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Predictive Model for the Carbon Concentration Profile of Vacuum Carburized Steels with Acetylene

Minsu Jung[1], Sehoon Oh[2], and Young-Kook Lee[1,*]

[1]Department of Materials Science and Engineering, Yonsei University,
262 Seongsanno, Seodaemun-gu, Seoul 120-749, Korea
[2]School of Mechanical Engineering, Chung-Ang University,
221 Heukseok-dong, Dongjak-gu, Seoul 156-756, Korea

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A predictive model for the carbon concentration profile in vacuum carburized steels with acetylene was proposed. The model involves the process and boundary conditions based on the characteristic of vacuum carburizing with acetylene and carbon diffusivity with an alloying element effect. In order to verify the predictive model, the carbon concentration profile of a cylindrical SCM415 steel specimen vacuum carburized with acetylene was calculated using the finite element method. The carbon concentration profile calculated with the alloying element effect, the carbon diffusivity in the Fe-C binary system proposed by Tibbetts, and multiple time steps of carburizing and diffusion exhibited good agreement with the measured carbon profile.

Keywords: vacuum carburizing, acetylene gas, carbon diffusivity, finite element method

1. INTRODUCTION

Carburizing is a type of surface hardening process that is used for various machine parts. Prediction and control of the effective case depth, microstructure, residual stress, and deformation of machine parts during a carburizing heat treatment require an accurate carbon concentration profile in steels because the carbon content affects the phase transformations and mechanical properties. Therefore, intensive and extensive investigations regarding the prediction of the carbon concentration profile in steels have been conducted mainly as they pertain to gas carburizing [1-5].

Recently, the carburizing process has gradually changed from gas carburization to vacuum carburization due to the excellent uniformity, repeatability, oxidation-free products, short carburizing time, and eco-friendly process of vacuum carburization [6,7]. In particular, vacuum carburizing with acetylene gas can reduce shooting considerably compared to the use of other carburizing gases [8,9].

Therefore, a predictive model of the carbon concentration profile in steels during and after vacuum carburizing with acetylene is required. Moreover, the diffusivity of carbon, one of the important factors in carburization, has been suggested as a function of the carbon concentration and the carburizing temperature [1-3]. However, there are few equations that concern carbon diffusivity when other alloying element effects are included.

In the present study, therefore, a predictive model of the carbon concentration profile that takes into account other alloying element effects is proposed for vacuum carburization with acetylene. The model is verified by comparisons between the measured and calculated carbon concentration profiles after vacuum carburizing with acetylene using a cylindrical SCM415 steel specimen.

2. SIMULATION MODEL

The carbon concentration profile of a carburized specimen can be predicted using the degree of carbon diffusivity, the carburizing process conditions, the boundary condition, and the specimen shape and dimensions as input data for the finite element method. Accurate carbon diffusivity and reasonable boundary conditions are important for a precise prediction of the carbon concentration profile.

2.1. Diffusivity of carbon

The diffusivity of carbon is reportedly a function of the temperature and carbon concentration [1-3]. In a strict sense, however, the effect of other alloying elements on the diffusivity of carbon should also be considered, as in most cases, vacuum carburizing is performed with alloy steels. In the present study, therefore, carbon diffusivity is derived as a function of the temperature and the concentrations of carbon

*Corresponding author: yklee@yonsei.ac.kr

and other alloying elements.

Variation of the carbon diffusivity with the activity coefficient of carbon is represented by Eq. 1, as originally proposed by Birchenall and Mehl [10].

$$D = D_0\gamma\left(1 + c\frac{d\ln\gamma}{dc}\right) \quad (1)$$

Here, D denotes the carbon diffusivity, D_0 is the carbon diffusivity in an infinite dilute solution, c is the carbon concentration, and γ is the activity coefficient of carbon.

The activity coefficient of carbon in a multi-component system was suggested by Wagner [11]:

$$\ln\gamma_c^* = \ln\gamma_c^0 + \Sigma x_i\frac{d\ln\gamma_c^i}{dx_i} = \ln\gamma_c^0 + \Sigma x_i\varepsilon_c^i \quad (2)$$

where γ_c^*, γ_c^0, and γ_c^i are the activity coefficients of carbon in a multi-component system, in a Fe-C binary system, and in a component i-C binary system, respectively. x_i is the mole fraction of component i. ε_c^i is an interaction coefficient defined as $d\ln\gamma_c^i/dx_i$.

