Carburization Process Modeling

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Outline

- History (1939 – 2005)
- Issues

1939

METALS HANDBOOK

1939 EDITION

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1939

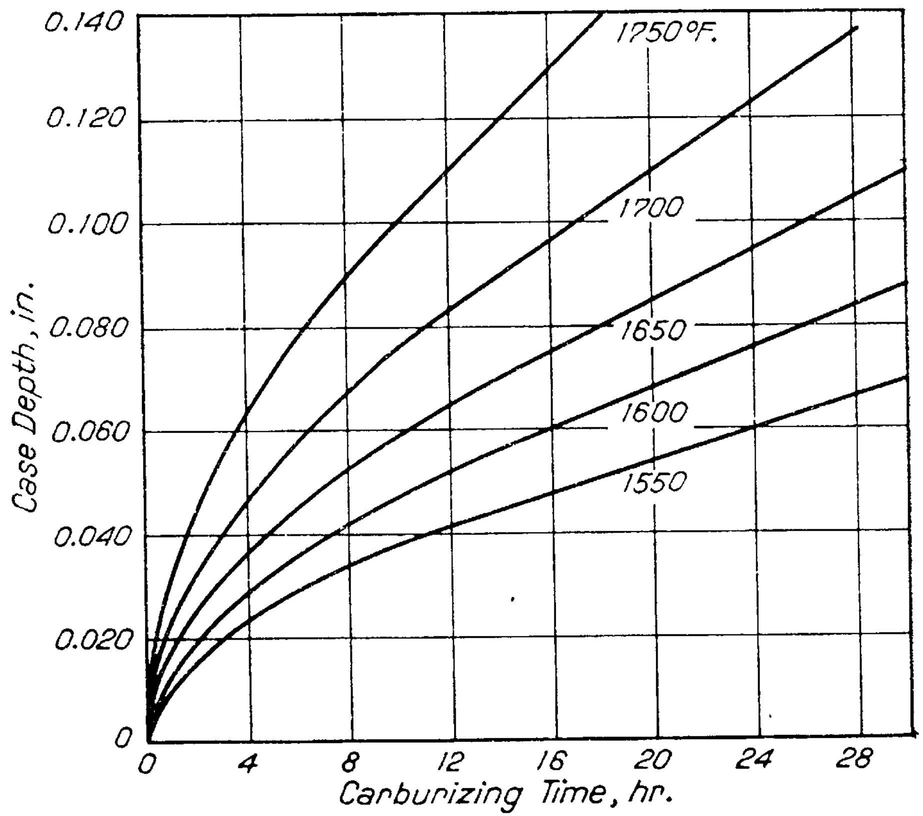

Fig. 5—Relation of Time and Temperature to Carbon Penetration. Carburized in vertical gas retort using natural gas (95-98% methane). Measurements made on triangular test specimen. S.A.E. steel 3115.

