doi.org/10.15407/tpwj2017.01.05

## MATHEMATICAL MODELING OF CHEMICAL COMPOSITION OF WELDING FUMES IN MANUAL ARC WELDING WITH HIGH-ALLOYED ELECTRODES

O.G. LEVCHENKO<sup>1</sup> and O.N. BEZUSHKO<sup>2</sup> <sup>1</sup>NTUU «Igor Sikorsky KPI» 37 Pobedy Prosp., 03056, Kiev, Ukraine <sup>2</sup>E.O. Paton Electric Welding Institute, NASU 11 Kazimir Malevich Str., 03680, Kiev, Ukraine. E-mail: office@paton.kiev.ua

A mathematical model of convective evaporation of metal from the melt surface was proposed for prediction of the composition of fumes formed in manual arc welding. Numerical analysis of the characteristics of the flow of multicomponent metal vapour in welding with high-alloyed chromium-nickel electrodes was performed. Rates of evaporation of welding fume components at application of electrodes for high-alloyed steel welding were established. Obtained mathematical model enables calculation of not only the relative mass fraction of toxic component in the fume, as it was possible up to now, but also of convective flows of welding fume components. 12 Ref., 2 Tables, 4 Figures.

*Keywords:* electric arc welding, coated electrodes, welding fumes, chemical composition, evaporation intensity, mathematical modeling

Manual arc welding is characterized by high values of temperature in the arc gap. A considerable part of the surface of metal of electrode drops and weld pool is in the boiling state and evolves a large amount of metal vapours into the arc zone, from which fumes harmful for the welder's body form as a result of vapour condensation and oxidation in working zone air.

The objective of this work was mathematical simulation of the composition of welding fumes (WF) forming in manual arc welding with high-alloyed



Figure 1. Dependence of pressure of saturated vapours of chromium, nickel, manganese and iron on temperature

© O.G. LEVCHENKO and O.N. BEZUSHKO, 2017

28

chromium-nickel electrodes based on physico-chemical properties of weld pool components.

Vapour pressure of different substances becomes higher with temperature rise. After a significant vapour pressure equal to atmospheric pressure (101325 Pa) has been reached, the substance starts boiling [1]. Dependence of saturated vapour pressure  $p_i$  near the molten metal surface on its temperature can be determined, using Kleiperon–Klausius equation [2]

$$p_{\rm s} = p_0 \exp\left[\frac{\lambda}{k} \left(\frac{1}{T_{\rm v}} - \frac{1}{T_{\rm s}}\right)\right],\tag{1}$$

where  $p_s$  is the saturated vapour pressure above the metal surface;  $p_0$  is the atmospheric pressure,  $T_b$  is the metal boiling temperature (temperature, at which saturated vapour pressure of this metal is equal to atmospheric pressure);  $T_s$  is the surface temperature,  $\lambda$  is the work function of atom in the melt, k is the Boltzmann constant. This equation holds, provided the vapour follows the ideal gas law, and molar volume of liquid  $V_i$  is much smaller than molar volume of vapour  $V_a$ .

Plotted graphic dependencies of saturated vapour flow of individual toxic elements, included into welding electrode composition (chromium, manganese, nickel and iron), on evaporating alloy surface temperature, according to equation (1) at  $T_s = 1500-3500$  K, are given in Figure 1. Analysis of the given data shows that during open arc welding process man-

ganese will be the first to evaporate the most intensively, followed by chromium, iron and nickel.

Calculations were performed using the values of atom work function  $\lambda$  and boiling temperature  $T_{\rm b}$ , at which pressure of the respective element saturated vapour is equal to atmospheric pressure [3, 4] (see Table 1).

