure 5.

The modeling of lines is limited to the temperature range from 650°C to 900°C. This range encompasses essentially all the interesting activity in steel. Above 900°C there is only austenite, no matter what the carbon content. Below 650°C an unchanging mixture of ferrite and cementite exists no matter what the carbon content. The upper limit on carbon composition in this worksheet is 1.0%. While steel can have more carbon than this, such compositions are not common in plain carbon steel. The lower limit on carbon content is 0.0218%, which is the furthest extent of the all ferrite region.

The worksheet makes all the determinations that can be made by hand. First, it determines which phases are present at a given state point. Possibilities are limited to austenite (γ iron), ferrite (α iron), and cementite (iron carbide). Second, the composition of each phase present is calculated. Third, if the state point is in a two phase region, a tie line calculation is performed to determine the relative amounts of the phases. Fourth, the primary (proeutectoid) phase is determined. This determination is based only on carbon content. If the steel is hypoeutectoid, the worksheet reports ferrite as the primary phase regardless of the temperature. Similarly, if the steel is hypereutectoid, the worksheet always reports iron carbide as the primary phase. If the state point is in the all austenite region, the worksheet is simply reporting the primary phase that will appear when the sample is cooled. Finally, if the state point is below the eutectoid temperature, the worksheet reports the amount of pearlite and the amount of primary phase present.

Mathcad Programming Statements

In many places, the worksheet must make decisions based on carbon content and temperature. This state point determines what phases are present and what equation should be

used for tie line calculations. Here is an example:

$$\%Fe_3C := \begin{cases} 0 & \text{if } \%C \leq 0.77\% \wedge \text{Temp} \geq 727 \\ (100\% - \% \gamma) & \text{if } \%C > 0.77\% \wedge \text{Temp} \geq 727 \wedge \text{Temp} < T_{cm} \\ (100\% - \% \alpha_2) & \text{if } \text{Temp} < 727 \\ 0 & \text{otherwise} \end{cases}$$

In the first line, the relative amount of iron carbide is zero if the carbon content is less than 0.77% (the steel is hypoeutectoid), and the temperature is above the eutectoid temperature. In the second line, if the steel is hypereutectoid (carbon content above 0.77%) and the temperature is above the eutectoid temperature, the relative amount of iron carbide is 100% minus the percentage of austenite, which has already been calculated. If the temperature is below the eutectoid temperature, the relative amount of iron carbide is calculated in the third line as 100% minus the relative amount of ferrite, which has already been calculated. Finally, if none of the conditions in the first three lines is met, the relative amount of iron carbide is set to zero. There are many other structures like this in the worksheet, and the general idea is the same.

Use of the Worksheet

The user need not be concerned with Figures 1 through 5. All he or she needs to do is enter the carbon content and temperature at the top of Figure 6. The table of output information appears in a table directly below the inputs. Finally, the phase diagram itself, with state point displayed as a red diamond, is displayed in Figure 7.

Output values are collected in a table shown just below the input values in Figure 6. In this example, at 675°C and a carbon content of 0.95%, the table appears as follows:

| | | |
|-----------------------|-----------|-----------|
| "" | "Phase 1" | "Phase 2" |
| "Name" | "ferrite" | "carbide" |
| "Composition (%C)" | 0 | 6.67 |
| "Relative Amount (%)" | 85.757 | 14.243 |
| "Primary Phase" | "carbide" | "" |
| "Amt Pri Phase (%)" | 3.051 | "" |
| "Amount Pearlite (%)" | 96.949 | "" |

As expected for hypereutectoid steel below the eutectoid temperature, the phases present are ferrite and iron carbide. The primary phase is iron carbide, which makes up 3% of the sample. The remainder of the sample is pearlite. In Mathcad, all numerical values in a table must show the same number of decimal places. In order to display three decimal places for the carbon content of ferrite, the table must be formatted to display three decimal places for all results. As a consequence the number of decimal places shown for the relative amounts of phases is often excessive. Figure 7 shows the phase diagram that appears at the end of the worksheet. Similar tables and phase diagrams can be generated for any carbon content between 0.0218% and 1% and temperatures between 650°C and 900°C. The worksheet has been tested in all regions of the diagram that fall within these limits, and the results are accurate.

Note that if the temperature is exactly 727°C, the phases present, their compositions, and their relative amounts are indeterminate. To avoid problems with the worksheet, it must be set to give arbitrarily chosen output at this temperature, but that output is not meaningful.

