

Resource-saving optimal control of energy-intensive process of work part thermochemical treatment

M Yu Derevyanov¹, M Yu Livshits¹ and E A Yakubovich²

¹Department of Heat-and-Power Engineering, Samara State Technical University, Molodogvardeyskaya St., 244, Samara, 443100, Russia

²Department of Metal science, powder metallurgy, nanomaterials, Samara State Technical University, Molodogvardeyskaya St., 244, Samara, 443100, Russia

E-mail: eyakubovich@mail.ru

Abstract. Paper discusses approach to the resource-saving optimal control algorithms development, which includes problem oriented mathematical modeling of the process, determination of the tolerance limits for controlling action changes and condition of thermochemical treatment process as a subject under control, optimality criteria formalization and determination. Specified and solved critical problems for resource-saving optimal control of energy-intensive thermochemical process of work parts treatment on the maximum accuracy and speed of operation criteria. Alternance optimization method was used for optimal control problems solution, which allows to determine not only interval of constancy size but also maximum achievable control accuracy in every subset of intervals. Analytical mathematical model of vacuum carburizing in an acetylene atmosphere with variable coefficients of mass transfer was developed, which takes into consideration different mechanisms of carbon mass transfer from the atmosphere into the work part surfaces at the saturation and diffusion stages. Dependences of the carburization accuracy on the optimal control parameters were constructed. Influence of the technological constraints on the control quality was analyzed. Suggested approach demonstrated high energy efficiency.

Key words: optimal control, mathematical model, carburizing, parametric identification, carbon distribution, surface hardening.

1. Introduction

Modern industry in order to improve wear resistance of metal parts uses hardening technologies, which lead to physical and mechanical properties of the part's surface change [1-3]. Carburizing is the most common among this kind of technologies, during which part surface saturates with carbon. Process can be accelerated significantly as the result of high temperature carburizing implementation (with high carbon potential at the first stage) under pressure lower than atmospheric (vacuum carburizing) [4-6].

Vacuum carburizing process control on the optimal algorithms can provide not only high equipment productivity but also improve quality of the part surface under hardening [7-9].

Objective of this paper is development of the optimal control algorithms, that consist of problem oriented mathematical process modeling, tolerance limits determination for controlling action changes and condition of carburizing process as a subject under control, optimality criteria formalization and determination.



2. Mathematical model of the vacuum carburizing process

Model of the carbon diffusion from the atmosphere through the part surface into the depth at a constant temperature, based on Fick's second law, can be described in the form of the differential equation of mass transfer [10-11]:

$$\frac{\partial C(x, \tau)}{\partial \tau} = \frac{\partial}{\partial x} \left(D(C, T) \cdot \frac{\partial C(x, \tau)}{\partial x} \right), \quad (1)$$

$$\forall \tau \in (0, t_k], \forall x \in (0, \infty),$$

where $C(x, \tau)$ - carbon concentration in the work part; T - carburizing temperature; $D(C, T)$ - coefficient of carbon diffusion into steel [10].

Assuming that coefficient of diffusion dependence on concentration is insignificant, the equation of diffusion within narrow range of carburizing process temperatures can be linearized:

$$D(C, T) = D = \text{const}; \quad (2)$$

$$\frac{\partial C(x, \tau)}{\partial \tau} = D \cdot \frac{\partial^2 C(x, \tau)}{\partial x^2}, \quad \forall \tau \in (0, t_k], \forall x \in (0, \infty), \quad (3)$$

As a boundary conditions, which most accurately represent physics of carbon transfer from a gaseous phase to the surface, apparently, can be taken boundary conditions of the III kind [10]:

$$-D \cdot \frac{\partial C(x, \tau)}{\partial x} \Big|_{x=0} = \beta(\tau) \cdot (\varphi(\tau) - C(x, \tau) \Big|_{x=0}). \quad (4)$$

