ALGORITHM FOR CARBON DIFFUSION COMPUTATION IN A VACUUM FURNACE EXPERIMENTAL METHODS PREDICT CARBURIZING TIMES.

ALGORITMO PER IL CALCOLO DELLA DIFFUSIONE DEL CARBONIO NELLA CEMENTAZIONE NEI FORNI A VUOTO

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Abstract

Times of boost and diffusion stages in a vacuum furnace were empirically determined by an experimental heat treatment cycle carried out with similar loads. One advantage that vacuum furnaces provide is good repeatability of the process parameters, yielding predictable case hardening results. In this work, an algorithm is developed mathematically to determine the theoretical time of diffusion in a vacuum furnace (after the boost period) to obtain a final 0.8% C at the surface of carburized samples. Three batches of gas carburized samples, with different levels of surface carbon and case depths, were subjected to increasing diffusion temperatures in a vacuum furnace.

Introduction

Case hardening in a vacuum furnace is carried out by three main techniques: plasma or ionic, lowpressure, and plasma-assisted, low-pressure processes. Although currently used in a variety of industrial applications, higher cost compared with gas carburizing is still a hindrance to further utilization. However, the vacuum process has the advantage of being pollution-free, which is he main reason why it can be put in series with other traditional machines in a production line. That allocation would not be possible with conventional gas carburizing furnaces because of oil and gas pollution concerns.

Full application of vacuum carburizing is hindered by the inability to regulate the surface carbon level. In contrast, this parameter is well controlled in the gas carburizing process using gas analysis by oxygen probes and infrared cells. In vacuum, proposed methods of carbon surface control are still experimental. Particularly promising is the direct surface analysis of carburizing workpieces by laser beam with continuous and real-time output. Currently, the only method that can be applied is the boost-diffusion technique (Fig. 1).





Fig.1 Schema di flusso del propano e dell'idrogeno durante un trattamento di cementazione secondo la

tecnica boost-diffusion

Boost-diffusion cycle

First step of the boost-diffusion process consists of carburization with sufficient gaseous hydrocarbon to saturate the austenite phase, while avoiding soot deposition on the surface. This is accomplished by knowing the amount of surface area to be carburized. In the case of a steel containing alloying metals that generate carbide, the level of carbon in the surface increases above the austenite saturation. The formation of some carbides instead of others is regulated by the entropy level of the reaction between carbon and metal. In the case of a positive enthalphy level, the reaction cannot succeed, as is the case with nickel.

At the end of the boost, the diffusion period starts. The propane flux is cut out and a vacuum is drawn in the furnace. The high carbon level at the surface (compared to the core) generates the diffusion phenomena. This decreases the surface level because the carbon migration from the surface to the core. In the theoretical case of infinite time and infinite thickness the surface carbon level may decrease to that of the core.

In contrast, carbon behavior is more complex in gas carburizing. In fact, after the boost period is carried out with a carbon potential near the austenite saturation level, the carbon potential of the carburizing gas is lowered to about 0.8 %. Here, the carbon flow toward the core is the same as in the vacuum process, but also starts another exchange between the surface and the gas that tends to decrease the surface carbon to 0.8%. So the process time is shorter, and the final, effective case depth is less than that achieved in a vacuum furnace.

An ionic case hardening cycle utilizing propane and hydrogen gas is shown in Fig.1. According to the boost-diffusion cycle, after every boost period a diffusion time follows to allow for carbon diffusion toward the core from the saturated austenite, so that the surface carbon content reaches the optimum range of 0.8%. The propane flow is directly proportional to the carburizing load surface and decreases exponentially with time.

The carbon penetration rate, V, at every time, h, of the carburizing process may be calculated theoretically by the Harris formula to determine the case depth penetration as a function of time:

 $p = 803 h^{1/2}/10^{3722/T}$; $V = dp/dh = (803.1/2 h^{1/2 - 1})/10^{3722/T} = 401.5/ (h^{1/2}.10^{3722/T})$, where h = carburizing time in hour, T = temperature K, V = carbon penetration rate, and p = case depth in mm.

This formula shows that as the carbon penetration rate approaches infinity, h approaches zero. In practice, the carbon solution rate is not as high because the carbonizing gas has to reach equilibrium with the steel surface.

Introduced by Wyss, a U factor, or carbon transfer coefficient, quantifies the capability of the carburizing atmosphere to exchange carbon with the steel surface (see fig.2).

Ionic carburizing reaches equilibrium more easily than gas carburizing or low pressure carburizing processes, because it is catalyzed by ionic discharge. For every m^2 of carburizing surface, the theoretical propane quantity is plotted in Fig.3,



Fig. 2 Carburising speed data in cm/sec 10⁻⁵, as function of atmosphere composition at 900°C.



