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Modeling of the Process of Welding Aerosol Formation Taking Place During Mining Equipment Fabrication

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Abstract. In the paper the authors formulate the thermodynamic model of welding aerosol formation. The thermodynamic parameters of chemical compounds and aerosol phases are calculated. The authors develop a program for numerical calculation of various elements emission under varied parameters changing the welding conditions.

1. Introduction

At the present moment practically in all branches of industry various kinds of welding including electroslag, contact, electron beam, plasma-arc welding, have become widely spread. Application of the given methods of metal working leads to formation of welding aerosol (WA) in the air of manufacturing areas. WA is a combination of the finest particles formed as a result of condensation of molten metal vapor, electrode coating, ingredients of the flux cored wire or fluxes. WA composition depends upon the components of welded and welding materials. Mainly, WA consists of iron and its oxides, as well as manganese, chrome, nickel, aluminum, cuprum, zinc, fluorine, silicon, nitrogen and other. By the nature of its formation the WA is a condensation aerosol and presents a disperse system where the dispersion phase is presented by fine particles of solids and the dispersion medium is the mixture of gases. So it is necessary to distinguish the solid component of the welding aerosol (SCWA) and the gas component of the welding aerosol (GCWA) in the WA composition [1].

Arc welding processes take place in the open type reactors (Fig. 1) where, effected by high temperature and infrared radiation, the components of coatings, fluxes and metals are intensively evaporated and then, in the process of oxidation and condensation outside the arc, they form submicron aerodispersion particles; thermochemical transformations of fluorides and fluorisilicates, reduction of carbon dioxide or incomplete oxidation of organic binders of coating and plasticizers with formation of HF and SiF₄, CO₂; nitrogen is oxidized (N₂ + O₂ + hv = 2NO₂); oxygen of the air turns into ozone (O₂ + hv => O⁺ + O⁺; O₂ + O⁺ = O₃). When completing the works associated with application of calcium carbide which, as a rule, is contaminated with calcium phosphate, phosphine is formed (PH₃). In case of welding (cutting) parts, units, constructions or materials covered with conserving agents, paint or (and) technological contaminators some other substances may also be released into the gaseous phase, such as: chlorine hydride (HCl), chlorine (Cl₂), phosgene (COCl₂), carbon tetrachloride (CCl₄), trichloroethylene (CCl₂=CHCl), sulphur dioxide and trioxide (SO₂, SO₃), hydrogen sulphide (H₂S), phosphorus (P₄), phosphoric anhydride (P₂O₅), phosphine (PH₃) and other toxic compounds.
It is known that 80-90% of the chemical composition of the SCWA is determined by the content of the welding electrode [1]. In the process of covered-electrode welding 1-3% of electrode material evaporates [3]. The rate of evaporation of the molten mass and the composition of WA are determined by the welding conditions and the welding method, composition of electrode coating, that of the base and filler metal. In the process of welding we usually observe not melting of pure metals but that of alloys, then, vapor will represent a mixture of gaseous components of the alloy. The lower the evaporation heat of the substance and the higher the heating temperature, the more intensive the evaporation process is. Thus, the greater part of the vapor will consist of components with lower evaporation heat. That means that separate components of multicomponent systems are evaporated selectively, for example, from the iron and manganese melts it is manganese to be evaporated first.

When covered-electrode welding metal sequentially passes first the stage of a drop and then the stage of a weld pool. When covered-electrode welding the same stages are also observed for the slag phase. The drop phase is characterized by higher degree of overheating and the specific surface exceeding the specific surface at the stage of the weld pool. Due to the temperature gradient effected by arc pressure and plasma flows convective mass transfer of the evaporated substances is completed from the area of the arc discharge. In the area of lower temperatures the vapor phase condenses and some products of condensation (metals and oxides with the lowest oxidation degree) are subjected to further oxidation. In the works of M. Kobayashi and others [4, 5] we conclude that WA results mainly from electrode metal evaporation (coating and core) in the area of the arc at the stage of the drop and the role of the melt at the stage of the weld pool is less significant. The formed vapor effected by arc pressure and plasma flows travels to the outside environment with lower temperature where it is condensed.

