A Computer Application In Materials Engineering Technology Course

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ABSTRACT

This paper describes the application of mathematical software, Mathcad™, in designing the heat treatment of steel. Such a software solution method is an effective teaching tool that finds many practical applications in engineering and technology. The Mathcad™ solution method assists engineering technology students, providing simplified solutions of complex diffusion equations and a graphical approach in modeling the heat treatment. The overall impression of the course from the student's perspective was favorable to the mathematical software method.

INTRODUCTION

Computer technology, as a tool for problem solving and data analysis, has been used in technical science curricula. To receive maximum benefit, students should be exposed to the use of computer technology and be encouraged to develop their competence in their field throughout the curriculum. This paper introduces diffusion mechanism in metals and present the most frequently encountered processing operation: the carburization of steels. Thus, the mathematical models in diffusion are presented along with practical examples in hypothetical carburization treatment. To minimize the mathematical difficulties, a graphical solution method in diffusion process is applied by the Mathcad™ software. This graphical solution method provides an effective tool to teach principles of diffusion for engineering technology students.

COMPUTER APPLICATION IN TEACHING

Materials science, the study of materials engineering and technology, has become an important addition to mechanical engineering technology education for the past decade. However, engineering technology students have historically shown the deficiency of knowledge in mathematics and science, which are the building blocks of materials science and technology. This deficiency of knowledge has caused a frustration for instructor to teach materials science and technology courses in the engineering technology program.

The advancement of computer technology has geared to change the method of instructional delivery in teaching, so the computer aided instructional method has given a significant impact to redesign the course materials in engineering and technical science curricula. The computer and the application software (such as Mathcad or MathLab) have been easily accessible for students and professors in campus. Recently, the manu-driven application software has assisted the students to provide solutions for relatively complex problems assigned in technical science courses. This situation clearly indicates that there is an opportunity for many improvements in the curriculum, particularly in materials courses, using the computer and the application software.

The application software (mathematical software, such as Mathcad™) provides a powerful tool to teach basic or applied fundamentals in engineering technology curriculum. The mathematical software makes course materials more modern, interesting, and realistic while retaining basic principles in the course contents. Since the Mathcad has the ability to enter formulas, variables, mathematical operations, graphs, and texts on the worksheet. Once a Mathcad model on the worksheet is properly built, mathematical formulas can be solved and thus, the solutions can be graphically displayed for many different examples. Using such a mathematical software method simplifies complex equations so that the engineering technology students can minimize the difficulties in understanding mathematical models in materials engineering technology. Thus, engineering and engineering technology educator considers the Mathcad an affective teaching tool for both solving mathematical models and knowledge management in many sciences and technology courses.

EXAMPLE AND ANALYSIS OF CARBURIZATION

The following examples show how relatively straightforward carburization process can be demonstrated for students to deliver basic concepts of carburization along with mathematical solution and graphical illustration when solved using the Mathcad software.

1) EXAMPLE IN FICK'S FIRST LAW

Steel surfaces can be hardened by carburization. A thin plate of the iron specimen is heated to 900 °C in furnace. During such a heat treatment, one side of the specimen in contact with a carbon-rich gas (CO/CO_2) mixture that maintains the carbon concentration at the surface at the initial concentration of 1.53×10^{21} atoms/cm^3. The other side of the specimen is in contact with the carbon concentration at 7.65×10^{20} atoms/cm^3. The thickness of the specimens is 1 mm. Compute the flux of carbon atoms into the steel specimen in the near-surface. Suppose that the carbon concentration gradient described in the above occurred at various heat treatment temperatures: 850°C, 900 °C, 950 °C, 1000 °C,1050 °C, and 1100 °C.

Mathcad™ Analysis:

The use of Mathcad software begins with the presentation of basic concepts and mathematical relationships (or models), which are followed by examples illustrating the concepts. Once students understand these concepts and then, they have to be able to extrapolate answers for solving given examples, using the Mathcad. Also, the necessity of graphical approach is emphasized for analyzing, interpreting, and evaluating the information. Thus, the students can combine the concepts and practices to approach problem-solving for complex technologic issues.

The flux of carbon atoms at 850 °C, 900 °C, 950 °C, 1000 °C, 1050 °C, and 1100 °C can be calculated on the Mathcad's worksheet in Fig. 1. The numerical solution in the example can be converted to the Mathcad’s document interface of a spreadsheet with a word processor. Thus, we can typeset equations on the screen exactly the way we see them in the textbook. The following example in Fig. 3 shows how to define a variable, use a graphical method, and evaluate the equation on the Mathacd™ worksheet. More details in the methods for working with formulas, numbers, text, and graphs, are included elsewhere [1].