Let us evaluate the resulting pressure of saturated vapours over the surface of an alloy, which is in the liquid state [5]. We will regard this alloy as a weak solution of chromium, manganese and nickel in iron. We will determine resulting pressure  $p_v$  as a sum of saturated vapour pressures above the alloy *i*-th component  $p_{is}$ , allowing for activity of the *i*-th component in the solution  $\alpha_i$ 

$$p_{\rm v} = \sum_{i} \alpha_i p_{i\rm s}.$$
 (2)

Iron activity can be determined, using Raoult law [2, 5]

$$\alpha_{\rm Fe} = X_{\rm Fe},\tag{3}$$

where  $X_{\text{Fe}}$  is the molar (atomic) fraction of Fe in the respective alloy. Note that Raoult law is applicable practically only for weak solutions, in which the saturated vapour behaves as an ideal gas, i.e. it is fulfilled the better, the lower the vapour pressure.

We will apply Henry's law to determine the activity of the vapour of dissolved substances Cr, Mn, Ni [2, 5]. Let us present impurity activities in the following form:

$$\alpha_{\rm Cr, Mn, Ni} = \gamma_i X_{\rm Cr, Mn, Ni}, \qquad (4)$$

where  $\gamma_i$  is the coefficient of activity of the *i*-th element;  $X_{Cr, Mn, Ni}$  is the molar (atomic) fraction of the respective dissolved element, i.e. its concentration in the alloy. In view of lack of data, let us assume that all the coefficients of activity are equal to a unity.

Thus, considering relationship (3) and assuming that  $\alpha_{Cr, Mn, Ni} = X_{Cr, Mn, Ni}$ , formulas (1) and (2) can be used to assess the saturated vapour pressure above the surface of an alloy, which is in the molten state, depending on  $T_s$ . Molar fraction of an element in the melt is calculated by the following relationship:

$$X_{im} = \frac{C_{im} : M_i}{\sum C_{im} : M_i},$$
(5)

where  $M_i$  is the atomic mass;  $C_{im}$  is the mass fraction of *i*-th element in the melt.

Let us study the features of evaporation of a multicomponent alloy in the case of high-alloyed electrodes of E-08Kh20N9G2B type (20 % Cr, 2 % Mn, 9 % Ni). Pressure of multicomponent saturated vapour over the melt for Cr, Mn, Ni and Fe is given in Figure 2.

Let us apply Knight model to determine the quantitative characteristics of the evaporation process (density, temperature and outflow velocity of the vapour)

ISSN 0957-798X THE PATON WELDING JOURNAL, No. 1, 2017

Table 1. Physical properties of molten metal components

Physical properties	Chemical element				
	Cr	Mn	Ni	Fe	
Atom work function in the melt, $\lambda$ , erg·10 <sup>-12</sup>	5.79	3.73	6.31	5.65	
Metal boiling temperature, $T_{\rm b}$ , K	2840	2424	3173	3008	

[6]. The model is based on the assumption that the vapour flow is one-dimensional and stationary. This model is actively applied for performance of numerical analysis of thermal and gas-dynamic characteristics of the vapor flow in laser welding [6–9]. Information about its application for manual arc welding is not available.

According to this model, there is a Knudsen layer of the thickness of several free path lengths vapour particles near the evaporated metal surface, beyond which (in the gas-dynamic flow region) a thermodynamic equilibrium is established. In [6–9] the following relationships were proposed, which relate density  $\rho_v$  and temperature  $T_v$  of vapour on Knudsen layer boundary with saturated vapour density  $\rho_{s,v}$  and evaporating surface temperature  $T_s$ 

$$\frac{T_{v}}{T_{s}} = 1 + \frac{m^{2}\pi}{32} \left( 1 - \sqrt{1 + \frac{64}{m^{2}\pi}} \right), \tag{6}$$

$$\frac{\rho_{v}}{\rho_{s,v}} = \sqrt{\frac{T_{s}}{T_{v}}} \left[ \left( m^{2} + \frac{1}{2} \right) e^{m^{2}} \operatorname{erfc}(m) - \frac{m}{\sqrt{\pi}} \right] + \frac{1}{2} \frac{T_{s}}{T_{v}} (1 - \sqrt{\pi} m e^{m^{2}} \operatorname{erfc}(m)),$$
(7)

where  $\operatorname{erfc}(m)$  is the probability integral. Value *m* is calculated by the following formula

$$m = \left(\frac{M_{\nu}u^2}{2kT_{\nu}}\right)^{1/2},\tag{8}$$



**Figure 2.** Temperature dependence of saturated vapour pressure above the surface of metal melt of E-08Kh20N9G2B type electrodes ( $X_{cr} = 0.213$ ;  $X_{Mn} = 0.02$ ;  $X_{Ni} = 0.085$ ;  $X_{re} = 0.683$ )