The ratio (q) of the activity coefficient of carbon in a multi-component system to that in a Fe-C binary system is represented by Eq. 2, as follows:

$$q = \frac{\gamma_c^*}{\gamma_c^0} = \exp(\Sigma x_i\varepsilon_c^i) \quad (3)$$

By combining Eqs. 1 and 3, D is re-written as follows:

$$D = D_0\gamma_c^*\left(1 + c\frac{d\ln\gamma_c^*}{dc}\right) = D_0q\gamma_c^0\left(1 + c\frac{d\ln(q\gamma_c^0)}{dc}\right) \quad (4)$$

Eq. 4 is re-written as Eq. 6 by substituting Eq. 5 for Eq. 4.

$$\frac{d\ln(q\gamma_c^0)}{dc} = \frac{1}{\gamma_c^0}\left(\frac{d\gamma_c^0}{dc}\right) = \frac{d\ln(\gamma_c^0)}{dc} \quad (5)$$

$$D = \left\{D_0\gamma_c^0\left(1 + c\frac{d\ln(\gamma_c^0)}{dc}\right)\right\} \times q \quad (6)$$

On the right side of Eq. 6, the term inside the braces is the carbon diffusivity in the Fe-C binary system, and q denotes the alloy element effect. The carbon diffusivity proposed by Tibbetts [3] was used for the carbon diffusivity in the Fe-C binary system:

$$D_c^o = 0.47\exp(-1.6c)\exp\left(-\frac{154.9 - 27.63c}{RT}\right)[cm^2s^{-1}] \quad (7)$$

Here, D_c^o is the carbon diffusivity in the Fe-C binary system, R is the gas constant (8.314×10^{-3} kJ mol^{-1}K^{-1}), and T is the temperature in Kelvin degrees.

Neumann and Person [12] proposed the q value as a function of the alloying elements,

$$q = 1 + [\%Si](0.15 + 0.033[\%Si]) - [\%Mn]\times0.0365 - [\%Ci](0.13 - 0.0055[\%Cr]) + [\%Ni](0.03 - 0.03365[\%Ni]) - [\%Mo](0.025 - 0.01[\%Mo]) - [\%Al](0.03 - 0.02[\%Al]) - [\%Cu](0.016 + 0.0014[\%Cu]) - [\%V](0.22 - 0.01[\%V]) \quad (8)$$

where the amount of alloying elements is in weight percent.

2.2. Boundary conditions

In vacuum carburization with acetylene, the acetylene gas readily dissociates into carbon and hydrogen according to the following chemical reaction [9]:

$$2Fe + C_2H_2 \rightarrow 2Fe(C) + H_2 \quad (9)$$

The dissociated carbon is immediately absorbed onto the surface of the steel, resulting in a rapid increase in the carbon concentration onto the surface of the specimen up to the maximum solubility of carbon in austenite at a given carburizing temperature. This indicates that vacuum carburization with acetylene is a diffusion-controlled process because the dissociation of acetylene and carbon absorption to the surface occur much faster than the carbon diffusion into the steel [9]. Therefore, in this study, during the carburizing time in which the acetylene gas is supplied into a vacuum furnace, the carbon concentration on the specimen surface is regarded as the maximum solubility of carbon in austenite at the carburizing temperature. On the other hand, during the diffusion time in which the acetylene gas is not provided in the vacuum furnace, the carbon flux on the specimen surface is regarded as zero.

The maximum solubility of carbon in austenite at the carburizing temperature should be calculated in a multi-component system to account for the alloying element effects for an accurate prediction of the carbon concentration profile.

3. SIMULATION AND EXPERIMENTAL PROCEDURES

The carbon diffusivity and boundary condition proposed in the present work were applied to a simulation of the carbon concentration profile of a cylindrical SCM415 steel specimen during vacuum carburization with acetylene. The chemistry of the steel was Fe-0.16%, C-0.25%, Si-0.7%, Mn-1.0%, and Cr-0.2% Mo in mass percent. The FEM simulation was conducted using the commercialized finite element software ABAQUS [13]. A cylindrical specimen, 50 mm in diameter and 100 mm in length, was used for the carburizing simulation and experimentation. An axisymmetric quadrilateral element was used with 294 nodes and 260 elements. The carburizing temperature was 1000 °C. The conditions for carburization and the carbon diffusion times are listed in Table 1.