1939

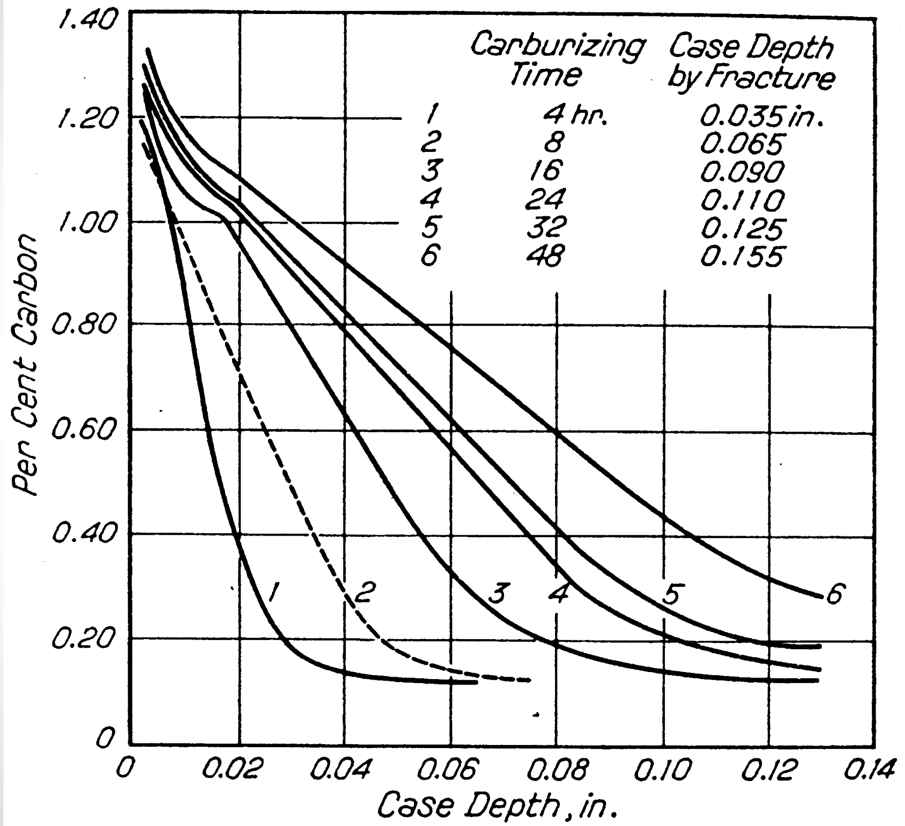

Fig. 1—Carbon Gradient Curves for S.A.E. Steel 3115. Carburized at 1700°F. in Hardwood Charcoal, Coke, Sodium Carbonate Compound.

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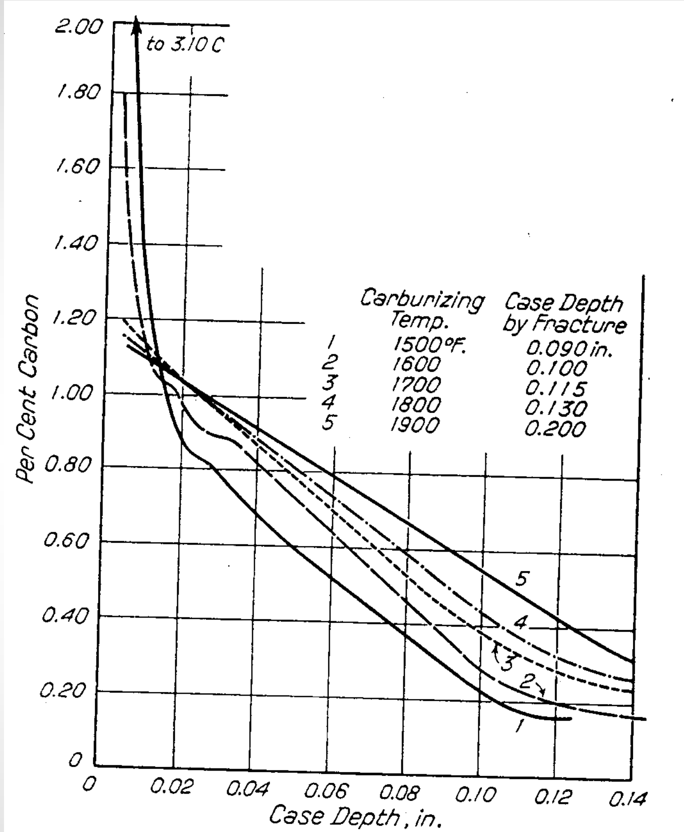

Fig. 2—Carbon Gradient Curves for S.A.E. Steel 3115. Carburized at different temperatures in same type compound as Fig. 1.

