Carburization Process Modeling

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Md. Maniruzzaman
Olly Karabelchikova
Outline

- History (1939 – 2005)
- Issues
1939

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1939

Fig. 5—Relation of Time and Temperature to Carbon Penetration. Carburized in vertical gas retort using natural gas (95-98% methane). Measurements made on triangular test specimen. S.A.E. steel 3115.
Fig. 1—Carbon Gradient Curves for S.A.E. Steel 3115. Carburized at 1700°F. in Hardwood Charcoal, Coke, Sodium Carbonate Compound.
1939

Fig. 2—Carbon Gradient Curves for S.A.E. Steel 3115. Carburized at different temperatures in same type compound as Fig. 1.
1948

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Fig. 1 Approximate solubility of carbon in austenite for eight steels
Y = 0, Core % C
Y = 1, Surface % C
X = 0, Surface
X = 1, Case Depth

Carbon spread equals surface % C minus core % C

Case Depth, inches = $0.025 \sqrt{t}$ for 1700 F
= $0.021 \sqrt{t}$ for 1650 F
= $0.018 \sqrt{t}$ for 1600 F

where $t = $ time in hours

Added carbon, lb per sq ft of surface area
= $0.2(\text{carbon spread})(\text{case depth})$

Fig. 2 Tabulation of case depth
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Metals Park, Ohio
Table 5. Values of Case Depth Calculated by the Harris Equation

<table>
<thead>
<tr>
<th>Time, $t$, hr</th>
<th>Case depth, in., after carburizing at 1600 °F</th>
<th>1650 °F</th>
<th>1700 °F</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.025</td>
<td>0.030</td>
<td>0.035</td>
</tr>
<tr>
<td>4</td>
<td>0.035</td>
<td>0.042</td>
<td>0.050</td>
</tr>
<tr>
<td>8</td>
<td>0.050</td>
<td>0.060</td>
<td>0.071</td>
</tr>
<tr>
<td>12</td>
<td>0.061</td>
<td>0.073</td>
<td>0.087</td>
</tr>
<tr>
<td>16</td>
<td>0.071</td>
<td>0.084</td>
<td>0.100</td>
</tr>
<tr>
<td>20</td>
<td>0.079</td>
<td>0.094</td>
<td>0.112</td>
</tr>
<tr>
<td>24</td>
<td>0.086</td>
<td>0.103</td>
<td>0.122</td>
</tr>
<tr>
<td>30</td>
<td>0.097</td>
<td>0.116</td>
<td>0.137</td>
</tr>
<tr>
<td>36</td>
<td>0.108</td>
<td>0.126</td>
<td>0.150</td>
</tr>
</tbody>
</table>

Case depth = $0.025 \sqrt{t}$ for 1700 °F; $0.021 \sqrt{t}$ for 1650 °F; $0.018 \sqrt{t}$ for 1600 °F.

For normal carburizing (saturated austenite at the steel surface while at temperature).
Effect of Time

F. E. Harris has developed a formula for the effect of time and temperature on case depth for normal carburizing (Metal Progress, Aug 1943):

\[
\text{Case depth} = \frac{31.6\sqrt{F}}{10^{0.056/T}}
\]

where case depth is in inches; \( t \) is time at temperature, in hours; and \( T \) is the absolute temperature, in degrees Rankine (°F + 460).

For a specific carburizing temperature, the relationship becomes simply:

\[
\text{Case depth} = K \sqrt{t}
\]

\[
= 0.025 \sqrt{t} \text{ for } 1700 \, ^\circ F
\]

\[
= 0.021 \sqrt{t} \text{ for } 1650 \, ^\circ F
\]

\[
= 0.018 \sqrt{t} \text{ for } 1600 \, ^\circ F
\]

Values of case depth calculated for times of 2 to 36 hr at three common carburizing temperatures are given in Table 5.

When carburizing is purposely controlled to produce surface carbon concentrations somewhat less than saturated austenite, the case depth will be slightly less than the Harris equation shows. The case depth determined by the equation is total case depth, and for case depths in the range from 0.040 to 0.070 in. it will correspond to a point on the carbon gradient where the carbon concentration is about 0.07% C higher than the carbon content of the core.

In addition to the time at carburizing temperature, several hours may be required for bringing the work to operating temperature. For work quenched directly from the carburizer, the cycle may be further lengthened to allow time for the work to cool from carburizing temperature to a quenching temperature of perhaps 1550 °F. Although some diffusion of carbon from case to core occurs during this time, diffusion is slower than it would be at the carburizing temperature. This period may be used deliberately as a moderate diffusion period, to lower the carbon concentration at the surface by maintaining an atmosphere of low carbon potential in contact with the work during this time.