In their works R. Heile and D. Hill [6] describe two possible mechanisms of WA formation. According to the first mechanism, components of electrode and base metals are melt and evaporated and the produced vapor is condensed after it leaves the high-temperature area of the arc and oxidizes. The second mechanism involves formation of volatile oxides under the action of the oxygen on the surface.
of molten electrode (for example, SiO). The oxygen can be found in the arc atmosphere when welding in the gas mixture (92% Ar + 6% CO₂ + 2% O₂). Formation of such oxides may lead to more intense formation of WA. The degree of involvement of each of the described above mechanisms changes according to the welding method and the shielding gas composition, with reduction of oxidizing potential of the shielding gas the second mechanism plays a less significant role in WA formation.

According to the data of modern physical and chemical research (X-ray diffraction, spectral and other methods of analysis) the composition of the solid component of the welding aerosol (SCWA) formed in the process of covered-electrode welding includes basic (Mn, Fe, Si, K, Na, Ca, Mg, Ti, Al, Cr, Ni, F) and impurity (As, Cu, Rb, Sn, Zr, Sr, Nb, Mo, Ag, Sb, Ba, Pb) as well as complex mixtures of metals, simple and composite oxides of metals, spinels MnFe₂O₄, CaFe₂O₄, (Fe,Mn)O-Fe₂O₃, K₂Cr₂O₇, Na₂Cr₂O₇, FeO₄ and other, fluorides (NaF, KF, K₃FeF₆, K₂SiF₆, CaF₂ and other), silicates (CaSiO₃, Si-O-Si-O-Si, Fe₃[SiO₄]₂, Mn₃[SiO₄] and other). Application of special steels with increased content of manganese (11…14.5 %) and other alloying components for mining equipment production (35L, 45L, 110G13L, 35HGSL, 30HGSA) increases the toxicity of the welding aerosol. The information about gross emissions of welding aerosol and its chemical composition is necessary to estimate the hygiene and sanitary work conditions effecting the people working in welding production. As a rule, these data is obtained with application of spectrophotometric method of analysis which is characterized by long time and complexity of experiment and, thus, it is important to be able to predict the working conditions of the welders without completing special experiments, by creating a thermodynamic model of welding aerosol formation.

2. Results and discussion

In the given paper we chose 30HGSA, 14HG2ASD and 14G2AS steels and welding wire Sv-08G2S and Sv-08GSM to estimate the welding aerosol composition and concentration as these grades of steel and types of welding wire are most frequently applied for welding mining equipment. The process was completed in CO₂ atmosphere. We estimated the mass concentrations of three elements (Fe, Mn, Si) which occur in the composition of SCWA produced when welding with the given wires, and the intensity of the given elements emission in the process of welding. The model allowing calculating the composition of SCWA was suggested by the authors [1,2]. The model is based on the equation which makes possible taking into consideration the equilibrium evaporation of the elements from the molten metal of the weld pool and nonequilibrium (explosion-like) transition of the components into the aerosol.

\[ C_i^a = \alpha_i C_i^p + (1 - \alpha_i) C_i^n, \]  

where \( C_i^a \) - concentration of the i-th element in SCWA,
\( C_i^p \) - concentration of the i-th element in the molten metal (in the composition of wire),
\( C_i^n \) - concentration of the i-th element in the saturated vapor over the molten,
\( \alpha_i \) - coefficient of nonequilibrium formation of the aerosol characterizing the amount of non-fraction component in the process of SCWA formation [2].