Fig.3 Carbon absorbing rate as a function of temperature (Montevecchi)

Fig.3 Velocità di assorbimento del carbonio in funzione della temperatura (Montevecchi)

based on 0.9% surface carbon (ref.1). With this parameter, the process is approximated because calculating the carburizing steel surface area is difficult and because the fixture surface can also absorb carbon, further complicating the calculation. Consequently, some table values were determined empirically, using the propane flow that would allow the entire carburized surface to reach austenite saturation.

Diffusion

The boost phase is difficult to run not only because it's related to the surface area of the components, but also because it is difficult to calculate using the algorithm related to that parameter. However, that is not the case with the time diffusion calculation after the boost phase.

The time necessary to decrease the carbon concentration from saturated austenite to 0.8% can be calculated from tables or theoretically. The decreasing rate of carbon concentration is related to the:

- diffusion rate of carbon in austenite
- case depth
- temperature
- piece thickness
- carbon differential between the core and surface of the component

For easier calculation, some parameters can be considered known or constant. For instance, thickness of the component being carburized can be assumed to always be over $10\times$ the required carburization depth. Similarly, the carbon level in the carburizing steel can be assumed to be about 0.16%; the level in the carburizing surface, about 0.8%.

Experimental details

16 Cr Ni 5 steel samples, 20 mm in diameter and 10 mm thick, were carburized to variable depths and with variable levels of surface carbon. The samples were heat treated in a vacuum furnace with an integral oil tank at a working pressure of about 2 mbar, the usual pressure for plasma carburizing. After 3 h of soaking time, they were oil quenched, then analysed to determine new values of surface carbon and case depth.

Three different batches were prepared to study the effects of:

• *surface carbon level* (batch 1). Carbon diffusion samples heat treated to 1070°C with a 3 h soak time, 1.5 mm case depth, and a surface carbon level from 0.69 to 1%.

- *case depth* (batch 2). Carbon diffusion samples heat treated to 1070°C, 3h soak time, surface carbon level 1%, and a case depth from 0.6 to 1.5 mm.
- *temperature* (batch 3). Carbon diffusion samples with a 1.5 mm case depth, 0.95% surface carbon, and a 3 h soak time at temperatures from 870 to 1070°C.

Results appear in Tables 1, 2, and 3 with relative trend diagrams 1, 2, 3.



Diagramma 1- 1° lotto. Influenza del tenore di C superficiale sul gradiente di variazione

Tabella 1 – 1° lotto. Variazioni di C superficiale su provini con profondità di cementazione 1,5 mm e

tenori di C superficiale indicati. I provini sono stati tenuti 3 ore a 1070°C in forno a vuoto.

Il valore corrispondente a 0.16% C è induttivo e puramente teorico.



Table 2 ; 2nd batch . Surface carbon variations on the sample with 1% C on surface and as shown case depth . Heat treated 3 h to 1070° C in vacuum furnace . The values indicated for 0 e ∞ case depth are only inductive and has been indicate for better understanding the trend of the chart curve

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Diagramma $2 - 2^{\circ}$ lotto. Influenza della profondità di cementazione sull'abbassamento del C

superficiale.

Tabella 2 – (2° lotto). Variazioni di C superficiale sui provini con C iniziale 1% e profondità di

cementazione indicate, tenuti 3 ore a 1070°C in vuoto. I valori di 0 e ∞ sono solo induttivi e sono stati

indicati per meglio comprendere l'andamento della curva.



Diagram 3 . 3rd batch . Influence of temperature on the surface carbon decreasing .

Temperature °C	C% at surface	Case depth (mm)	Time (hour)	C% final value at surface	Δ C%
870	0.95	1.5	3	0.90	0.05
970	0.95	1.5	3	0.75	0.20
1070	0.95	1.5	3	0.55	0.40
00	0.95	1.5	3	- 0.16	0.79

Table 3 . $3^{rd}\,$ batch . Surface C variation on samples with 0.95 % C , held 3 h $\,$ in vacuum furnace at indicated temperatures .

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Diagramma $3 - 3^{\circ}$ lotto. Influenza della temperatura sulla diminuzione del tenore superficiale del C.

Tabella 3 (3° lotto). Variazioni di C superficiale su provini con C superficiale 0.95% tenuti per 3 ore

in un forno a vuoto alle temperature indicate.

In some tables, experimental values were completed with some limits value obtained by inductive reasoning to better understand the examined phenomena.

Diffusion time

The necessary time to lower the carbon surface content (after the boost time) to 0.80% is defined by the surface carbon level, case depth, and process temperature. The trend of these three parameters (Fig.3,4,5) can be expressed mathematically, as follows:

• *Time* t_1 to lower the %C from the boost level to 0.80%, calculated at 1070°C by trends shown in Table 1 is $t_1 = K (\%C - 0.8) / \%C$ where $t_1 =$ hours, K = 5.2, and %C = surface carbon level after the boost phase.