Here $\beta(\tau)$ - coefficient of mass transfer; $\varphi(\tau)$ - carbon potential of an atmosphere, φ_{max} - maximum permissible level of the carbon potential of an atmosphere on process capability of furnace and soot formation:

$$\varphi_{max} \geq \varphi(\tau) \geq 0. \quad (5)$$

Taking into the consideration insignificant depth $x = h_d$ of the diffusion layer in comparison with work part dimensions and relatively short time of carburizing $t = t_k$, much shorter than full saturation time, one can consider work part as a semi-infinite solid with adiabatic conditions:

$$\frac{\partial C(x, \tau)}{\partial x} \Big|_{x \rightarrow \infty} = 0. \quad (6)$$

Initial distribution of carbon concentration in the layer can be considered constant:

$$C(x, 0) = C_0 = \text{const}. \quad (7)$$

It is necessary to prevent intense carbide forming, that reduces surface wear resistance, in the process of carburizing.

$$C_{max}^{\kappa} \geq C(\tau). \quad (8)$$

Here C_{max}^{κ} - maximum permissible, on carbide content, level of carbon concentration in the work part, which is defined by the carburized layer embrittlement.

Boundary condition of the third kind (4) determines diffusing element flow through the separation surface «metal – saturating atmosphere» and considers it proportional to the difference of concentration on the surface $C(0, \tau)$ and equilibrium with an environment $\varphi(\tau)$.

3. Optimal control problem statement

During diffusion saturation there is no necessity and technical capabilities to provide the given profile $C^*(x)$ accurate realization at the process end, because some uncontrolled disturbances always present in the work environment: initial carbon content variations in steel C_0 , atmosphere's gas composition instability, atmosphere flow irregularity and so on [10,12,13]. In addition, there is a possibility that given profile $C^*(x)$ is not a part of the boundary value problem solutions (3), (4), (6), (7), which, in general, suggests that it is inaccessible in principle.

Therefore, in real conditions permissible range of parameters change and model status (3), (4), (6), (7), required resulting state of the carburizing process transforms from the given concentration distribution $C^*(x)$ into some region Ω_c - «tube» of permissible deviations $C^*(x) \pm \varepsilon$, that is characterized by Chebyshev measure [14-16]:

$$\rho_c = \max_{x \in [0, \infty)} |C^*(x) - \varepsilon|. \quad (9)$$

Naturally, in order to obtain a maximal wear resistance deviation value of ε must be minimal. Therefore, for controlled object (3), (4), (6), (7), under constraint conditions (5) – (8), problems are being formulated:

Speed of an operation problem:

$$J_\tau^{opt} = \min_{\varphi(\tau)} t_k \Big|_{C(x, t_k) \in \Omega_c}; \quad (10)$$

Maximum accuracy problem:

$$J_\varepsilon^{opt} = \min_{\varphi(\tau)} \max_{x \in [0, h_d]} |C(x, t_k) - C^*(x)|. \quad (11)$$

Stated problems are problems of optimal control with right variable end point of trajectory in the infinite dimensional non-smooth region of permissible resulting conditions.

$$\Omega_c = \left\{ C(x, \tau) : \max_{x \in [0, h_d]} |C(x, t_k) - C^*(x)| \leq \varepsilon \right\}$$

4. Optimal control problems solving method

Solution to the problems (10), (11) by the alternance optimization method (AOM) [15-17], determine both the optimal control $v^0(\tau) = \varphi(\tau) \equiv \varphi(\Delta_n^{(i)}) \in R^n$, $i = 1, 2, \dots, n$, in the form of piecewise constant function with i intervals of constancy Δ_i , and maximal attainable in every i -th subset accuracy

$$\varepsilon = \varepsilon_{min}^{(i)} = \max_{\varphi(\Delta_n^{(i)})} |C(x, t_k, \Delta_i) - C^*(x)| \quad (12)$$

of uniform approximation to the profile which is given as satisfying conditions of operational requirements $C^*(x)$.