Summary

Like the isomorphous phase diagram worksheet described in the earlier article, this worksheet is intended as a tool for the instructor in a basic materials science course. Display of the state point is easily suppressed, and the printed phase diagram can be given to students as part of a test or homework assignment. The

instructor can quickly and easily prepare the solution key. Only the last two pages of the worksheet need be printed. The last page contains the phase diagram, and the next to last page contains the input values and the output table.

References

1. Wiggins, Edwin G., "Isomorphous Phase Diagrams in Mathcad, A Powerful Tool for Instructors" *Computers in Education Journal*, Vol. XVII, no. 3, p.106.

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. As a representative of SNAME, Ed Wiggins served on the Technology Accreditation Commission, the Engineering Accreditation Commission, and the Board of Directors of the Accreditation Board for Engineering and Technology (ABET). A Centennial Medallion and a Distinguished Service Award recognize his service to SNAME.

The worksheet models the iron-iron carbide phase diagram in the vicinity of the eutectoid point (650C to 900C and 0.0218%C to 1%C).

Above 727C there are 3 lines to be represented: the α boundary, the A_3 and the A_{cm} . For the α boundary, a straight line is sufficiently accurate. First equations are developed for these lines. The line for the α boundary is developed as follows:

Below 727C there is a different α boundary at the left and 6.67%C at the right.

So, the α boundary above 727C is represented as a straight line. Here are the endpoints.

$$x_1 := \begin{pmatrix} 0 \\ 0.0218 \end{pmatrix} \% \quad y_1 := \begin{pmatrix} 912 \\ 727 \end{pmatrix}$$

The line function calculates the intercept and the slope.

| | Intercept | Slope |
|-------------------------------------|--------------------------|-------------------------------------|
| $\alpha_1 := \text{line}(x_1, y_1)$ | $\alpha_{1_0} = 912.000$ | $\alpha_{1_1} = -8.486 \times 10^5$ |

The function for the α boundary above 727C is simply:

$$a_1(x) := \begin{cases} \alpha_{1_0} + \alpha_{1_1} \cdot x & \text{if } x < 0.0218\% \\ 727 & \text{otherwise} \end{cases}$$

For the A_3 line, cubic spline interpolation is used. Here are the data points.

$$x_2 := \begin{pmatrix} 0 \\ 0.2 \\ 0.4 \\ 0.6 \\ 0.77 \end{pmatrix} \% \quad y_2 := \begin{pmatrix} 912 \\ 828 \\ 781 \\ 750 \\ 727 \end{pmatrix}$$

$$vs := \text{cspline}(x_2, y_2)$$

Here is the continuous function for the A_3 line.

$$A_3(x) := \text{interp}(vs, x_2, y_2, x)$$

Figure 1 (a)

A_3 and α Boundary Curve Fit Above 727°C

For the A_{cm} line, cubic spline interpolation is used again. Here are the data points

$$x_4 := \begin{pmatrix} 0.77 \\ 0.9 \\ 1 \end{pmatrix} \% \quad y_4 := \begin{pmatrix} 727 \\ 782 \\ 820 \end{pmatrix}$$

$$vt := \text{cspline}(x_4, y_4)$$

Here is the continuous function for the A_{cm} line.

$$A_{cm}(x) := \text{interp}(vt, x_4, y_4, x)$$

The A_3 and the A_{cm} lines are combined into a single function below.

$$A(x) := \begin{cases} A_3(x) & \text{if } x < 0.77\% \\ A_{cm}(x) & \text{if } x \geq 0.77\% \end{cases}$$

For the α boundary below 727C, another straight line is used.

$$x_3 := \begin{pmatrix} 0 \\ 0.0218 \end{pmatrix} \% \quad y_3 := \begin{pmatrix} 675 \\ 727 \end{pmatrix}$$

The line function calculates the intercept and slope.

$$\alpha_2 := \text{line}(x_3, y_3) \quad \alpha_{2_0} = 675.000 \quad \alpha_{2_1} = 2.385 \times 10^5$$

The function for the α boundary below 727C is simply:

$$a_2(x) := \begin{cases} \alpha_{2_0} + \alpha_{2_1} \cdot x & \text{if } x < 0.0218\% \\ 727 & \text{otherwise} \end{cases}$$

Figure 1 (b)
Acm and α Boundary Curve Fit Below 727°C

Composition of Fe₃C

Carbide := 6.67%

A range variable for the x coordinate in the phase diagram below.