1948

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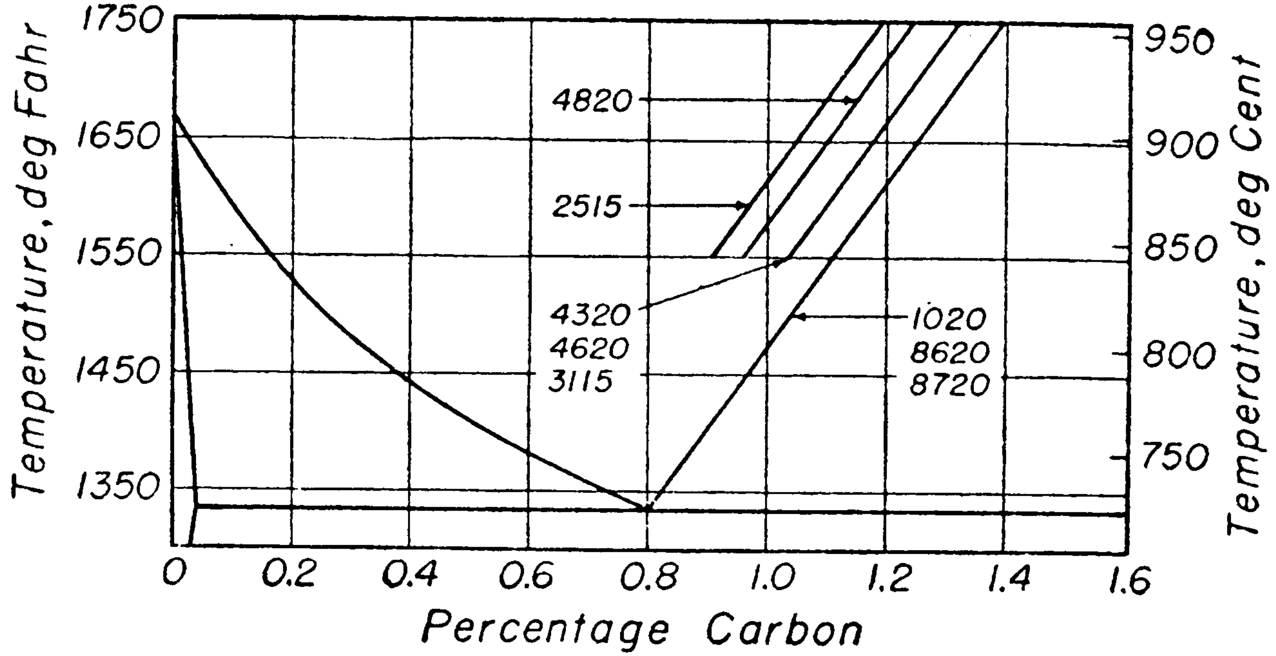
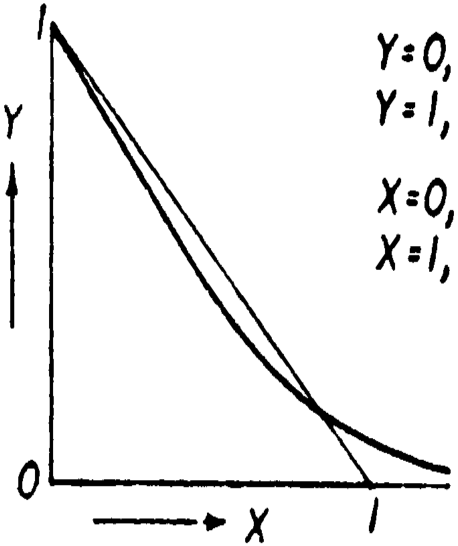


Fig. 1 Approximate solubility of carbon in austenite for eight steels

Metals Handbook - Harris - 1948



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 (carbon spread)(case depth)

Fig. 2 Tabulation of case depth

8th Edition- 1964

METALS
HANDBOOK

8th Edition

VOL. 2

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Table 5. Values of Case Depth Calculated by the Harris Equation

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

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).

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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):

$$\text{Case depth} = \frac{31.6\sqrt{t}}{10^{(6700/T)}}$$

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:

$$\begin{aligned}\text{Case depth} &= K\sqrt{t}\\ &= 0.025\sqrt{t} \text{ for 1700 F}\\ &= 0.021\sqrt{t} \text{ for 1650 F}\\ &= 0.018\sqrt{t} \text{ for 1600 F}\end{aligned}$$

