Vacuum Carburizing Process: Identification of Mathematical Model and Optimization

M Yu Derevyanov, M Yu Livshits, E A Yakubovich

Samara State Technical University, 244, Molodogvardeiskaya Av., Samara, 443100, Russia

E-mail: mder2007@mail.ru

Abstract. This paper deals with individualizing the surface-hardening vacuum carburizing process based on optimal process control. The authors’ parametric identification determined that the mathematical model for the vacuum carburizing process requires the use of different mass-transfer coefficients at the stages of saturation and diffusion. The authors analyzed the effect that the optimal surface-hardening process conditions have on the structures and properties of drill-bit steels.

1. Introduction

The operability and durability of components depend on the aggregate effect of many factors, including design features, operating conditions, workmanship, and the metallurgical quality of materials used in manufacturing [1,2]. For purposes of this discussion, hardening processes based on thermochemical treatment are especially important. Their efficiency is enhanced by using high-temperature vacuum carburization at a pressure below atmospheric [3,4].

Under standard requirements, the vacuum carburizing process (with subsequent heat treatment) must make the surface layer highly hard and durable and provide high component strength under contact loads as well as under repeated bending and torsional exposure. Traditional design methods for vacuum carburizing processes involve setting key parameters (saturation point, hold time, and the composition and saturating activity of the environment), relying conventionally on the standard average quality performance of the hardened layer [3]. That approach cannot always satisfy the variable market requirements for efficiency indicators of the carburizing process.

The actual practice of process-induced hardening increasingly poses the problem of individually designing process conditions to make it possible to obtain individual and group, rather than average, properties of components applicable to the operating conditions of those components. This problem includes developing efficient methods for mathematical modeling of vacuum carburizing processes and computer-aided techniques for calculating and designing process parameters that meet, with the required accuracy, the specified individual properties of the hardened layer. In its salient aspects, the problem can be solved by applying the modern theory and technology of optimal control [5,6].

The primary concept underlying the idea of individualizing process design consists in coordinating two dialectically conflicting aspects—process capabilities of equipment on the one hand and operating requirements for the carburized layer on the other, aiming to achieve the extremal values of criteria for operational and economic optimality of the vacuum carburizing process. The extremum of those criteria is mostly attained with a combination of primary process parameters that differ from those in standard process instructions and design solutions.

2. The mathematical model of the vacuum carburizing process

The mathematical model for carbon diffusion from the atmosphere through the surface of the component into its depth at a constant temperature, given the slight dependence of diffusion...
coefficient $\delta$ on carbon concentration $C(x, \tau)$ and according to Fick’s second law [3,7,8], can be made in relative units as a differential equation for mass-transfer:

$$\frac{\partial \Theta(\ell, \vartheta)}{\partial \vartheta} - \frac{\partial^2 \Theta(\ell, \vartheta)}{\partial \ell^2} = 0,$$

(1)

where $\Theta(\ell, \vartheta) = C(\ell, \vartheta) \cdot \alpha_m^{-1}$; $\ell = x \cdot x_m^{-1}$, $0 \leq \ell \leq 1$; $\vartheta = \tau \cdot \delta \cdot x_m^{-1}$, $0 \leq \vartheta < \infty$; $\alpha_m$ is the maximal allowable level of the atmosphere’s carbon potential for the process capabilities of the oven; and $x_m$ is the maximal depth of the carburized layer, and it is determined by the operating properties of the carburized product; for example, for the vacuum carburizing process for drill-bit roller cones, $x_m = 1.7 \cdot 10^{-3}$ m [9].

Boundary conditions of the third kind for equation (1) reflect carbon transition from the gas phase to the surface [3]:

$$\frac{\partial \Theta(\ell, \vartheta)}{\partial \ell} \bigg|_{\ell=0} = B(\vartheta) \cdot [\Phi(\vartheta) - \Theta(\ell, \vartheta)] \bigg|_{\ell=0}, \quad \vartheta \in (0, \infty),$$

(2)

where $B(\vartheta) = x_m \cdot \eta(\vartheta) \cdot \delta^{-1}$; $\eta(\vartheta)$ is the mass-transfer coefficient; $\Phi(\vartheta) = \alpha(\vartheta) \cdot \alpha_m^{-1}$; and $\alpha(\vartheta)$ is the atmosphere’s carbon potential.

Processes taking place in the product’s depth characterize adiabatic conditions of the second kind:

$$\frac{\partial \Theta(\ell, \vartheta)}{\partial \ell} \bigg|_{\ell=\infty} = 0, \quad \Theta(\ell, \vartheta) \bigg|_{\ell=\infty} = \Theta_0, \quad \vartheta \in (0, \infty).$$

(3)

The initial distribution of carbon concentration in layer $C_0$ equals:

$$\Theta(\ell, \vartheta) \bigg|_{\vartheta=0} = \Theta_0 = \text{const},$$

(4)

where $\Theta_0 = C_0 \cdot \alpha_m^{-1}$.