$$x := 0\%, 0.01\%.. 1\%$$

Redefine α_1 and α_2 for convenience below.

$$\alpha_a(z) := \alpha_{1_0} + \alpha_{1_1} \cdot z$$

$$\alpha_b(z) := \alpha_{2_0} + \alpha_{2_1} \cdot z$$

In the α and γ region:

$$T_3 := A_3(\%C) \quad T_3 = 699 \quad \text{The temperature on the A3 line at the system composition.}$$

The phase compositions are calculated by a solve block. Here are the guess values.

$$\alpha := 0.02\% \quad \gamma_1 := 0.4\% \quad \beta := 0.02\%$$

Given

$$\alpha_a(\alpha) = \text{Temp}$$

$$\alpha_b(\beta) = \text{Temp}$$

$$\begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} := \text{Find}(\alpha, \beta) \quad \alpha_1 = 0.028\% \quad \alpha_2 = 0.0000\%$$

For any given system temperature only one of the α s is valid. The ferrite variable below contains the valid one.

$$\text{ferrite} := \begin{cases} \alpha_1 & \text{if Temp} \geq 727 \\ \alpha_2 & \text{if Temp} < 727 \end{cases}$$

$$\text{ferrite} = 0.0000\% \quad \text{The ferrite composition}$$

Figure 2 (a)
Calculation of Ferrite and Cementite Phase Compositions

The second part of the A3 function below is phony but necessary for some of the calculations below. Continuous values above %C of 0.0218% are required.

$$A_3(x) := \begin{cases} A_3(x) & \text{if } x \leq 0.77\% \\ (727 - 100x) & \text{otherwise} \end{cases}$$

Given

$$A_3(\gamma_1) = \text{Temp}$$

$$\gamma_1 := \text{Find}(\gamma_1) \quad \gamma_1 = 52.000\% \quad \gamma \text{ composition for hypoeutectoid steel at Temp}$$

In the γ and iron carbide region:

$$T_{cm} := A_{cm}(\%C) \quad T_{cm} = 801 \quad \text{The } A_{cm} \text{ temperature at the sample composition}$$

$$\gamma_2 := 0.9\% \quad \text{a guess value}$$

Given

$$A_{cm}(\gamma_2) = \text{Temp}$$

$$\gamma_2 := \text{Find}(\gamma_2) \quad \gamma_2 = 0.67\% \gamma \text{ composition for hypereutectoid steel at Temp}$$

There are two values of γ composition above, but only one is valid. The statements below select the proper one.

$$\gamma := \begin{cases} \gamma_1 & \text{if } \text{Temp} < T_3 \wedge \text{Temp} > 727 \wedge \%C < \gamma_1 \\ \gamma_2 & \text{if } \text{Temp} < T_{cm} \wedge \text{Temp} > 727 \wedge \%C > \gamma_2 \\ \%C & \text{otherwise} \end{cases}$$

$$\boxed{\gamma = 0.95\%}$$

Figure 2 (b)
Calculation of Austenite Phase Composition

Tie line calculation above 727C

$$\% \gamma_1 := \frac{\%C - \alpha}{\gamma_1 - \alpha} \quad \boxed{\% \gamma_1 = 1.8\%}$$

$$\% \alpha_1 := 100\% - \% \gamma_1 \quad \% \alpha_1 = 98.2\%$$

$$\% \gamma_2 := \frac{6.67\% - \%C}{6.67\% - \gamma_2} \quad \boxed{\% \gamma_2 = 95.3\%}$$

$$\% \text{Fe}_3\text{C} := 100\% - \% \gamma_2 \quad \% \text{Fe}_3\text{C} = 4.651\% \quad \text{Valid only for hypereutectoid}$$

There are 2 values of relative amount of γ above, but only one is valid. The statement below select the proper one.

$$\% \gamma := \begin{cases} \% \gamma_1 & \text{if Temp} < T_3 \wedge \text{Temp} > 727 \wedge \%C < \gamma_1 \\ \% \gamma_2 & \text{if Temp} < T_{\text{cm}} \wedge \text{Temp} > 727 \wedge \%C > \gamma_2 \\ 0 & \text{if Temp} < 727 \\ 100\% & \text{otherwise} \end{cases}$$

$$\boxed{\% \gamma = 0.0\%}$$

Tie line calculation below 727C

Given

$$\alpha_b(\alpha) = \text{Temp}$$

$$\alpha_2 := \text{Find}(\alpha)$$

$$\alpha_2 = 0.0000\%$$

$$\% \alpha_2 := \frac{\text{Carbide} - \%C}{\text{Carbide} - \alpha_2}$$

$$\% \alpha_2 = 85.757\% \quad \text{The relative amount of } \alpha \text{ IF the steel is below } 727\text{C}$$