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

$$\text{Diffusion time} = \text{Total} - \text{Carburizing time}$$

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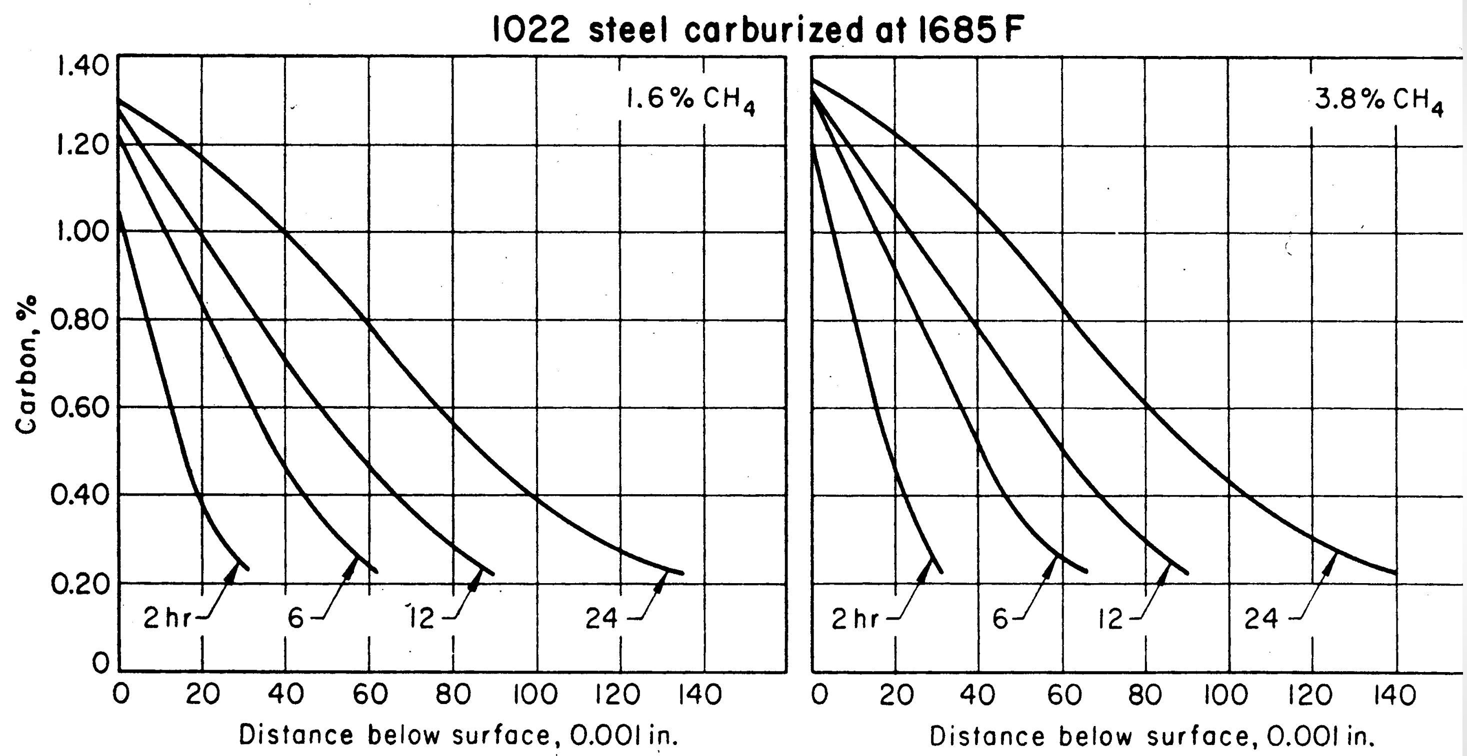

Fig. 3. Carbon gradients in test bars of 1022 steel carburized at 1685 F in 20% CO – 40% H_2 gas with 1.6 and 3.8% CH_4 added (H. M. Heyn)