During the process, a carbide network may develop on the component’s surface. That network is highly fragile and therefore decreases wear resistance of the component, hence the limitation on the maximal carbon concentration $C_m$:

$$\Theta(\ell, \vartheta) \leq \Theta_m, \quad \forall \vartheta \in \left[0, \vartheta^{(i)}\right], \forall \ell \in [0, \infty),$$

(5)

where $\Theta_m = C_m \cdot \alpha_m^{-1}$, and the limitations on the maximal consumption of acetylene, whose dissociation determines the carbon potential of the oven atmosphere, are:

$$0 \leq \Phi(\vartheta) \leq 1.$$  

(6)

In the technologically justified case of pulsed carburization conditions, the relationships in figure 1 apply [10]:

$$\Phi(\vartheta) = \begin{cases} 1, & \vartheta \in \left(\vartheta^{(i-1)}, \vartheta^{(i)}\right), \text{ at } i = 1, 3, 5... \\ 0, & \vartheta \in \left(\vartheta^{(i)}, \vartheta^{(i+1)}\right), \text{ at } i = 2, 4, 6... \end{cases}, \quad i = 1, 2, ..., J.$$  

(7)
3. Formulating the problems of optimal control

The problem of optimal control over vacuum carburizing consists in determining the carbon distribution profile \( \Theta(\ell, \vartheta) \) that does not differ significantly from specified profile \( \Theta^*(\ell) \), which ensures that the operating requirements for the product are met. But it is neither technically feasible nor necessary to obtain precise profile \( \Theta^*(\ell) \) at the end of the process because in practice, several uncontrolled disturbances always occur, such as variations in the initial carbon content in steel, \( \Theta_0 \); the unstable gas composition of the atmosphere; and irregularities in the atmosphere flow. Further, specified profile \( \Theta^*(\ell) \) may not belong to the solutions to the boundary problem (1)–(4), which means it cannot be achieved at all.

As a result, under actual conditions of the allowable ranges for the parameters and states of model (1)–(4), the required resulting state of carburizing process \( \Theta^*(\ell) \) is specified as area

\[
\{\vartheta \in \Omega = \Theta^0(\ell) - \epsilon, \epsilon > 0\},
\]

which is characterized by the Chebyshev measure [11]:

\[
\xi = \max_{\vartheta \in [0,1]} |\Theta(\ell, \vartheta_0) - \Theta^*(\ell)|. \tag{8}
\]

Therefore, for the controlled object (1)–(4), subject to limitations (5) and (6), the following can be formulated:

- The problem of maximal efficiency:

\[
J^{opt}_{\vartheta} = \min_{\vartheta^{opt}} \left. \xi(\ell, \vartheta_0) \right|_{\vartheta \in [0,1]}, \tag{9}
\]

where \( \vartheta^{opt} \) is the time the process ends (fig. 1)

- The problem of maximally accurate control:

\[
J^{opt}_{\epsilon} = \min_{\vartheta \in [0,1]} \left. \max_{\vartheta \in [0,1]} |\Theta(\ell, \vartheta_0) - \Theta^*(\ell)| \right. \tag{10}.
\]

4. Parametric identification for the mathematical model of the vacuum carburizing process

To solve extremal problems (9) and (10), one needs to identify parameters \( \alpha_{\max}, \eta(\tau), \) and \( \delta \), which are part of the corresponding relative parameters of mathematical model (1)–(4).

To determine the carbon potential inside the oven, \( \alpha_{\max} \), one of active-identification methods — the foil-sample method — is used [12,13,14]. From two experiments, with identical saturation times at \( 0, \vartheta_0 \) (fig. 1) and with a single maximal-saturation stage, \( i = 1 \) at (7), the authors determined the maximal carbon potential of the oven atmosphere, \( \alpha_{\max} = 4.1\% \) C or \( \Phi(\vartheta) = 1 \).
To determine mass-transfer coefficient $\eta(\tau)$ and diffusion coefficient $\delta$, the authors also carried out several experiments with identical carburization times at $[0, \vartheta^2]$ (fig. 1) and with two-stage process $i = 1,2$ at (7). Figure 2 shows the identification results obtained with the least-square technique, with constant relative coefficient $B(\vartheta) = B_1 = const$ and known atmospheric carbon potential $\Phi(\vartheta) = 1$. As figure 2 illustrates, the difference between the experimental and calculated profiles at mass-transfer coefficient $B(\vartheta) = B_1 = const$ is about 25%, which is an impermissible value. The difference results from the nuances of vacuum carburizing—as opposed to, for instance, gas carburizing—mostly due to the mechanism of mass-transfer of carbon from the atmosphere onto the component’s surface. With gas carburizing, that mechanism does not vary as a function of the process stage, and only the intensity of carbon saturation changes. With vacuum carburizing, mass-transfer processes at saturation stage $i = 1,3,5...$ and diffusion stage $i = 2,4,6...$ differ significantly [15].