AOM procedure assumes the determination of unknown optimal parameters Δ_i , $\varepsilon_{min}^{(i)}$, t_k , on the basis of solving auxiliary definiens system of transcendental equations:

$$\begin{cases} \theta(z, t_k)|_{z=z_{kj}} = \pm \varepsilon_m^{(i)} \\ \frac{\partial \theta(z, t_k)}{\partial z} \Big|_{z=z_{kj}} = 0, \end{cases} \quad (13)$$

where $\theta(z, t_k) = (C(x, t_k) - C^*(x)) / (\varphi_{max} - C_0)$; $\varepsilon_m = \varepsilon / (\varphi_{max} - C_0)$; $z = x/h$, $\varphi_{max} = \max_{\tau} \varphi(\tau)$.

Here z_{ej} - points of extremum of the function $\theta(z, t_k)$, $z_b = 1, h_d$ - boundary points of the function $\theta(z, t_k)$, while $i = 1, 2, \dots, S$; $S = i$, at $\varepsilon_{m_{min}}^{(i-1)} \geq \varepsilon_m^* \geq \varepsilon_{m_{min}}^{(i)}$; $S = i + 1$, at $\varepsilon_m = \varepsilon_{m_{min}}^{(i)}$; $z_{kj} = z_{ej} \cup z_b$; $t_k = \sum_{i=1}^S \Delta_i$.

Therefore, in order to solve the definiens system (13) it is necessary to obtain direct solution of the boundary problem (3), (4), (6), (7), for control $\varphi(\tau)$ [18]:

$$\varphi(\tau) = \begin{cases} \varphi_{max}, \tau \in (t_i, t_{i+1}), \text{ at } i = 0, 2, 4, \dots \\ 0, \tau \in (t_i, t_{i+1}), \text{ at } i = 1, 3, 5, \dots \end{cases} \quad (14)$$

In order to take into consideration an initial carbon distribution before each following interval, it is reasonable to use Green function method [10].

In this manner, solution of the linear non-homogeneous boundary problem (3), (4), (6), (7), at any point of time $\tau > t_\gamma$, can be written as follows:

$$C(x, \tau) = \int_0^\infty f(\xi) \cdot G(x, \xi, \tau) d\xi - D \cdot \int_0^\tau g(\tilde{\tau}) \cdot G(x, 0, \tau - \tilde{\tau}) d\tilde{\tau}, \quad (15)$$

where $f(\xi) = C(\xi, \tau)|_{\tau=t_\gamma}$ - carbon concentration distribution at a switching moment $\tau = t_\gamma$, where $\gamma = 0, 1, 2, \dots$ - interval number, while $t_0 = 0$ - starting moment of time; $\xi, \tilde{\tau}, \eta$ - intermediate values, $G(x, \xi, \tau)$ - Green function for the problem (3), (4), (6), (7) [10, 18]:

$$G(x, \xi, \tau) = \frac{1}{2 \cdot \sqrt{\pi \cdot D \cdot \tau}} \cdot \left\{ e^{\left[\frac{(x-\xi)^2}{4 \cdot D \cdot \tau} \right]} + e^{\left[\frac{(x+\xi)^2}{4 \cdot D \cdot \tau} \right]} - 2 \cdot \beta(\tau) \cdot \int_0^\infty e^{\left[\frac{(x+\xi+\eta)^2}{4 \cdot D \cdot \tau} - \frac{\beta(\tau)}{D} \right]} d\eta \right\}, \quad (16)$$

$$g(\tau) = -\frac{\beta(\tau)}{D} \cdot \varphi(\tau). \quad (17)$$

Then, to obtain the distribution function $C(x, \tau)$ from n -th intervals it is necessary to convolute the solution for $n-1$ th interval with Green function (16), moreover, as can be seen from (15), on the odd intervals it will be needed an introduction of the complimentary summand in the form of convection flow $g(\tau)$ (17) and Green function $G(x, 0, \tau - \tilde{\tau})$ with intermediate variable $\xi = 0$, which is the equivalent of zero depth of carbon penetration:

$$C_n(x, \tau) = \int_0^\infty C_{n-1}(\xi, \tau) \cdot G(x, \xi, \tau) \Big|_{\tau=t_n} d\xi - D \cdot \int_0^\tau g(\tilde{\tau}) \cdot G(x, 0, \tau - \tilde{\tau}) d\tilde{\tau}. \quad (18)$$

Formula (18) describes carbon distribution in the carburized layer at an arbitrary point of time with n -th number of controlling actions.