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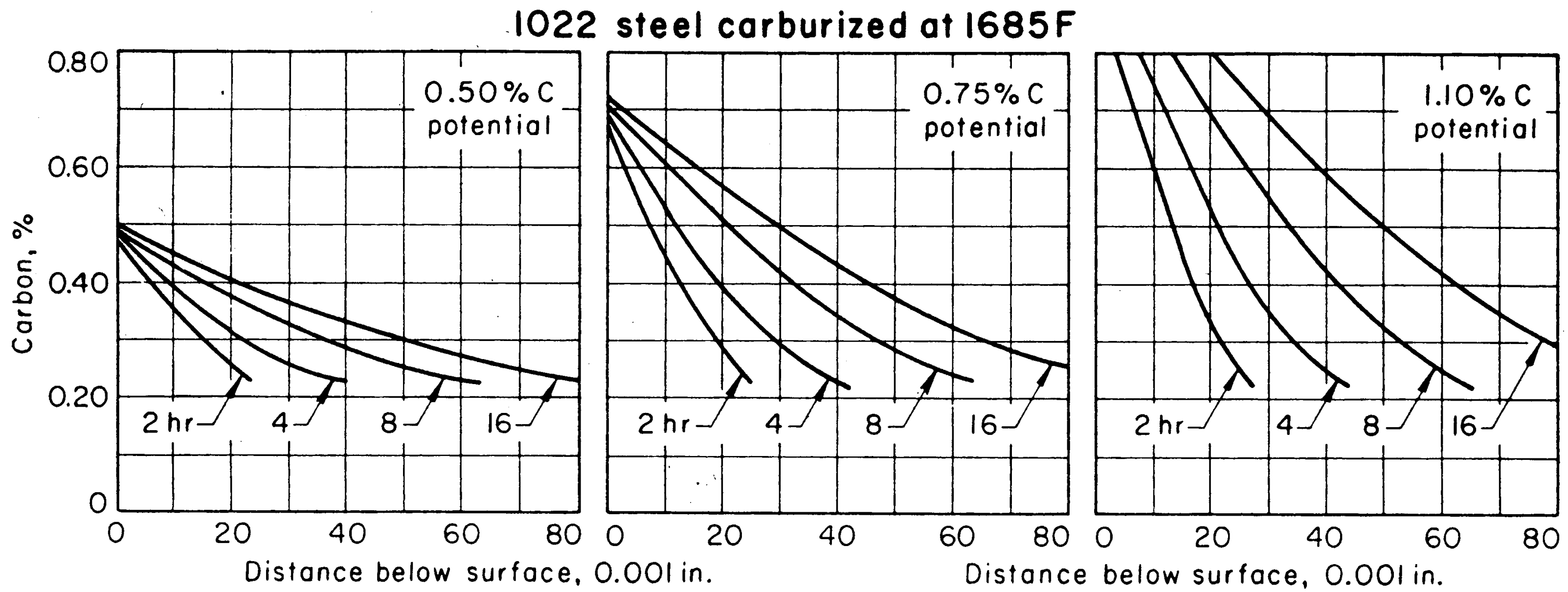

Fig. 4. Carbon gradients in 1022 steel carburized at 1685 F with 20% CO – 40% H_2 gas containing enough H_2O to produce the carbon potentials shown, 0.50, 0.75 and 1.10% C (H. M. Heyn)

Volume 4 - 1991

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Volume 4
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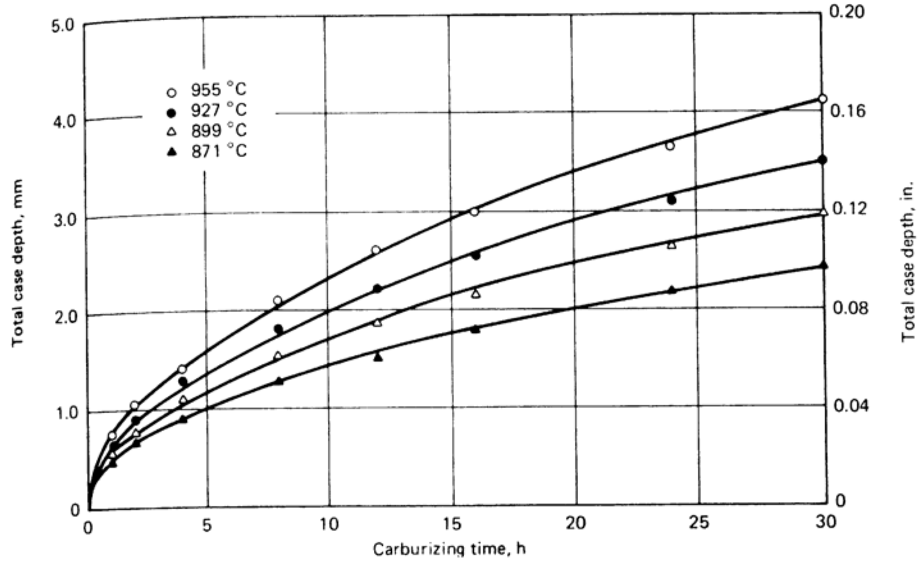
10 'Diffusion of Carbon in Austenite
12 'Tibbetts' Expression for the Diffusion Constant of Carbon
15 DEF FNDFC(T,WC) = .47*EXP(-1.6*WC - (37000! - 6600*WC)/(1.987*T))
20 INPUT "Temperature in Degrees C  ",TC
30 INPUT "Time in Hours  ",TH
40 INPUT "Carbon Potential, wt. pct.  ",CP
50 INPUT "Surface Reaction 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(0) + CL(1))/2
170   DB = FNDFC(T,WC)
180   ETA = .75*CL(0) + .25*CL(1) + L1*(BETA*(CP - CL(0))
            + DB*(CL(1) - CL(0))/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(0) = 4*(ETA - .25*C(1))/3  :  V% = 0
290   FOR I% = 0 TO 31
300     CL(I%) = C(I%)
310 NEXT I%,J%
320 PRINT "Depth, mm","Wt. Pct. C","Depth, mm.","Wt. Pct. C"
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