![Graph showing experimental and calculated carbon concentration profiles](image)

**Figure 2.** Comparison of the experimental and calculated carbon concentration profiles at $\delta = 9.29 \cdot 10^{-11} \text{ m}^2 \cdot \text{s}^{-1}$ and $\Phi(\vartheta) = 1$

At the saturation stage, acetylene molecules interact with the steel surface:

$$C_2H_2(\text{gas}) \xrightarrow{\text{catalysis}} C_2H_2(\text{ solids}) \xrightarrow{\text{catalysis}} CH + CH \xrightarrow{\text{catalysis}} C + C + H + H \rightarrow H_2.$$ \hspace{1cm} (11)

At the diffusion stage of vacuum carburizing, no carburizing atmosphere is present, and carbon sublimes from the component’s surface into the vacuum. The physics of carbon removal from the steel surface to the atmosphere differs for gas carburizing and vacuum carburizing. As a result, for purposes of calculating process conditions for vacuum carburizing, different coefficients $B(\vartheta) = B_{1 \sim 3,5...}$ and $B(\vartheta) = B_{2 \sim 4,6...}$ should be used for odd and even intervals, respectively, because of different mass-exchange conditions on the surface at the stages of saturation and diffusion:

$$B(\vartheta) = \begin{cases} B_1, \tau \in (t_{i-1}, t_i), \text{ for } i = 1,3,5... \\ B_2, \tau \in (t_{i-1}, t_i), \text{ for } i = 2,4,6... \end{cases}.$$ \hspace{1cm} (12)

Identification with the least-square technique at (11) with different mass-transfer coefficients for the 14XH3MA steel gives an accuracy not worse than 5% (fig. 2), and that satisfies the conventional accuracy requirements for mathematical models.
5. Solutions obtained for optimal problems
Reference [15] describes in detail the results of parameterizing optimal problems (9) and (10) and their solution with an alternance optimization method [8]. The solution reduces to finding quantity \( i \) and duration \( \Delta^0_i \), \( n = 1, 2, \ldots, i \) for intervals of control continuity \( \Phi(\vartheta) = \Phi^0(\Delta^0_i) \) and the error attainable in each \( i \)th control subset and equal to

\[
\varepsilon = \varepsilon^{(i)} = \max_{\vartheta \in \Delta} \left| \Theta(l, \vartheta) - \Theta^*(l) \right| \tag{12}
\]

which is the error of uniform approximation of resulting profile \( \Theta(l, \vartheta) \) to concentration profile \( \Theta^*(l) \) based on the conditions to satisfying the operation requirements.

For a technically justified situation with the most rational (in terms of wear resistance) carbon distribution profile during the carburizing of 14XH3MA steel roller cones to a depth of \( 1.7 \times 10^{-3} \) m, the individual vacuum carburizing process determined under the above method consists of four alternating active-saturation intervals with the maximal allowable atmospheric carbon potential \( \alpha_{\text{max}} = 4.1\% \) and subsequent diffusion without a carburizing atmosphere. The alternating intervals last for \( \Delta_1 = 2760s; \Delta_2 = 4980s; \Delta_3 = 90s \) and \( \Delta_4 = 150s \).

Reference [16] evaluates the nuances of structures and properties of steels most used in drill-bit manufacturing. Comparing the mechanical properties and impact hardness of drill-bit 14XH3MA and 15H3MA grades for the standard vacuum carburizing process and for the optimal (individualized) vacuum carburizing process shows that, given the final heat treatment (high tempering at 640°C, air cooling, hardening at 780°C in oil, and low tempering at 180°C), the properties and indicators under study are identical (do not differ significantly). Analysis of the core microstructure after the conventional and the individualized vacuum carburization following heat treatment confirms that the core of 14XH3MA consists of sorbite and disperse ferrite; and of 15H3MA, of sorbite-like perlite and disperse ferrite.

6. Conclusion
Individualizing the design of process conditions for the vacuum carburizing of drill-bit steels with the proposed mathematical model and optimization algorithms reduces the duration of the vacuum carburizing process by 13% and makes carburization as accurate as possible while keeping resource consumption to a minimum and preserving the required primary properties that determine the strength of drill-bit components. In a mass-production environment, this might serve as an indicator of economic efficiency and an important stimulus promoting practical use.

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