The numerical computation on the worksheet is necessary for plotting temperature versus flux graphs. Figs. 2-1 and 2-2 show graphical illustrations in the flux change as a function of carburizing temperature based on the worksheet computation. After mathematical formulas are entered, the results of the flux changes are calculated and thus, the graphical solution can be generated in the same worksheet. The ease of graphical expression is an advantage of the Mathcad solution method so that students can easily recognize the temperature effects on the flux change of carbon atoms in a diffusion process. As the carburizing temperature increases, the diffusion coefficient and the flux of species increase as well (Fig. 2-1 and 2-2). For example, the bar graph (Fig. 2-2) shows that the flux of carbon in austenite at 950 °C (1223 K) is about 68 % greater than at 850 °C (1123 K). In higher carburizing temperatures, the thermal energy supplied to the diffusing carbon atoms permits the atoms to overcome the activation energy barrier and easily move to neighboring lattice sites [2,3]. In conclusion, the rate at which carbon can be added to the steel specimen, is controlled by the diffusivity of carbon.

2) EXAMPLE IN FICK'S SECOND LAW

A gear made of AISI 1020 steel is to be strengthened by the carburizing treatment process. In carburizing, the steel gear is placed in a carbon-rich atmosphere that provides a 1.0 % of the carbon solution at the surface. The carburizing temperature is 950 °C. Develop the carbon profile after 1, 3, 6, and 10 hours in the design of the carburizing treatment process for this steel gear.

Mathcad™ Analysis:

In this example, the diffusion zone is small compared with typical gear dimensions so that the assumption of a semi-infinite solid is applicable to analyze the carburization treatment by Fick’s second law.

The carbon concentrations for different carburizing treatment times are computed on the Mathcad worksheet (Fig. 3). The results of the carbon concentration profile at 1 hour, 3 hours, 6 hours, and 10 hours are graphically shown in Figure 4. The concentration of carbon depends both on location (*x*) and time (*t*). For example, the concentrations of carbon (C_X) at the location of x = 0.01 cm below the surface after 1 hour, 3 hours, 6 hours, and 10 hours are 0.821 %, 0.896 %, 0.926 %, and 0.943 %, respectively. The concentrations of carbon (C_X) at the location of x = 0.05 cm below the surface after 1-, 3-, 6-, and 10-hours are 0.324 %, 0.530 %, 0.650 %, and 0.723 %, respectively. These results show that higher carbon concentration can be obtained at a desired distance below the surface of steel gear by increasing the carburizing time . The increase in the carburizing time can boost the carbon concentration at the surface so that the surface of the steel gear can be hardened through a subsequent quenching and tempering heat treatment [3-7]. The carburizing time can be also reduced by increasing the carburizing temperature to accomplish the desired surface property in steel. However, we have to consider heating time to determine whether an increase in carburizing temperature will results in overall savings. The case depth resulting from the carburization process is visible and measurable in a metallographic study. However, the microstructural investigation of case hardened steel is beyond the scope of this paper.

EDUCATIONAL BENEFITS

The Mathcad software has been used in materials engineering technology courses at Indiana University-Purdue University, Fort Wayne. In particular, the Mathcad provides an effective tool to teach principles in materials and processes to the lower level of undergraduate students, who are not well prepared in mathematics. Using such a software method simplifies complex equations so that students can minimize the difficulties in understanding mathematical models in materials engineering technology. It also allows students to directly write laboratory reports on the worksheet. The students say that the Mathcad™ solution method makes them clearly understand the lecture contents and laboratory exercise in the carburization of steels.

CONCLUSION

Diffusion in the heat treatment of steels is expressed in Fick's first and second laws. The analysis and simulation of carburizing processes are performed using the Mathcad solution method. Thus, engineering technology students are able to analyze and simulate complex diffusion phenomena in hypothetical heat treatment systems.

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Figure 1. Mathcad worksheet for solving example in Fick's first law .

The concentrations of carbon atoms are given:

$$C1 := 1.53 \cdot 10^{21}$$

$$C2 := 7.65 \cdot 10^{20}$$

The thickness of the steel specimen is given:

$\Delta x := 0.1$

The activation energy (q), the diffusivity (Do), and the gas constant(g) are:

$q := 142000$
$Do := 0.2$
$R := 8.314$

Calculate the flux of carbon atom at various temperatures: 850, 900, 950, 1000, 1050, and 1100 celsius degrees.

$i := 850, 900 .. 1100$

The conversion of temperture from Celsius degree to Kelvin degree:

$T_i := i + 273$

We can calculate the diffusion coefficient at various temperatures:

$$D_i := Do \cdot \exp\left(-\frac{q}{R \cdot T_i}\right)$$

Using Fick's firs law gives:

$$J_i := D_i \cdot \left[\frac{(C1 - C2)}{\Delta x}\right]$$

The flux of carbon at various temperatures can be calculated. Here Table 2 is constructed to plot the flux (J: atoms/cm ^{2} sec) versus temperature (K) graph.