The maximum solubility of carbon (1.39 wt.%) in austenite at 1000 °C, as calculated by Thermo-Calc [14] including the alloying element effect, was taken as the boundary condition during the carburizing time. Additionally, during the

diffusion time, the boundary condition was regarded as zero carbon flux. The initial carbon concentration of the specimen was 0.16 wt.%. The q value of the SCM415 steel was calculated using Eq. 8 as 0.885. Finally, the carbon diffusivity of the SCM415 steel was:

$$D = \left[0.47\exp(-1.6c)\exp\left(-\frac{154.9-27.63c}{RT}\right)\right]\times 0.885 \tag{10}$$

Vacuum carburization was experimentally performed using a vacuum furnace (ECM, Fulgura Duo 996TG). Specimens having the same shape and dimensions as that used for the FEM simulation were placed at the center of a five-layer tray measuring 600 × 600 × 900 mm^3. The tray was transferred into a heating chamber of 800 × 800 × 1100 mm^3 and was heated to 1000 °C under a pressure of 5×10^{-2} torr. The specimens were carburized at 1000 °C in an acetylene atmosphere of (5 to 10) torr according to the carburization conditions and diffusion times listed in Table 1. After vacuum carburization, the specimens were cooled by blowing nitrogen gas at 17 bar.

The middle part in the longitudinal direction of each carburized cylindrical specimen was sliced so that a disk 2 mm thick was obtained. The carbon concentration profile in the disk specimen was measured along the radial direction from the surface using an electron probe micro-analyzer (EPMA, Shinadzu, EPMA 1600). The EPMA was operated at 15 kV and 150 nA. The spot size of the electron beam used in the EPMA process was 1 μm in diameter. Various carbon steels containing (0.2 to 1.0) wt.% carbon were employed as standard samples for a precise quantitative analysis of the carbon concentration prior to the measurement of the carbon concentration profile of the disk specimen of the vacuum carburized SCM415 steel.

4. RESULTS AND DISCUSSION

Figure 1 shows the calculated carbon concentration distributions on the surface (Fig. 1(a)) and on the axis-symmetric plane (Fig. 1(b)) of the SCM415 cylindrical specimen vacuum carburized at 1000 °C. The calculated results reveal that the carbon concentration is higher in the order of the edges, top and bottom, and side of the cylindrical specimen.

Figure 2 shows the calculated and measured carbon concentration profiles in the radial direction from the surface at the middle part of the cylindrical specimen. The carburized depth was approximately 1.5 mm. The carbon concentration profile was calculated twice using the carbon diffusivities with and without the alloying element effect. The calculated carbon concentration profiles are in good agreement with the measured values. Particularly, the carbon concentration profile calculated with the alloying element effect is closer to the measured profile. This indicates that the alloying elements in steels affect the diffusivity and concentration pro-