On the base of the given equation and on the base of the results of experimental measurements of SCWA amount and composition, also basing on the equations for determining composition and concentration of elements in vapor according to works [7,8], in paper [2] coefficients \( \alpha \) for three basic elements (Fe, Mn, Si) under various arc power were estimated. Basing on the obtained coefficients in [2] the authors suggest to solve the problem of SCWA determining for wires with different composition and for the whole range of arc power. In [1] the authors provide numerical results of SCWA composition and the results of calculations of element concentration in the saturated vapor. Proceeding from the meaning of the introduced coefficient \( \alpha \), its values, in our opinion, must range from zero to
one, but the authors obtain negative values of the coefficient according to experimental results and calculations.

According to [7,8] concentration of elements in the saturated vapor over the molten can be obtained from the correlation of vapor pressure under the certain temperature of the molten. The mole composition of the saturated vapor is found from the correlation

\[ M_i^n = P_i^{om} \cdot [M]_i / (\sum_i P_i^{om} \cdot [M]_i), \]

where \( P_i^{om} = P_i^y / P_{Fe}^y \), relative pressure of vapor of the i-th element is considered as relation of vapor pressure of the given element over this element melt to vapor pressure of iron over the iron melt, \([M]_i\) - element concentration in the melt (wire).

Vapor pressure was estimated from Clausius-Clapeyron relation

\[ P_i^y = \exp \left( \frac{-\Delta H_i}{RT} + C_i \right), \]

where \( \Delta H_i, C_i \) - heat of element evaporation and constant of integration, accordingly, which are taken from the table data or found from the data on vapor pressure of the elements under the given temperature.

Molar concentration is transformed into the mass one according to the equation

\[ C_i^n = M_i^n \cdot A_i / (\sum_i M_i^n \cdot A_i), \]

where \( A_i \) - atomic mass of the given element.

The values of element concentrations in the vapor over the melt found by us do not correspond to the results obtained by Levchenko [2] which we relate to significant disagreement of reference data applied by different authors.

In [2] the author also suggests applying approximation of \( \alpha \) coefficient dependence upon arc power to obtain the formula for SCWA elements concentration influenced by the varied welding conditions. To take into consideration the effect of arc power upon elements concentration in the vapor under equilibrium evaporation we need to consider the influence of power upon the temperature of welding wire drops. This influence can be taken into consideration if we put down and solve the heat balance equation which is a nontrivial task which requires considering the welding method, welding conditions, environment, welding productivity and wire cross-section, so temperature change can be obtained only by estimation. In general, to find the SCWA composition we need to apply a thermophysical model which takes into consideration formation of chemical compounds in the process of welding and the welding conditions.

In simplified form by analogy with the model in [2], we suggest changing the expression (1) in such a way not to break the physical meaning of the required coefficients

\[ C_i^a = \beta \alpha_i C_i^p + (1 - \beta)C_i^n, \]

where \( \beta \) - coefficient, characterizing the amount of nonequilibrium aerosol formation which is similar in meaning to coefficient \( \alpha \) in works [1,2], depends upon the welding conditions and parameters and it is the same for all required elements. The values of the coefficient are within the range from 0 to 1.

\( \alpha_i \) - non-fract coefficient of aerosol composition under its non-equilibrium formation, actually is a characteristics of concentration change of each element in relation to the melt composition. The coefficient cannot be negative.

Finding the SCWA composition according to the expression above is a complicated problem as it depends upon two unknown coefficients which, in their turn, depend upon the welding conditions and,
thus, are hard to obtain experimentally. In this regard we have to introduce some suppositions concerning the dependence of coefficient $\beta$ upon arc power. Basing on the results of SCWA composition measurements in work [1] and calculation of the coefficient, and also understanding that small input power leads to the growth of nonequilibrium component of welding aerosol, we took the changes of coefficient $\beta$ from 0.7 to 0.5 under changing the input power from 4.5 kW to 13 kW. Coefficients $\alpha_i$ were calculated under such supposition on the base of measurements results of SCWA composition in work [1]. The coefficients obtained for Sv-08G2S wire and concentration of elements in SCWA from work [1] and the calculated concentration of elements in the saturated vapor under equilibrium evaporation for the capacity of 13 kW are provided in Table 1.