• *Time* t_2 to bring the carbon to 0.8% as a function of the case depth. In this case, the value must be equal to 1 with the case depth equal to 1.5 mm. The equation is $t_2 = 1.4$ ^(p-1.5) where p = case depth in mm after the boost.

• *Time t*₃ to lower the carbon to 0.8% as a function of temperature must be equal to 1 at 1070°C. Here, the Arrhenius equation is utilized as $t_3 = e^{(Q/1.987 \cdot T)}/a$, where T = temperature K, Q = activation energy (34,500 cal /mole for γ iron), e = natural logarithm base, and 1.987 = gas constant, cal/mole•K. The final equation becomes $t_3 = e^{(34,500/1.987 \cdot T)}/411,850$.

Diffusion time t_d can then be expressed as a function of the boost time t_b:

Eq. 1 $t_{d} = [K (\%C - 0.8) / \%C] [1.4^{(p-1.5)}] [e^{(34,500/(1.987))}/411,850]$

Substituting numerical values into this equation makes it possible to calculate the diffusion time required to lower the surface carbon from 1.7%, that's the saturated austenite level for a carburizing process at 1050°C (1323°K), to 0.8%. In this case we consider, for example, case depth 1.4 mm. $t_{d=}[5.2 (1.7 - 0.8)/1.7] [1.4^{(1.4 - 1.5)}] [(1/411,850)e^{(34,500/(1.987 \cdot 1323)}] = 3.23 h$

Further calculations

Per Equation 1, the diffusion time of carbon in a vacuum furnace is defined as a function of the surface carbon content after the boost, the case depth, and the temperature. It is possible to calculate the total times of boost-diffusion in a vacuum furnace to obtain a desired case depth with a 0.8% surface carbon level by utilizing the Harris formula to yield case depth as function of the working temperature and time.

The total time t_t to obtain a targeted case depth with a 0.8% surface carbon content by the boostdiffusion process is derived from the boost time t_b added to the diffusion time t_d and can be expressed as: **Eq. 2** $t_t = t_b + t_d$, or $t_b = t_t - t_d$, or $t_d = t_t - t_b$. Using the Harris formula if the temperature is known, time t_t can be calculated, while the diffusion time t_d can be calculated as a function of the case depth value and the % C obtained after the boost.

Total case depth time

Time t_t can be calculated reversing the Harris formula where t_t = hours, T = temperature K, and p = case depth in mm.

Eq.3
$$t_t = p^2 (10^{3722/T})^2 / 803^2 = p^2 (10^{7444/T}) / 803^2$$

The % C, which is the austenite carbon saturation value after the boost period, can be calculated as a function of the Kelvin temperature by the following formula:

Eq.4 % C sat = $-0.70597 + 7.21 \times 10^{-4} \text{ T} + 6.13 \times 10^{-7} \text{ T}^2 + 1.67 \times 10^{-10} \text{ T}^3$

The case depth p, after the boost, can then be calculated with the Harris formula:

Eq.5 $p = 803(t_b^{1/2})/10^{3722/T}$, where T = temperature K, p = case depth mm, and t = time in hours. Subsequently t_d can be expressed as function of t_b by substituting these values in Eq.1.

Boost time

Substituting the expressions obtained in Eq. 1 and Eq. 3 for the t_t and t_d parameters in Eq. 2 results in a unique uncertainty for t_b .

The new equation is synthetically, even if not mathematically correctly expressed , shown in Eq.6

Eq.6
$$t_b = p^2 (10^{7444/T}) / 803^2 - \left[K (\% Csat - 0.8) / \% Csat \right] \left[1.4^{(**-1.5)} \right] \left[e^{(34500/1:987 \text{ T})} / 411.850 \right]$$

where $\% Csat$ is the **Eq.4** and ** is the **Eq.5**

Using a computer makes it possible to approximate the calculations for the total time of boost and diffusion required to obtain the needed case depth with 0.80% C in the surface.

Conclusions

In the vacuum carburising process, on the steel surface, a carbon saturation of the austenite occurs.

After this phenomena a time of diffusion will be necessary to allow the penetration of the carbon downward the core, until the surface reach the target of 0.8% C concentration.

The boost diffusion time was until now experimentally obtained and reported on tables that was utilised by technicians to set up the carburising program on the furnace computer.

In this work, instead, the time calculation is mathematically planned and start from temperature and case depth set up of the process, with this parameter the computer aboard furnace can calculate the boost and diffusion time automatically.

The diffusion algorithm has been calculated by breaking up ad analyse mathematically the experimental data achieved by the behaviour of the carbon, while is going from surface toward the core. Three parameters have been analysed:

- Surface carbon concentration
- Case depth
- Temperature

The boost time is instead calculated using metallurgical equations take from literature, adapted to calculation requirement.

The final algorithms are complex, but with the huge calculation power of the modern computer this is not a problem.

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