**Figure 3.** Dependence of convective vapour flows of chromium (1), iron (2), manganese (3), and nickel (4) on drop surface temperature

where u is the weight-average velocity of outflow from the metal surface.

Weight-average velocity of outflow from the metal surface was calculated by the following formula

$$u = \frac{s_0 \left(\frac{p_m^0}{p_0} - 1\right)}{\gamma_0 \sqrt{1 + \frac{\gamma_0 + 1}{2\gamma_0} \left(\frac{p_m^0}{p_0} - 1\right)}},$$
(9)

where  $p_0$  is the atmospheric pressure;  $\gamma_0 = 1.4$  is the constant of air adiabatic;  $s_0 = 331.5$  m/s is the velocity of sound in the air;  $P_m^0$  is the vapour pressure on Knudsen layer boundary.

Calculation of convective flow of vapour was performed by the following formula:

$$J_{p,i} = \alpha_i \frac{p_s}{p_v} \frac{M_i}{M_v} j_{\rho}, \qquad (10)$$

where  $p_v$  is the resultant pressure, calculated by formula (2);  $p_i$  is the saturated vapour pressure over the *i*-th component from formula (1);  $\alpha_i$  is the activity of the *i*-th component, calculated by formulas (3, 4);  $M_v$ is the average mass of an atom of multicomponent vapour  $M_v = \sum_{i=1}^n M_i \frac{\alpha_i p_s}{p_v}$ ,  $j_\rho$  is the full evaporation flow  $j_\rho = \rho_v Ms \approx \rho_v u$ .





 Table 2. Intensity of WF component formation in welding with coated electrodes of E-08Kh20N9G2B type

Electrode type —	Formation intensity, $V_a$ ·10 <sup>-5</sup> , kg/s				
E-08Kh2ON9G2B (ANV-65u grade)	CrO <sub>3</sub>	Cr <sub>2</sub> O <sub>3</sub>	Mn	Ni	
	0.018337	0.025005	0.020004	0.003334	

Obtained graphic dependencies of convective flows  $J_i$  of chromium, manganese, nickel and iron on drop surface temperature are given in Figure 3.

As is seen from Figure 3, in the temperature range from 2900 to 3400 K, the highest evaporation flow is characteristic for chromium and iron. To determine the evaporation intensity of these elements, we will assume that the drop evaporation area is the same as that of a sphere with a diameter equal to electrode diameter. Diameter of electrodes, used to perform experimental welding, was equal to 4 mm. Then, the area of a spherical welding drop was calculated by formula  $S_{drop} = \pi d^2$  and was equal to  $5.0265 \cdot 10^{-5}$  m<sup>2</sup>.

We will write the evaporation flow of the *i*-th element in the following form

$$J_i = V_i S_{\text{drop}}.$$
Hence,  $V_i = J_i S_{\text{drop}}.$ 
(11)

Experimental data [10] of the intensity of formation (precipitation) of chromium, manganese, nickel and iron in welding with coated electrodes of E-08Kh20N9G2B type, are given in Table 2.

Experimental data were used to plot the diagrams of the intensity of WF component formation.

As is seen from the obtained results, the summary value of the intensity of chromium compound formation prevails over the values of other harmful components that is confirmed by calculated data of the intensity of chromium evaporation (Figure 4).