Figure 3 (a)
Tie Line Calculations Part 1

The statements below calculate the relative amount of Fe₃C for various cases

$$\%Fe_3C := \begin{cases} 0 & \text{if } \%C \leq 0.77\% \wedge \text{Temp} \geq 727 \\ (100\% - \% \gamma) & \text{if } \%C > 0.77\% \wedge \text{Temp} \geq 727 \wedge \text{Temp} < T_{cm} \\ (100\% - \% \alpha_2) & \text{if } \text{Temp} < 727 \\ 0 & \text{otherwise} \end{cases}$$

$$\%Fe_3C = 14.243\%$$

$$\%Pearlite := \begin{cases} \frac{\%C - \alpha_2}{0.77\% - \alpha_2} & \text{if } \%C \leq 0.77\% \wedge \%C \geq \alpha_2 \wedge \text{Temp} < 727 \\ \frac{\text{Carbide} - \%C}{\text{Carbide} - 0.77\%} & \text{if } \%C > 0.77\% \wedge \text{Temp} < 727 \\ 0 & \text{otherwise} \end{cases}$$

$$\%Pearlite = 96.9\%$$

The statement below determines what the primary phase is

$$\text{PriPhase} := \begin{cases} \text{"ferrite"} & \text{if } \%C < 0.77\% \\ \text{"carbide"} & \text{if } \%C > 0.77\% \\ \text{"NA"} & \text{otherwise} \end{cases}$$

The statement below calculates the amount of primary phase for various case:

$$\text{AmtPriPhase} := \begin{cases} (100\% - \%Pearlite) & \text{if } \text{Temp} < 727 \\ \% \alpha_1 & \text{if } \text{Temp} \geq 727 \wedge \%C \leq 0.77\% \\ 100\% - \% \gamma & \text{if } \text{Temp} \geq 727 \wedge \%C > 0.77\% \\ 0 & \text{if } \% \gamma = 100\% \end{cases}$$

$$\text{PriPhase} = \text{"carbide"}$$

$$\text{AmtPriPhase} = 3.1\%$$

Figure 3 (b)
Tie Line Calculations Part 2

The statement below determines the identity of one of the phases present.

$$\text{Phase}_1 := \begin{cases} \text{"ferrite"} & \text{if } \text{Temp} \leq T_3 \wedge \%C \leq 0.77\% \wedge \text{Temp} > 727 \\ \text{"carbide"} & \text{if } \text{Temp} \leq T_{cm} \wedge \%C \geq 0.77\% \wedge \text{Temp} > 727 \\ \text{"ferrite"} & \text{if } \text{Temp} < 727 \\ \text{"austenite"} & \text{otherwise} \end{cases}$$

$$\text{Phase}_1 = \text{"ferrite"}$$

The statement below determines the identity of the other phase present. If only one phase is present, it must be γ . Both Phase_1 and Phase_2 will evaluate to "austenite."

$$\text{Phase}_2 := \begin{cases} \text{"austenite"} & \text{if } \text{Temp} \geq 727 \\ \text{"carbide"} & \text{otherwise} \end{cases}$$

$$\text{Phase}_2 = \text{"carbide"}$$

The statement below determines the composition of Phase_1

$$\text{CompPhase1} := \begin{cases} \text{ferrite} & \text{if } \text{Temp} \leq T_3 \wedge \%C \leq 0.77\% \wedge \text{Temp} > 727 \\ 6.67\% & \text{if } \text{Temp} \leq T_{cm} \wedge \%C \geq 0.77\% \wedge \text{Temp} > 727 \\ \text{ferrite} & \text{if } \text{Temp} < 727 \\ \gamma & \text{otherwise} \end{cases}$$

$$\text{CompPhase1} = 0.000\%$$

The statement below determines the composition of Phase_2

$$\text{CompPhase2} := \begin{cases} \gamma & \text{if } \text{Temp} \geq 727 \\ \text{Carbide} & \text{otherwise} \end{cases}$$