Volume 4 - 1991



Time, h	871 °C (1600 °F)		899 °C (1650 °F)		927 °C (1700 °F)		955 °C (1750 °F)	
	mm	in.	mm	in.	mm	in.	mm	in.
1	0.46	0.018	0.53	0.021	0.64	0.025	0.74	0.029
2	0.64	0.025	0.76	0.030	0.89	0.035	1.04	0.041
4	0.89	0.035	1.07	0.042	1.27	0.050	1.30	0.051
8	1.27	0.050	1.52	0.060	1.80	0.071	2.11	0.083
12	1.55	0.061	1.85	0.073	2.21	0.087	2.59	0.102
16	1.80	0.071	2.13	0.084	2.54	0.100	2.97	0.117
24	2.18	0.086	2.62	0.103	3.10	0.122	3.66	0.144
30	2.46	0.097	2.95	0.116	3.48	0.137	4.09	0.161

Fig 3 Plot of total case depth versus carburizing time at four selected temperatures. Graph based on data in table

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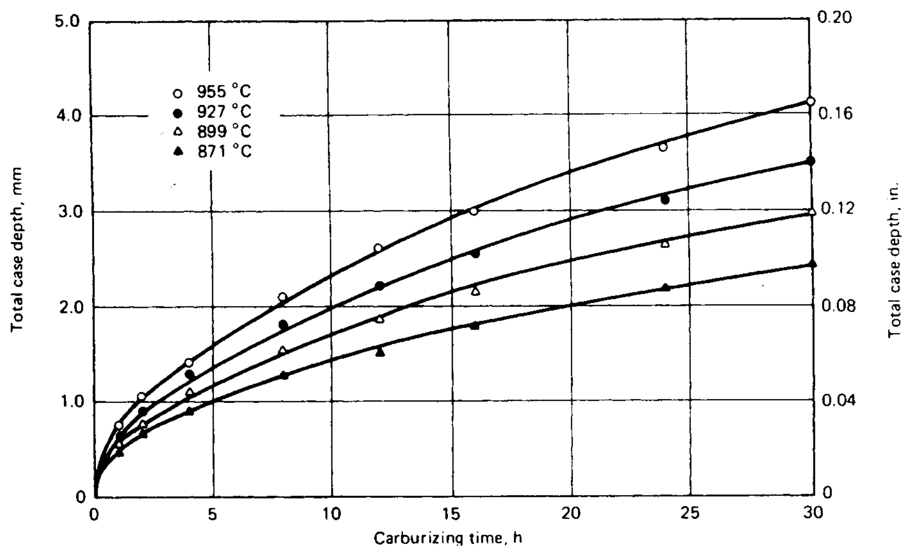


Time, h	871 °C (1600 °F)		899 °C (1650 °F)		927 °C (1700 °F)		955 °C (1750 °F)	
	mm	in.	mm	in.	mm	in.	mm	in.
1	0.46	0.018	0.53	0.021	0.64	0.025	0.74	0.029
2	0.64	0.025	0.76	0.030	0.89	0.035	1.04	0.041
4	0.89	0.035	1.07	0.042	1.27	0.050	1.30	0.051
8	1.27	0.050	1.52	0.060	1.80	0.071	2.11	0.083
12	1.55	0.061	1.85	0.073	2.21	0.087	2.59	0.102
16	1.80	0.071	2.13	0.084	2.54	0.100	2.97	0.117
24	2.18	0.086	2.62	0.103	3.10	0.122	3.66	0.144
30	2.46	0.097	2.95	0.116	3.48	0.137	4.09	0.161