F. E. Harris has also developed a method for calculating the carburizing time and diffusion time to produce a carburized case of predetermined depth and carbon concentration at the surface (Metal Progress, Aug 1943):

\[
\text{Carburizing time} = \text{Total time} \left( \frac{C - C_i}{C_0 - C_i} \right)^2
\]

and

\[
\text{Diffusion time} = \text{Total} - \text{Carburizing time}
\]
Fig. 3. Carbon gradients in test bars of 1022 steel carburized at 1685 F in 20% CO–40% H₂ gas with 1.6 and 3.8% CH₄ added (H. M. Heyn)
Fig. 4. Carbon gradients in 1022 steel carburized at 1685 F with 20% CO – 40% H₂ gas containing enough H₂O to produce the carbon potentials shown, 0.50, 0.75 and 1.10% C (H. M. Heyn)
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Heat Treating

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316 / Surface Hardening of Steel

10 'Diffusion of Carbon in Austenite
12 'Tibbetts' Expression for the Diffusion Constant of Carbon
15 DEF FNDFC(T,W) = .47*EXP(-1.6*WC - (37000 - 660*W)*WC)/(1.987*T)
20 INPUT "Temperature in Degrees C ",TC
20 INPUT "Time in Hours ",TH
40 INPUT "Carbon Potential, wt. pct. ",CP
50 INPUT "Surface Reaction Rate Constant ",BETA
60 INPUT "Initial Carbon Content of Steel ",C0
70 T = TC + 273.15 : TSEC = TH*3600
80 DT = 15 : DX = .01
90 DIM C(31), CL(31)
100 L1 = 2*DT/DX : L2 = DT/DX^2
110 NN% = INT(TSEC/DT) : V% = 0
120 FOR I% = 0 TO 31
130 CL(I%) = C0
140 NEXT I%
150 FOR J% = 1 TO NN%
160 WC = (CL(J%) + CL(1))/2
170 DB = FNDFC(T,WC)
180 ETA = .75*CL(J%) + .25*CL(1) + L1*(BETA*(CP - CL(J%)) + DB*(CL(1) - CL(J%))/DX)
190 FOR I% = 1 TO 30
200 IF (V% = 0) THEN GOTO 220
210 C(I%) = C0 : GOTO 270
220 DA = DB
230 WC = (CL(I%) + CL(I%+1))/2
240 DB = FNDFC(T,WC)
250 C(I%) = CL(I%) + L2*(DB*CL(I%+1) - (DA+DB)*CL(I%) + DA*CL(I%-1))
260 IF (ABS(C(I%) - C0) < .00005) THEN V% = 1
270 NEXT I%
280 C(J%) = 4*(ETA - .25*C(1))/3 : V% = 0
290 FOR I% = 0 TO 31
300 CL(I%) = C(J%)
310 NEXT I%,J%
330 FOR I% = 0 TO 15
340 PRINT USING "#.##### "; DX*I%*10, C(I%), DX*(I%+15)*10, C(I%+15)
350 NEXT I%
360 END

Fig 5 Finite-difference computation of the diffusion of carbon in austenite using BASIC computer program
Fig 3. Plot of total case depth versus carburizing time at four selected temperatures. Graph based on data in table.

<table>
<thead>
<tr>
<th>Time, h</th>
<th>871 °C (1600 °F)</th>
<th>899 °C (1650 °F)</th>
<th>927 °C (1700 °F)</th>
<th>955 °C (1750 °F)</th>
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<tbody>
<tr>
<td></td>
<td>mm</td>
<td>mm</td>
<td>mm</td>
<td>mm</td>
</tr>
<tr>
<td>1</td>
<td>0.46</td>
<td>0.018</td>
<td>0.53</td>
<td>0.021</td>
</tr>
<tr>
<td>2</td>
<td>0.64</td>
<td>0.025</td>
<td>0.76</td>
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Metals Handbook®

DESK EDITION
Second Edition

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**Fig. 1** Plot of total case depth versus carburizing time at four selected temperatures. Graph based on data in table.

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Fig. 2  Reducing effect of increased process temperature on carburizing time for 8620 steel. Case depth: 1.5 mm (0.060 in.)
Fig. 3  Carbon gradients for 1020 and 8620 steels carburized at three temperatures.
Diffusion Modeling of the Carburization Process

J. I. GOLDSMITH AND A. E. MOREN

Mathematical models have been developed for simulating the carburization process. One model simulates carburization in low alloy steels where temperature, time, surface carbon content, and diffusion coefficient vary during the process. Two step and vacuum carburization are among the treatments considered. The other model simulates the effect of major ternary alloying additions such as Mn, Cr, Ni and Si during carburization. The importance of the off diagonal or cross diffusion coefficient $D_{ij}$ on carbon diffusion is calculated. The Crank-Nicolson finite difference equations are used to provide numerical stability and flexibility. Calculated carbon profiles for low alloy steels were compared with experimental data available in the literature. Agreement between calculated and measured data was very good. Chromium and silicon have large cross coefficient effects and it is predicted that they have a large influence on the amount of carburization which will occur. Experimental data for carburization treatments of Fe-C-Cr alloys are in excellent agreement with model predictions of major increases in effective surface carbon content and the formation of carbides in austenite at the carburization temperature. These computer models are relatively easy to apply and can be used to design carburization treatments for specific alloy steels.
Analytical Models for the Gas Carburizing Process