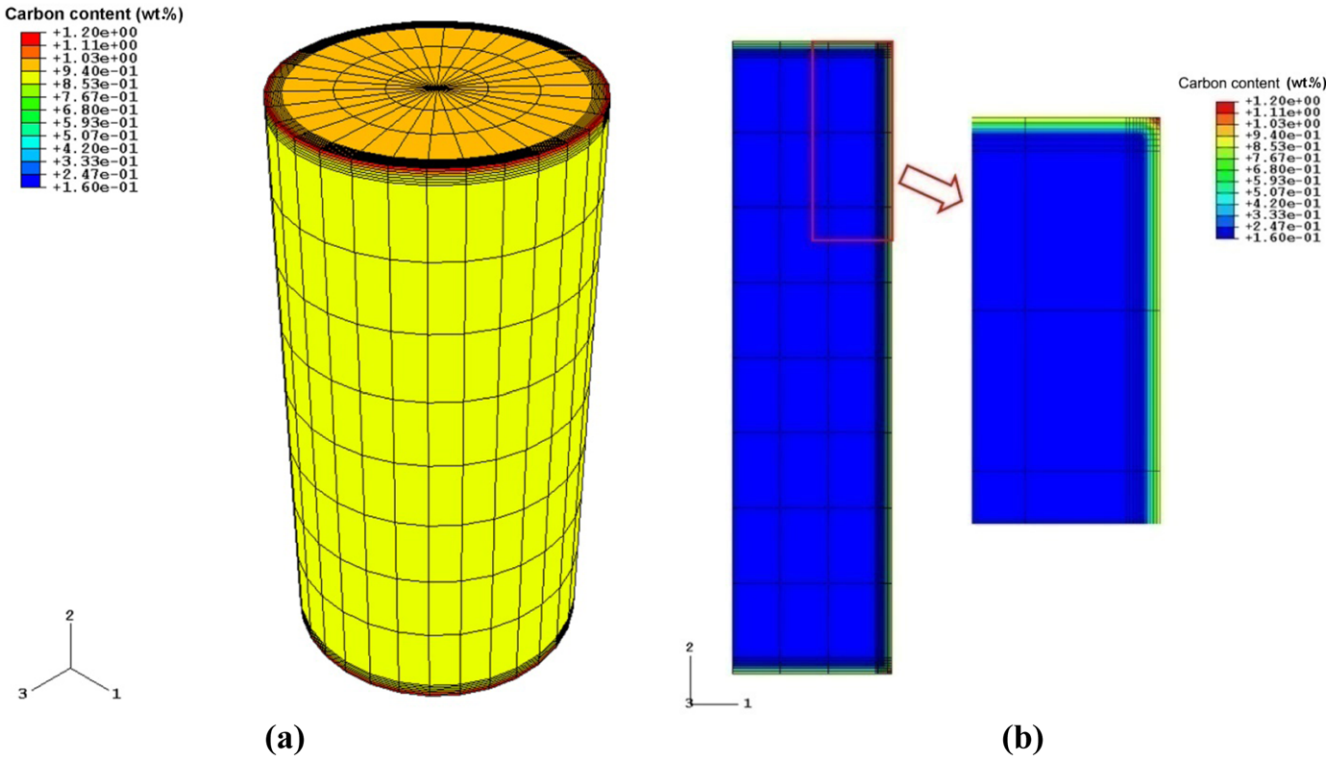

Fig. 1. The predicted carbon concentration distributions at the surface (a) and at the axis-symmetric plane, which is the half of the vertical cross section (b) of the SCM415 cylindrical specimen vacuum carburized at 1000 °C.

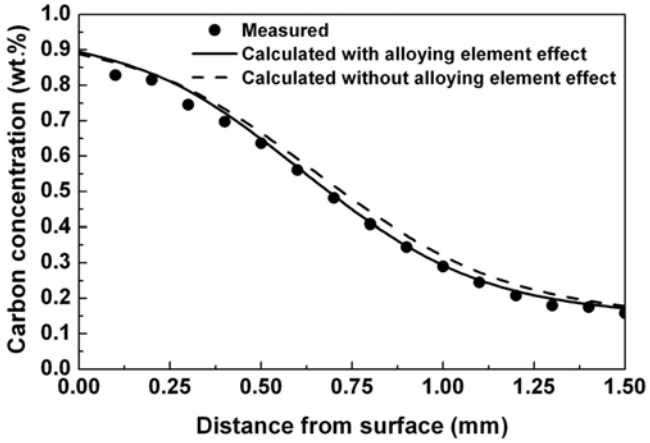

Fig. 2. The calculated and measured carbon concentration profiles in the radial direction of the SCM415 steel vacuum carburized at 1000 °C. The calculations were conducted using carbon diffusivity with and without alloying element effect.

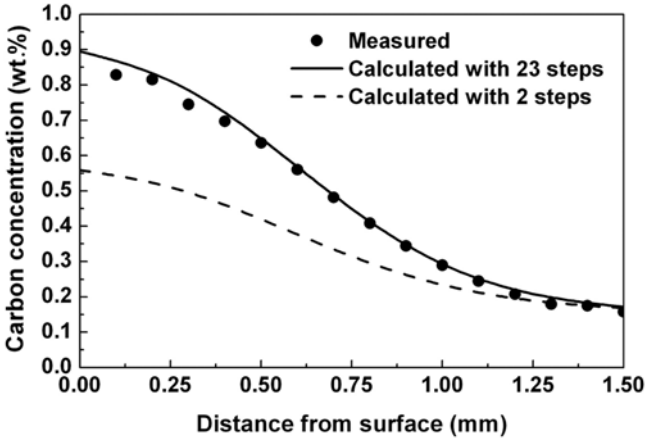

Fig. 3. Comparison between the carbon concentration profiles calculated with 23 carburizing and diffusion steps and with two carburizing and diffusion steps, respectively.