Table 2. Temperature (K) Versus Flux (J)

T_i	J_i
$1.123 \cdot 10^3$	$3.798 \cdot 10^{14}$
$1.173 \cdot 10^3$	$7.263 \cdot 10^{14}$
$1.223 \cdot 10^3$	$1.317 \cdot 10^{15}$
$1.273 \cdot 10^3$	$2.279 \cdot 10^{15}$
$1.323 \cdot 10^3$	$3.785 \cdot 10^{15}$
$1.373 \cdot 10^3$	$6.057 \cdot 10^{15}$

Figure 2. 1) The line and 2) bar graphs for flux (J) versus temperature (K)

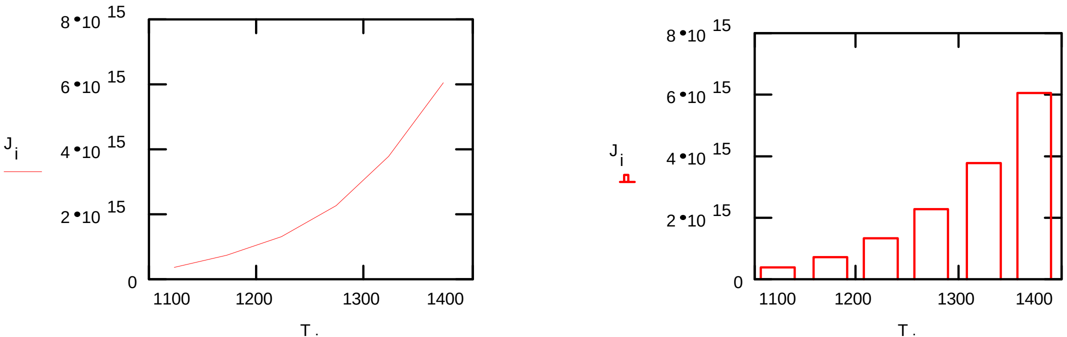

Figure 2.1: line graph

Figure 2.2: bar graph

Figure 3. Mathcad worksheet interfaced with text for solving eaxmple in Fick's second law.

Mathhacad shows equations as we see them in book. By defining variables and functions, we can link equations together and use intermediate results in further calculations.
In example, the initial carbon concentration is Co = 0.2 % and the boundary condition at the surface of the specimen is Cs = 1.0 %: Defining Cs, type Cs and then, press the colon key (:). Mathcad shows the colon as the definition symbol ":=." Then type 1 (%) as the carbon concentration at the surface. And define Co ":=" 0.2 (%) as the initial carbon concentration.

$$Cs := 1 \qquad Co := 0.2$$

Using Equation (6), we can compute the diffusivity (D) of carbon atoms (cm2/s) at 1223 K:

$$D := 0.2\cdot\exp\left[\frac{-142000}{(8.314)\cdot(1223)}\right]$$

Now that we can calculate the diffusivity by pressing the letter "D" and the equals sign "=." Mathcad returns results as shown:

$$D = 1.722\cdot 10^{-7}$$

Mathcad can do repeated calculations called a range variable. To define a range variable, type the variable name, location = x, followed by the colon key (:). Type 0 at the location = 0, i.e, the surface of the specimen. Then type the step size 0.01 cm. Press semicolon key (;). Mathcad shows semicolon as two periods ".." to indicate a range. And complete the range definition by typing 0.1 cm.

$$x := 0, 0.01 .. 0.1$$

The above definition indicates that the carbon concentration can be calculated by taking the values.
x = 0, 0.01, 0.02, 0.03, 0.04..., and 0.1cm.

Also we define the carburizing time: type the letter t1, the colon key (:), and then, 1 hour (t1 = 3600 seconds). Thus we can define other values for 3 hours (t3), 6 hours (t6) and 10 hours (t10).

$$t1 := 3600 \qquad t3 := 10800 \qquad t6 := 21600 \qquad t10 := 36000$$

The concentration of carbon at various locations, x (cm), after 1 hour (t1 = 3600 sec), 3 hours (t2 = 10800 sec), 6 hours (t6 = 21600 sec), and 10 hours (t10 = 36000) can be calculated using the defined equation:

$$C(x, t1) := Cs + (Co - Cs)\cdot\operatorname{erf}\left(\frac{x}{2\cdot\sqrt{D\cdot t1}}\right) \qquad C(x, t3) := Cs + (Co - Cs)\cdot\operatorname{erf}\left(\frac{x}{2\cdot\sqrt{D\cdot t3}}\right)$$

$$C(x, t6) := Cs + (Co - Cs)\cdot\operatorname{erf}\left(\frac{x}{2\cdot\sqrt{D\cdot t6}}\right) \qquad C(x, t10) := Cs + (Co - Cs)\cdot\operatorname{erf}\left(\frac{x}{2\cdot\sqrt{D\cdot t10}}\right)$$

Table 3. Carbon concentration calculation results at various locations

x	C(x , t1)	C(x , t3)	C(x , t6)	C(x , t10)
0	1	1	1	1
0.01	0.821	0.896	0.926	0.943
0.02	0.656	0.794	0.853	0.886
0.03	0.515	0.698	0.782	0.83
0.04	0.405	0.609	0.714	0.776
0.05	0.324	0.53	0.65	0.723
0.06	0.271	0.46	0.589	0.672
0.07	0.237	0.401	0.534	0.624
0.08	0.218	0.352	0.483	0.578
0.09	0.208	0.312	0.437	0.535
0.1	0.204	0.281	0.397	0.495

Figure 4. The carbon concentration profile for various carburizing times.