C.A. STICKELS

Mathematical models for carburizing in batch and continuous furnaces are described. Both the steady-state model for continuous furnaces and the time-dependent model for batch furnaces are based on material balances, with thermodynamic equilibrium of the constituents of the furnace atmosphere assumed. The instantaneous rate of carburizing is taken to be proportional to the difference between the carbon potential of the furnace atmosphere and the surface carbon content of the work load. Computer programs incorporating these models were written which predict furnace operating characteristics for any assumed process. The continuous furnace model predicts the pattern of internal gas flow within the furnace and computes the natural gas (or air) additions to each zone needed to achieve the desired carbon potentials and satisfy the carbon demand. The batch furnace model describes how the furnace atmosphere changes in composition during carburizing as a result of the interaction of the instantaneous carbon demand and the rate of supply of carburizing gases to the furnace. Examples of the use of these programs are given, and the limitations of the predictions are discussed.
Microstructural and Compositional Evolution of Compound Layers during Gaseous Nitrocarburizing

HONG DU, MARCEL A.J. SOMERS, and JOHN ÅGREN

Compound layers developed at 848 K during gaseous nitrocarburizing of iron and iron-carbon specimens were investigated for several combinations of N and C activities imposed at the specimen surface by gas mixtures of NH₃, N₂, CO₂, and CO. The microstructural evolution of the compound layer was studied by light microscopy and by X-ray diffraction analysis. Composition-depth profiles were determined by electron probe (X-ray) microanalysis. Layer growth kinetics was investigated by layer thickness measurements. The influence of the N and C activities on the microstructural and compositional evolution and the growth kinetics of the compound layers formed is discussed for the iron substrate. The results indicate that the microstructure is governed by a fast C and a slow N absorption at the surface in an early stage of gaseous nitrocarburizing. The influence of carbon in the substrate on the microstructural and compositional evolutions and on the growth kinetics was evaluated from comparing the results obtained for a normalized Fe-0.8C alloy with those for iron under identical nitrocarburizing conditions.
Commercial Models are currently Available - alphabetically

- DANTE
- DEFORM
- DICTRA
- SYSWELD

- Use FEA for heat and diffusion as well as deformations and strains
- Provide data to the models via some database
Carburization Modeling

- Carburization rates are controlled by:
  - Mass transfer coefficients at the surface
  - Carbon diffusion in the steel
Surface boundary condition
Flux Balance

\[ h_m \left( a_c^{\text{gas}} - a_c^{\text{surface}} \right) = -D \frac{d a_c^{\text{surface}}}{d x} \]
Mass transfer coefficient $h_m$

- The mass transfer coefficient $h_m$ controls the rate that carbon is absorbed by the steel.
- It depends on temperature, alloy composition, surface chemistry and oxides.
- We want to enhance the surface reactions between the gas and the steel by controlling surface condition and chemistry.
Carbon Diffusion Coefficient

- The diffusion coefficient $D(T, a_c)$ controls the rate that carbon can diffuse in the steel.
- It depends on temperature, alloy composition and carbon concentration.
- We need to maximize the diffusion coefficient by increasing temperature and controlling alloy compositions.
Fishbone diagram for Carburization

Method
- Gas
- Vacuum
- Time, Temp.
- Pressure
- Gas circulation

Alloy
- Composition
- TTT
- CCT
- TTP

Surface
- Finish
- Chemistry
- Oxide
- Mass transfer coeff.
- Diffusion coeff.

Output
- Case Depth ($\tau$)
- Carbon Conc. ($x, \tau$)
- Hardness ($x, \tau$)

Furnace
- Gas
- Temp.
- Part

Vacuum
- Size
- Racking
- Gas

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Alloy Effects

- Designation and real composition
  - Transformation diagrams
  - Carbon diffusion coefficient $D(T, a_c)$
  - Surface chemistry
  - Mass transfer coefficient $h_m(T, a_c)$
  - Carbon activity
Surface Condition

- Surface chemistry
- Oxide formation
- Roughness
- Mass transfer coefficient $h_m(T,a_c)$
Gas

• Composition
  - Endogas
  - Methane/propane etc.
  - Other gases or liquids
  - Activity of carbon
  - Equilibrium?

• Boost/diffuse?
Temperature

- Single or boost/diffuse?
- Profile in furnace
- Profile in part
- Carbon Diffusion coefficient $D(T, a_c)$
- Mass transfer coefficient $h_m(T)$
Carburization Modeling Issues

- Do we know \( D(T,c) \) ?
- How well do we need to know \( D(T,c) \)?
- Databases?
- Do we know \( h_m(T) \) ?
- How well do we need to know \( h(T) \)?
- Databases?
- Phase Transformation kinetics?
- Databases?