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

Desk Edition-1998

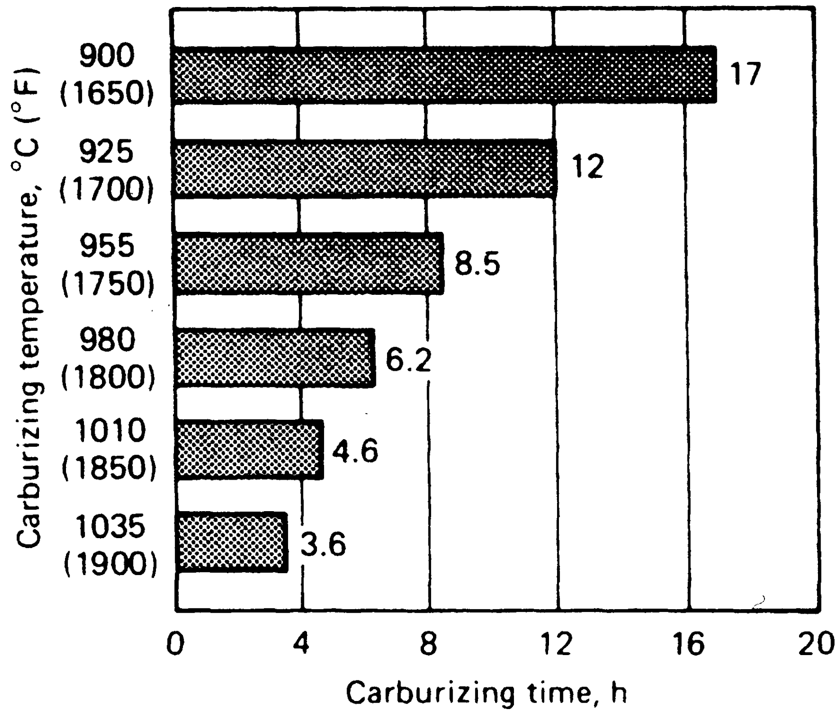


Fig. 2 Reducing effect of increased process temperature on carburizing time for 8620 steel. Case depth: 1.5 mm (0.060 in.)

Desk Edition - 1998

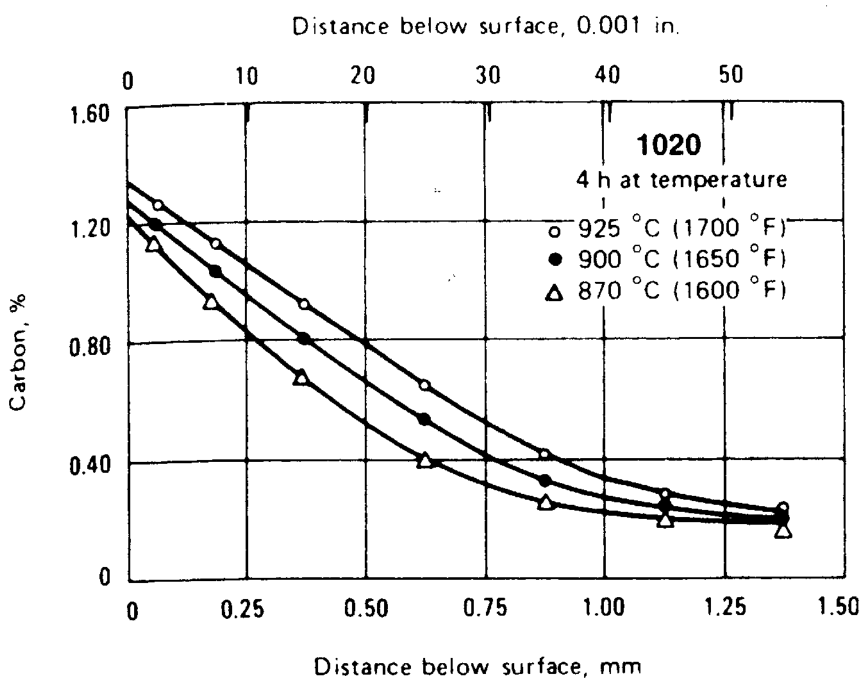


Fig. 3 Carbon gradients for 1020 and 8620 steels carburized at three temperat

1978 – Met Trans

Diffusion Modeling of the Carburization Process

J. I. GOLDSTEIN 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_{12}^3 on carbon diffusion is calculated. The Crank-Nicolson finite difference equations are used to provide numerical stability and flexability. 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.