$$\text{CompPhase2} = 6.670\%$$

Figure 4
Determine of Compositions of Phases Actually Present

The statement below determines the relative amount of Phase₁

$$\text{AmtPhase1} := \begin{cases} \% \alpha_1 & \text{if } \text{Temp} \leq T_3 \wedge \%C \leq 0.77\% \wedge \text{Temp} > 727 \\ \% \text{Fe3C} & \text{if } \text{Temp} \leq T_{cm} \wedge \%C \geq 0.77\% \wedge \text{Temp} > 727 \\ \% \alpha_2 & \text{if } \text{Temp} < 727 \\ \% \gamma & \text{otherwise} \end{cases}$$

The statement below determines the relative amount of Phase₂

$$\text{AmtPhase2} := \begin{cases} \% \gamma & \text{if } \text{Temp} \geq 727 \\ \% \text{Fe3C} & \text{otherwise} \end{cases}$$

The matrix below assembles the values for the table that follows.

$$\text{Phases} := \begin{pmatrix} & "" & \text{"Phase 1"} & \text{"Phase 2"} \\ \text{"Name"} & & \text{Phase}_1 & \text{Phase}_2 \\ \text{"Composition (\%C)"} & & \text{CompPhase1} \cdot 100 & \text{CompPhase2} \cdot 100 \\ \text{"Relative Amount (\%)} & & \text{AmtPhase1} \cdot 100 & \text{AmtPhase2} \cdot 100 \\ \text{"Primary Phase"} & & \text{PriPhase} & "" \\ \text{"Amt Pri Phase (\%)} & & \text{AmtPriPhase} \cdot 100 & "" \\ \text{"Amount Pearlite (\%)} & & \% \text{Pearlite} \cdot 100 & "" \end{pmatrix}$$

Figure 5
Determination of Amounts of Phases Actually Present

At the following state point (enter values below)

$\%C \equiv 0.95\%$

$\text{Temp} \equiv 675$

Values are as follows

| | "" | "Phase 1" | "Phase 2" |
|----------|------------------------|-----------|-----------|
| | "Name" | "ferrite" | "carbide" |
| | "Composition (\%C)" | 0 | 6.67 |
| Phases = | "Relative Amount (\%)" | 85.757 | 14.243 |
| | "Primary Phase" | "carbide" | "" |
| | "Amt Pri Phase (\%)" | 3.051 | "" |
| | "Amount Pearlite (\%)" | 96.949 | "" |

Figure 6
User Inputs and Mathcad Outputs

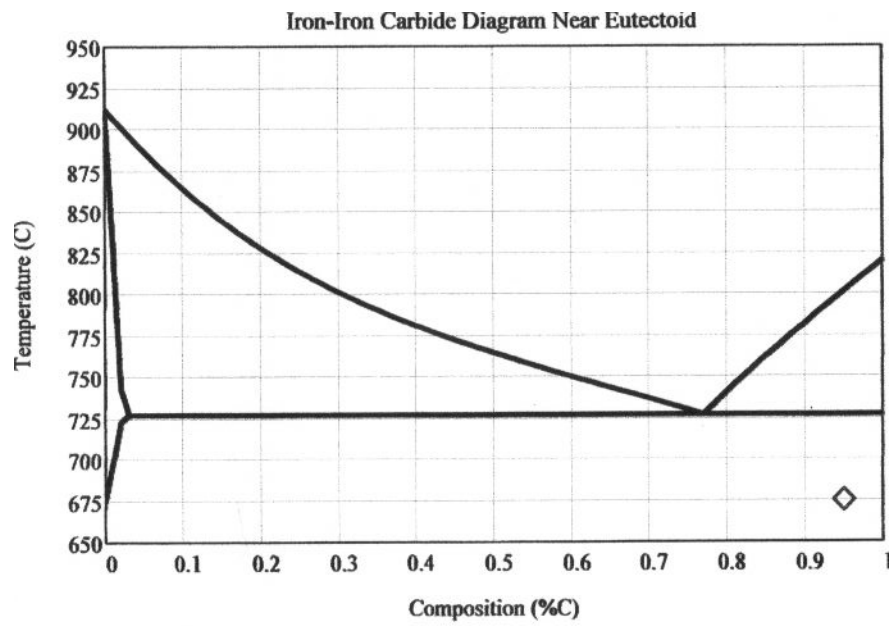


Figure 7
Phase Diagram With State Point