Table 1. Carburizing and diffusion times used in this study

Step	Carburizing time (min.)	Step	Diffusion time (min.)
1	0.8	2	0.2
3	0.8	4	0.2
5	0.8	6	1.5
7	0.9	8	2.8
9	0.9	10	3.7
11	0.8	12	4.7
13	0.8	14	5.7
15	0.8	16	6.6
17	0.8	18	7.5
19	0.8	20	8.6
21	0.8	22	9.6
		23	25.4

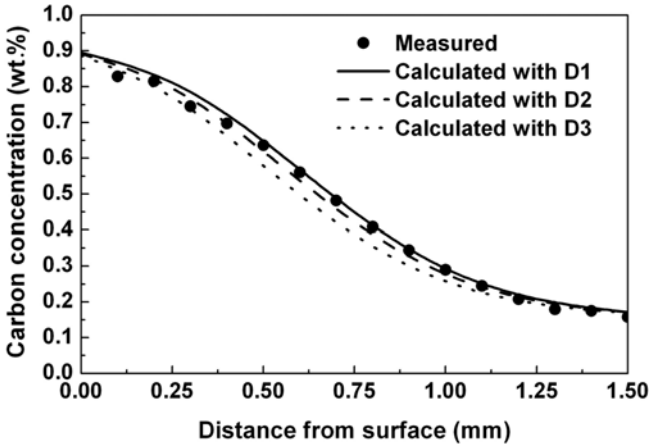

Fig. 4. Comparison of the carbon concentration profiles calculated with different carbon diffusivities in Fe-C binary system. D1, D2, and D3 are carbon diffusivities proposed by Tibbetts [3], Collin [2] and Goldstein [1], respectively.

file of carbon.

For the calculation of the carbon concentration profile, many time steps of carburizing and diffusion were used, as listed in Table 1, causing complexity in the boundary condition. Therefore, to avoid the generation of complicated boundary conditions and to conserve calculation time, the carbon concentration profile was re-calculated with only two steps of carburizing and diffusion. For the carburizing step, the total time of 11 carburizing steps in Table 1 was regarded as the carburizing time of one carburizing step. For the diffusion step, the total time of 12 diffusion steps was taken as the diffusion time of one diffusion step.

Figure 3 shows the carbon concentration profiles calculated with the simplified and actual time steps of carburizing and diffusion. The calculated carbon concentration profile with two steps of carburizing and diffusion exhibits a considerable difference compared to the measured profile. In the carburization process with the actual time steps, because the carburizing and diffusion time steps are repeated, the carbon concentration on the surface, which was consumed during the previous diffusion step, is resupplied during the next carburizing step. However, during the carburization process using the two simplified time steps, during one carburizing step, the carbon concentration at the surface is the maximum solubility of carbon in austenite at 1000 °C; it is consumed by diffusion upon the next diffusion step. Therefore, the carbon concentration calculated with the two simplified time steps is much less than that calculated with the actual time steps.

Accurate calculation of the carbon diffusivity in different temperature and carbon concentration ranges for vacuum carburization is important in the prediction of the carbon concentration profile. The carbon concentration profiles were calculated with other carbon diffusivities proposed by Collin *et al.* [1] (D2), Goldstein and Moren [2] (D3), and

Tibbetts' [3] carbon diffusivity (D1). These are compared in Fig. 4. The carbon concentration profile calculated with D1 shows good agreement with the measured profile, most likely because D1 was derived using carbon diffusivities measured in the temperature ranges of 975 °C to 1075 °C and carbon concentrations up to 1.3 wt.%, which are similar to the values used with vacuum carburization.

5. CONCLUSIONS

For an accurate prediction of the carbon concentration profile in vacuum carburized steels with acetylene, carbon diffusivity is proposed as a function of the temperature and concentrations of both the carbon and the other alloying elements present. The boundary condition was taken considering multiple time steps of carburizing and diffusion along with rapid dissociation and absorption of the acetylene gas.

The carbon concentration profiles in a cylindrical specimen of vacuum carburized SCM415 steel with acetylene were calculated using the following conditions: carbon diffusivities with and without the alloying element effect (q value), various carbon diffusivities in a Fe-C binary system, and the number of carburizing and diffusion time steps. The carbon concentration profile calculated with the alloying element effect (q value), the carbon diffusivity in the Fe-C binary system proposed by Tibbetts, and the multiple time carburizing and diffusion steps showed the highest level of agreement with the measured profile.

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