Due to the fact that integrand in the first summand (18) is a convolution of a complex function $C_{n-1}(\xi, \tau)$ with a Green function $G(x, \xi, \tau)$, the calculation of such integrals becomes a sophisticated problem. To solve this problem, it is worthwhile to use integrand approximation $C_{n-1}(\xi, \tau)$.

In particular case, for example, for a single interval control ($i = 1$), according to (7):

$$f(\xi) = C(\xi, \tau)|_{\tau=t_0} = C_0. \quad (19)$$

In this manner, from the equation (15) with consideration of (19) solution for the single interval control is obtained:

$$C_I(x, \tau) = \int_0^{\infty} C_0 \cdot G(x, \xi, \tau) d\xi - D \cdot \int_0^{\tau} g(\tilde{\tau}) \cdot G(x, 0, \tau - \tilde{\tau}) d\tilde{\tau}. \quad (20)$$

For the double interval control ($i = 2$) initial distribution at the switching moment $\tau = t_1$:

$$f(\mu) = C_I(\mu, \tau)|_{\tau=t_1}, \quad (21)$$

and $\tau = t_2$ should be introduced into (16), here μ - intermediate variable.

Carbon distribution for the double interval control is described by the general equation (15) with consideration that for the second interval controlling action is $\Phi(\tau)|_{\tau=t_2} = 0$, and then in (17) $g(\tau) = 0$.

For the double interval control we obtain:

$$C_{II}(x, \tau) = \int_0^{\infty} C_I(\mu, \tau)|_{\tau=t_1} \cdot G(x, \mu, \tau)|_{\tau=t_2} d\mu. \quad (22)$$

In (22) instead of $C_I(\mu, \tau)|_{\tau=t_1}$ approximation can be used and that will simplify further calculations significantly.

For the triple interval control ($i = 3$) solution can be written as follows:

$$C_{III}(x, \tau) = \int_0^{\infty} C_{II}(\varpi, \tau)|_{\tau=t_3} \cdot G(x, \varpi, \tau)|_{\tau=t_2} d\varpi - D \cdot \int_0^{\tau} g(\theta) \cdot G(x, 0, \tau - \theta) d\theta. \quad (23)$$

Likewise, analytical problem solution for the quadruple interval control ($i = 4$) is as follows:

$$C_{IV}(x, \tau) = \int_0^{\infty} C_{III}(\psi, \tau)|_{\tau=t_4} \cdot G(x, \psi, \tau) d\psi. \quad (24)$$

5. Results and Discussion

In order to solve formulated extremum problems (10), (11) by solving the auxiliary system (13) it is necessary to identify parameters (coefficients of diffusion D and mass transfer $\beta(\tau)$) of the mathematical model (3), (4), (6), (7) [13].

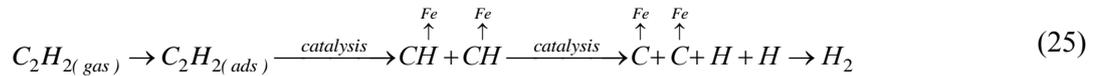
Identification procedure is based on the least squares method, which determined values $\beta(\tau)$ and D . Identification results with the constant coefficient of mass transfer $\beta(\tau) = \beta_1 = const$ and with carbon potential $\varphi_{max} = 4.1\%C$, determined by a foil test method, presented in Figure 1.

Comparison of the estimated and experimental carbon profiles for steel 14HN3MA (14CrH3Mo) suggests that the difference between experimental and estimated profile with mass transfer coefficient $\beta(\tau) = \beta_1 = const$ is around 40%, which is intolerable.