Using the proposed mathematical model, it is possible to predict the intensity of formation of the above WF components in welding with high-alloyed chromium-nickel electrodes. Here, it should be taken into account that the vapour formed from molten metal drop is transferred into the weld pool, where is partially condenses, and the rest is dissipated beyond the arc, forming fumes as a result of vapour condensation in air. Thus, the results of experimental determinations of the quantity of evolved WF show just that part of metal vapour from which the fumes form. Therefore, in order to precise the actually predicted value of the intensity of WF component evolution, we will use the coefficient of  $K_{yy}$  ratio of experimental value of evolution intensity of *i*-th element  $V_{iexp}$  to its calculated evaporation intensity V

$$K_{vi} = V_{iexp} / V_{icalc}$$

Calculated value of evaporation intensity  $V_{icalc}$  was used at the temperature of  $T_v = 3000$  K. As experimental values of chromium evaporation intensity are given for trivalent and hexavalent chromium, we will sum them up for their comparison with calculated data. Obtained data of the coefficients of evaporation intensity of the *i*-th element  $K_{vi}$  for chromium, manganese and nickel, respectively, in welding with electrodes of 08Kh20N9G2B type with basic coating with metal deoxidation-alloying through the electrode rod are as follows:  $K_{vCr} = 6.08 \cdot 10^{-4}$ ;  $K_{vMn} = 9.09 \cdot 10^{-4}$ ;  $K_{vNi} = 4.54 \cdot 10^{-4}$ .

Verification of mathematical model accuracy showed that relative error of component ratios in the compositions of vapour and WF does not exceed 30 % that is due to the assumptions taken during development of this modeling system.

## Conclusions

Thus, the proposed mathematical model enables calculation of not only the relative mass fraction of the toxic component in percent, as it was possible up to now [11], but also calculation of the convective flows of WF components, that allows prediction of the main hygienic index of welding consumables without experimental studies, namely the intensity of WF component formation [12] and determination on its basis of the degree of the risk of harmful action of the process of welding by these consumables on the welder's body.

- 1. Potapov, N.N. (1989) *Consumables for arc welding*. Vol. 1: Shielding gases and welding fluxes: Refer. Book. Moscow: Mashinostroenie.
- Landau, L.D., Lifshits, E.M. (1976) *Theoretical physics*. Vol. 5: Statistic physics. Pt 1. Moscow: Nauka.
- 3. Nesmeyanov, A.N. (1961) Vapour pressure of chemical elements. Moscow: AN SSSR.
- 4. (1976) *Tables of physical magnitudes*: Refer. Book. Ed. by I.K. Kikoin. Moscow: Atomizdat.
- 5. (1969) *Course of physical chemistry*. Vol. 1. Ed. by Ya.I. Gerasimov. Moscow: Khimiya.
- 6. Knight, C.J. (1979) Theoretical modeling of rapid surface vaporization with back pressure. *AIAA J.*, **17**, 519–523.
- 7. Krivtsun, I.V., Sukhorukov, S.B., Sidorets, V.N. et al. (2008) Modelling of the processes of evaporation of metal and gas dynamics of metal vapour inside a keyhole in laser welding. *The Paton Welding J.*, **10**, 16–22.
- Zhao, H., Debroy, T. (2001) Weld metal composition change during conduction mode laser welding of aluminum alloy 5182. *Metallurg. and Materials Transact. B*, 32B, 163–172.
- Mundra, K., Debroy, T. (1993) Calculation of weld metal composition change in high-power conduction mode carbon dioxide laser-welded stainless steels. *Metal. Transact. B*, 24B, 145–155.
- Yushchenko, K.A., Levchenko, O.G., Bulat, A.V. et al. (2007) Sanitary and hygienic characteristics of covered electrodes for welding high-alloy steels. *The Paton Welding J.*, **12**, 35–38.
- Podgaetsky, V.V., Golovatyuk, A.P., Levchenko, O.G. (1989) About mechanism of welding fume formation and prediction of its composition. *Avtomatich. Svarka*, 8, 9–12.
- 12. DSTU ISO 15011-4:2008: Health protection and safety in welding and related processes. Laboratory method of sampling of fumes and gases. Pt 4: Form for fumes data record. Valid from 2008-08–15. Kyiv: Derzhspozyvstandart Ukrainy, 2011.

Received 17.11.2016