### Table 1 – Results of calculations

| Element | Mo | Ni | Cr | Mn | Si | Fe |
|---------|----|----|----|----|----|----|
| $C^n_{i}, \%$ | 0 | 12.72 | 0.13 | 23.83 | 5.47 | 57.85 |
| $C^a_{i}, \%$ | - | - | - | 15.66 | 7.54 | 76.78 |
| $\alpha_i$ | - | - | - | 1.82 | 13.31 | 1.1 |

Proceeding from the linearity of coefficients dependence upon capacity in formula (5) we obtained the formula for concentration of elements in SCWA depending upon the wire composition and input power (similar to [1,2], coefficient 0.68 used in these works was not used by the authors of the given paper as its physical meaning is unknown and its application was not reasoned by the authors).

Calculation of saturated vapor composition and that of element concentrations in SCWA according to (5) was programmed and the program allows obtaining the dependences of element concentration in SCWA upon the capacity and the wire composition inserted by the user. In the process of program checking we applied two models of calculation of the saturated vapor composition over the melt described in [7]. As a result we chose the model described in the first part (equations (2)-(4)).

Also, we programmed the algorithm of calculation of intensity and specific emission of SCWA components on the base of equations taken from work [2]

$$V_i = 0.167 \cdot 10^{-6} \cdot I \cdot U \cdot (\beta_0 - K \cdot I \cdot U) \cdot C^n_{i}, \text{ g/min}$$ (6)

where $I \cdot U$ - welding arc power, kW;

$\beta_0, K$ - coefficients of linear approximation of specific rate of SCWA formation dependence upon the arc power.

$$G_i = V_i / G_p, \text{ g/kg}$$ (7)

where $G_p$ - productivity of welding material diffusion, kg/min.

Results of calculating the SCWA composition and intensity of emission for three metals (Mn, Si, Fe) are shown in figures 2-7. The changes in concentration of the given elements correlate with experimental data in [2].

The dramatic impact upon the cooling rate of metal vapor and, thus, upon quantity distribution of particles in the welding aerosol, is produced by temperature distribution and the flow rate in the arc [9].

Thus, the results prove that intensity of manganese, iron and silicon emission in SCWA when welding the considered steels applied for mining equipment production is maximal under arc power from 8 to 12 kW which allows making recommendations about choosing the welding conditions. Besides, taking into consideration the peculiarity of SCWA mixing under two physical phenomena taking place in the process of welding, we obtained a valid expression for SCWA composition allowing forecasting total emission and intensity of SCWA emission [10]. At the same time, due to two coefficients
in the model depending upon welding conditions, their experimental estimation is complicated. For more accurate solution of this problem we need to develop a thermophysical model of the welding process taking into consideration formation of chemical compounds and phases. This model could describe nonequilibrium formation of welding aerosol and its amount in the emitted aerosol. We think that for correct predictive modeling we also need to consider the equation of temperature dependence of melt drops upon the applied power. To obtain such dependence we need to derive an equation of heat balance which can be solved with application of a number of experimentally obtained values.

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The opportunities for detailed analysis of particles formation and distribution of particles according to their dimensions are provided by digital modeling [11]. Application of digital modeling as contrasted to most welding experiments may allow establishing a clear cause-and-effect link.

![Figure 2](image1.png)  
**Figure 2** – Dependence of manganese concentration in SCWA upon arc power

![Figure 3](image2.png)  
**Figure 3** – Dependence of silicon concentration in SCWA upon arc power
3. Conclusion

The developed model allows calculating the amount of various elements emitting changing due to alteration of parameters effecting the welding conditions. In contrast to experiments we can separately consider the intensity and type of current, type of electrode metal transition, etc. to estimate separate phenomena, such as coarse-droplet transfer with short circuit of the arc space and overheating of electrode end resulting from it, without additionally effecting data variableness. The given results will lay the foundation for developing a complex model of welding aerosol formation allowing considering the welding method, welding conditions and environment.

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