Cause for this discrepancy can be explained by vacuum carburizing specifics as opposed to, for example, gaseous, firstly, because of the mass transfer mechanism of carbon from an atmosphere to the

work part surfaces. Mechanism of the carbon mass transfer process, during gas carburizing, remains constant at all process stages. Only carbon saturation intensity changes. During vacuum carburizing processes of the mass transfer at saturation stage $i = 1, 3, 5, \dots$ and diffusion stage $i = 0, 2, 4, \dots$ vary significantly [13].

At the diffusion stage acetylene molecules interact with steel surface:



Carburizing atmosphere at a diffusion stage of a vacuum carburizing is not present, and carbon sublimes from the work part surface into vacuum. Physics of a carbon removal from a metal surface into atmosphere during vacuum and gas carburizing is different. Therefore, in technological mode calculations of vacuum carburizing should be used different coefficient values $\beta(\tau) = \beta_1|_{i=1,3,5,\dots}$ and $\beta(\tau) = \beta_2|_{i=2,4,6,\dots}$ for even $i = 0, 2, 4, \dots$ and for odd $i = 1, 3, 5, \dots$ intervals due to different conditions of mass transfer on the surface, at the saturation and diffusion stages:

$$\beta(\tau) = \begin{cases} \beta_1, \tau \in (t_i, t_{i+1}), \text{ at } i = 0, 2, 4, \dots \\ \beta_2, \tau \in (t_i, t_{i+1}), \text{ at } i = 1, 3, 5, \dots \end{cases} \quad (26)$$

Identification of the model (3)-(5) by the least squares method in conditions (25) with different mass transfer coefficients for steel 14HN3MA (14CrH3Mo) (Figure 1), ensures accuracy at least 5% according to (9).

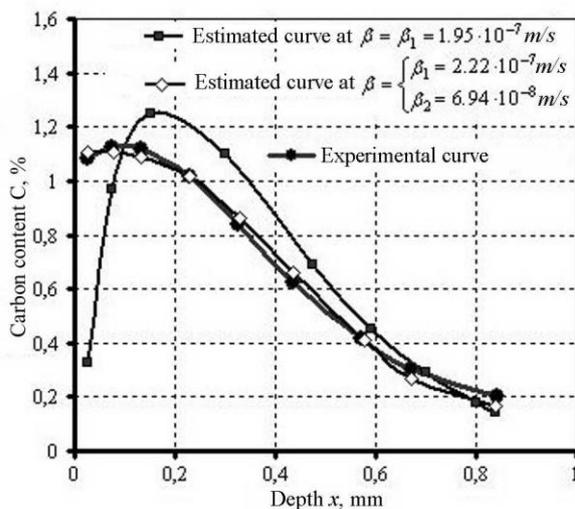


Figure 1. Comparison of experimental and estimated carbon concentration profiles at $D = 6.44 \cdot 10^{-11} m^2 \cdot s^{-1}$, $\varphi_{max} = 4.1 \%C$.

Examined model of vacuum carburizing (18) under controlling action (14) doesn't take into consideration influence of soot formation, in other words, free carbon precipitation on the surfaces of work parts and structural parts of a furnace, which obstructs uniform access of carbon atoms to a steel surface. Therefore, control $\varphi(\tau)$, in combination with (5), should be under constraints (Figure 2):

$$\varphi_{min} \leq \varphi(\tau) \leq \varphi_{max}, \quad (27)$$

$$\varphi_{min} \leq \varphi(\tau) \leq \varphi_{con}(\tau), \quad (28)$$

$$\varphi_{con}(\tau) = a\tau^2 + b\tau + c, \quad \tau \in (t_i + \Delta^0, t_{i+1}), i = 0, 2, 4, \dots \tag{29}$$

$$\varphi_{min} = const \tag{30}$$

Here φ_{min} - the maximum value of carbon potential, determined by furnace atmosphere irregularity; coefficients a, b, c designated in accordance with a furnace type, work parts characteristics and saturated atmosphere; Δ^0 - duration of constraint (14).