1988 – Met Trans

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.

1998 – Met Trans

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 NH_3, N_2, CO_2, 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 ell 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

$$h_m\left(a_c^{gas} - a_c^{surface}\right) = -D\frac{da_c^{surface}}{dx}$$

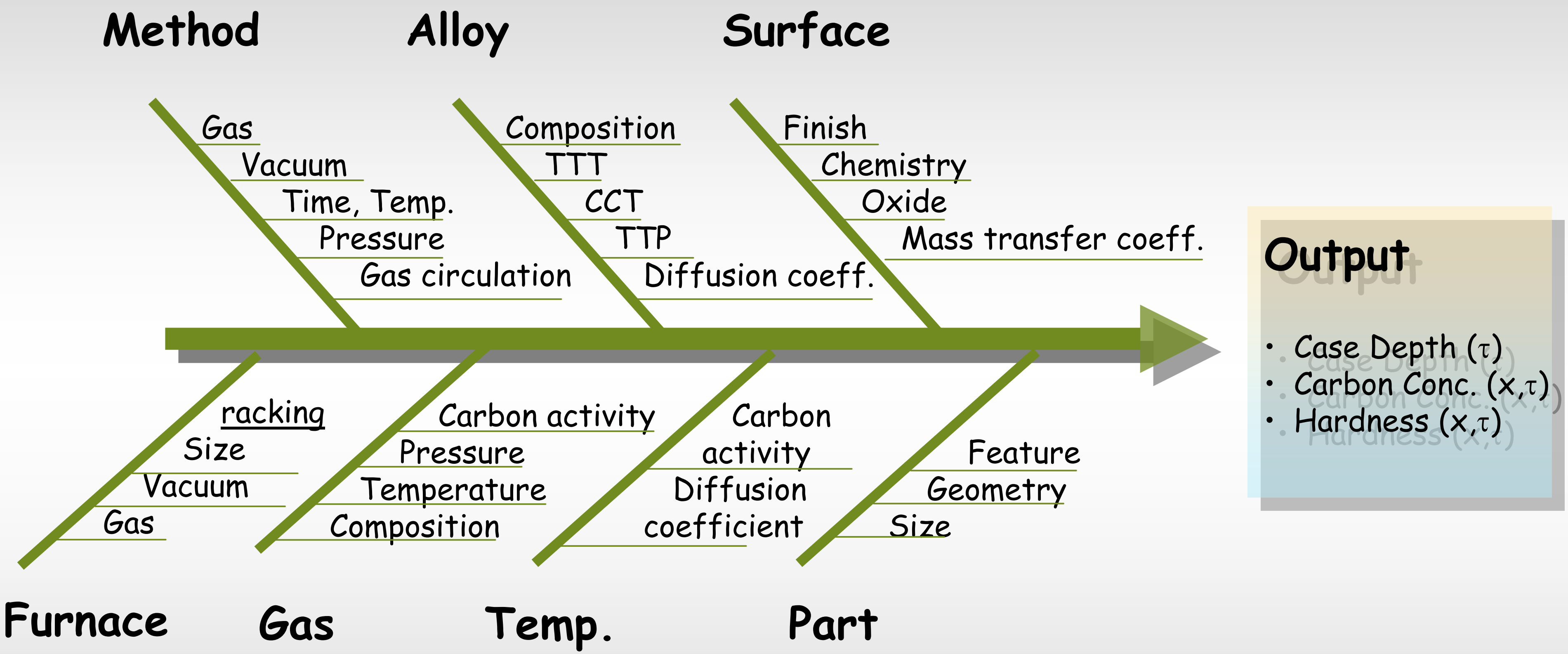
Mass transfer coefficient h_m

- 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



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 $hm(T)$?

Carburization Modeling Issues

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