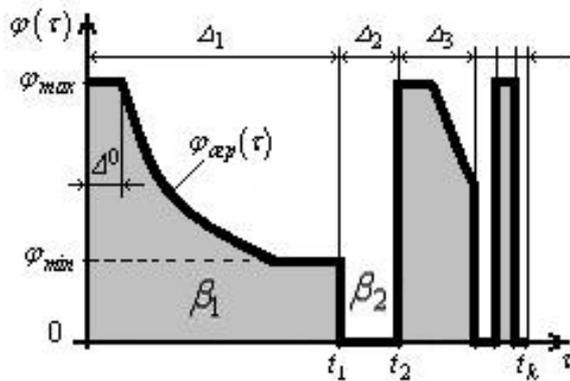


Figure 2. Controlling action $\varphi(\tau)$ for $i=6$ with a soot formation constraint.

For the real industrial technology of the vacuum carburizing formulated optimal problems (10), (11) have been solved for the model (3), (4), (6), (7) in variable coefficients condition $\beta(\tau)$ under controlling action $\varphi(\tau)$ (5) without soot formation influence. Below presented dependencies of the interval durations Δ_i of optimal vacuum carburizing process on the carburization accuracy ε without soot formation constrains consideration (figure 3) and with technological limitations consideration (5), (27) – (30) on the controlling action $\varphi(\tau)$ of soot formation (figure 4).

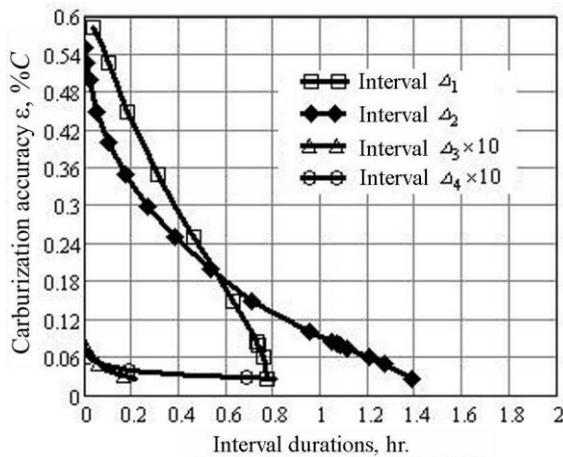


Figure 3. Dependencies of the interval of constancy durations Δ_i on the carburization accuracy ε without soot formation constrains.

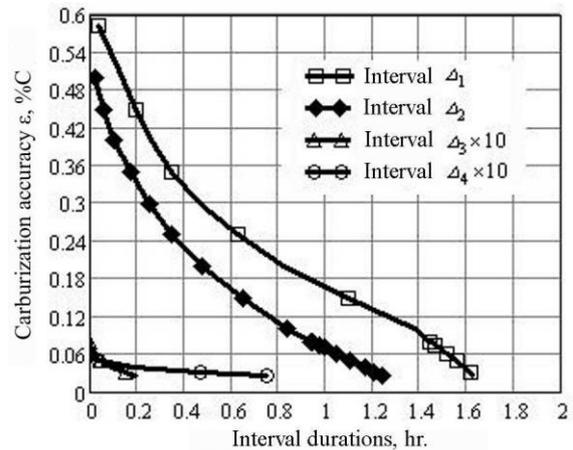


Figure 4. Dependencies of the interval of constancy durations Δ_i on the carburization accuracy ε with soot formation constrains.

Coefficient values, used in calculations, $\beta_1=2.22 \cdot 10^{-7} \text{m} \cdot \text{s}^{-1}$, $\beta_2=6.94 \cdot 10^{-8} \text{m} \cdot \text{s}^{-1}$, $D=6.19 \cdot 10^{-11} \text{m}^2 \cdot \text{s}^{-1}$, $\varphi_{max} = 4.1 \% \text{C}$.

6. Conclusion

Obtained dependencies analysis (Figure 3 and Figure 4) allows to make a conclusion that consideration of the soot formation influence increases process duration slightly and therefore expenses on fuel. However, long and systematic use of carburizing technology, taking into consideration possible soot formation, allows decrease significantly labor intensity and cost for soot formation removal from the furnace surfaces.

Process optimization allows to synthesize flexible resource saving customized TCT technology, that ensures specific operation requirements with maximum possible accuracy in a minimum time and minimum resource usage [19]. Efficiency of such algorithms is verified by their introduction into the industry [11, 12].

Acknowledgments

Research is conducted with the assistance of RFBR grants (project 17-08-00593, 19-08-00232)

References

- [1] Lakhtin M Yu and Arzamasov B N 1985 *Ximicheskaya termoobrabotka metallov* [Chemical Heat Treatment of Metals] (Moscow: Metallurgiya) [In Russian]
- [2] Edenhofer B 1999 *Heat Treatment of Metals* **26(1)** 1-5
- [3] Semenov M Yu, Smirnov A E and Ryzhova M Yu 2013 *Metal Science and Heat Treatment of Metals* **1** 38-42
- [4] Kula P, Pietrasik R and Dybowski K 2005 *J. of Materials Processing Technology* **164-165** 876-81
- [5] Kula P, Kaczmarek Ł, Dybowski K, Pietrasik R and Krasowski M 2013 *Vacuum* **87** 26-9
- [6] Lee-Der Liu and Fan-Shiong Chen 2003 *Materials Chemistry and Physics* **82(2)** 288-94
- [7] Lee-Der Liu and Fan-Shiong Chen 2004 *Surface and Coatings Technology* **183(2-3)** 233-8
- [8] Bataev I A, Golkovskii M G, Losinskaya A A, Bataev A A, Popelyukh A I, Hassel T and Golovin D D 2014 *Applied Surface Science* **322** 6-14
- [9] Kazuyuki Yada and Osamu Watanabe 2013 *Computers & Fluids* **79** 65-76
- [10] Derevyanov M Yu, Lipkind V Ya, Lifshits M Yu 2010 *Bulletin of Samara State Technical University. Ser. Eng.* **26** 187-95 [In Russian]
- [11] Livshits M Yu and Yakubovich E A 2016 *Materials Science Forum* **870** 647-53
- [12] Derevyanov M Yu, Livshits M Yu and Yakubovich E A 2017 *IOP Conf. Ser.: Earth and Envir. Sci.* **87** 082012
- [13] Derevyanov M Yu, Livshits M Yu and Yakubovich E A 2018 *IOP Conf. Ser.: Mater. Sci. Eng.* **327** 022022
- [14] Derevyanov M Yu, Pleshivtseva Yu E, Kordyukova L S and Rapoport A V 2019 Using DEA models to measure the efficiency of energy saving projects *IOP Conf. Ser.: Mater. Sci. Eng.* **552** 012020
- [15] Pleshivtseva Yu E and Rapoport E Ya 2009 The successive parameterization method of control actions in boundary value optimal control problems for distributed parameter systems *J. of Computer and Systems Sciences Int.* **48 (3)** 351-62
- [16] Rapoport E Ya 2013 Minimax optimization of stationary states in systems with distributed parameters *J. of Computer and Systems Sciences Int.* **52 (2)** 165-79
- [17] Pleshivtseva Yu E and Rapoport E Ya 2013 Joint optimization of interrelated thermophysical processes in metal working systems based on system quality criteria *Optoelectronics, Instrumentation and Data Processing* **49 (6)** 527-35
- [18] Pleshivtseva Yu E and Rapoport E Ya 2018 Parametric Optimization of Systems with Distributed Parameters in Problems with Mixed Constraints on the Final States of the Object of Control *J. of Computer and Systems Sciences Int.* **57(5)** 723-37
- [19] Zhao Y et al. 2015 *Alloys, Metallurgical and Materials Transactions* **46** 2218-23