Modeling of heat and mass transfer and electrons scattering in electron beam welding and additive manufacturing

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Abstract. The mathematical formulation of electron beam melting and liquid metal transfer model in wire-based additive manufacturing with temperature dependencies of thermophysical properties is described. A description of the model algorithmic implementation based on the use of numerical methods for solving the Navier-Stokes equations system and the Volume of Fluid (VOF) method for tracking the free surface of a liquid on the cubic mesh cells is given. An iterative method for calculating the pressure field that ensures the fulfillment of the incompressibility condition for a viscous fluid is described. The paper also paid attention to the description of methodology for calculating the forces acting on the free surface of the melt, including surface tension forces and metal vapor pressure forces. One of the key elements of the proposed model is method for volumetric distribution of electron losses calculating, considering their scattering during the interaction of an electron beam with a curved melt surface. Electron beam focusing influence on the distribution of energy losses and the dynamics of penetration channel formation has been studied. An algorithm for visualizing the free surface of the melt based on the use of the Gaussian function, is described.

1. Introduction

Metal transfer caused by concentrated heat source action, such as the focused electron beam, is a difficult object to study [1–3]. The reasons for this are, on the one hand, a high temperature and high flow velocities in the area of the steam-gas channel, and on the other hand, the presence of intense optical radiation and metal vapors. These factors limit the possibilities of experimental research, for example, the use of sensors such as pyrometers [4] or cameras [5]. These methods are well suited for practical applications in the future and can be used to create a new control and monitoring systems for welding and additive manufacturing.

However, if the study requires detailed data on the temperature and flow velocity fields, then these methods can have only limited application since they provide only indirect information about the process on the monitored molten pool surface. For this reason, the methods of mathematical modeling are very relevant, because they allow obtaining comprehensive data on the processes in the molten pool after carrying out some series of computational experiments [6–7].

In recent decades, different fundamental works in the field of computational fluid dynamics have been published, which describe algorithms for solving transfer problems. Among them are the books and articles, which were written by S. V. Patankar and D. B. Spalding [8], as well as other authors who developed and generalized the results of long-term researches [9–10].
Development of computer technology and introduction of the mentioned numerical methods is allowed modern researchers to develop computer models for studying heat transfer processes in welding with concentrated heat sources [11].

Currently, the main interest for researchers is represented by models that allow one to study the processes of heating and metal transfer with non-stationary spatial and energy parameters of heating sources such as electron beam or laser beam. Obviously, to create such a model, it is necessary to consider the processes of electron scattering (including rescattering in the formed vapor-gas channel), their influence on the temperature distribution of free surface, the deformation of this surface, and their mutual influence on each other.

2. Description of the Model: Heat and Mass Transfer

The model is based on the Euler approach – the fluid is considered as a continuous medium, and its vector and scalar characteristics are determined at fixed points in the Cartesian coordinate system (Figure 1). It uses a grid with cubic cells, and liquid medium characteristics can be determined both in the volume of the cells and on their outer faces. This approach makes it convenient to describe the transfer of heat and mass between cells and calculate the necessary vector and scalar fields [8]. Such scalar values as temperature $T$, K; pressure $P$, Pa; relative volume fraction $L$ are calculated in the centers of cubic control volumes. On the faces of cubic elements, it is convenient to calculate the projections of heat fluxes and flow velocities, which are usually determined in the so-called “fractional” cells.

![Figure 1. Spatial discretization of the continuous medium used in the model.](image)

The most important equation for solving is the equation of fluid motion, which relates the acceleration acquired by fluid particles at the point under consideration with the action of external and internal forces. It should be noted that since the coordinate system is stationary, and the fluid itself is moving relative to it, the equation will contain a convective term – the second term on the left side:

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} = -\frac{1}{\rho} \nabla p + \mu \nabla^2 \mathbf{v} + \frac{f_{st}}{\rho} + \frac{f_{rec}}{\rho} + \mathbf{g},$$

where $\mathbf{v}$ is the velocity, m/s; $\rho$ is the density, kg/m$^3$; $\mu$ is the kinematic viscosity, m$^2$/s; $f_{st}$ and $f_{rec}$ are the volumetric surface tension and vapor pressure forces respectively, N/m$^3$; $\mathbf{g}$ is the gravity acceleration, m/s$^2$; $t$ is time, s. When using the finite difference solution algorithm, it is convenient to rewrite equation (1) in the form of projections onto the coordinate axes.
\[
\frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \mu \left( \frac{\partial^2 v_x}{\partial x^2} + \frac{\partial^2 v_x}{\partial y^2} + \frac{\partial^2 v_x}{\partial z^2} \right) + f_{u.x} + f_{rec.x} \frac{\rho}{\rho}
\]
\[
\frac{\partial v_y}{\partial t} + v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \mu \left( \frac{\partial^2 v_y}{\partial x^2} + \frac{\partial^2 v_y}{\partial y^2} + \frac{\partial^2 v_y}{\partial z^2} \right) + f_{u.y} + f_{rec.y} \frac{\rho}{\rho}
\]
\[
\frac{\partial v_z}{\partial t} + v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} = -\frac{1}{\rho} \frac{\partial p}{\partial z} + \mu \left( \frac{\partial^2 v_z}{\partial x^2} + \frac{\partial^2 v_z}{\partial y^2} + \frac{\partial^2 v_z}{\partial z^2} \right) + f_{u.z} + f_{rec.z} \frac{\rho}{\rho} - g,
\]
where the subscripts \(x, y\) and \(z\) correspond to the projections of vector quantities onto the Cartesian axes.

To calculate the pressure included in equation (1) in accordance with the current practice of solving such problems, one of the splitting schemes in terms of physical factors must be used [8; 12]. At the predictor step, the flow velocity field is determined taking into account only the pressure field calculated at the previous time step. Then it is necessary to calculate the pressure field that satisfies the incompressibility condition and ensures the formation of a solenoidal velocity field. We denote the speed calculated at the predictor step by the index “\(p\)”, and the speed calculated at the correcting step by the index “\(c\)”, then the incompressibility condition must be met after the completion of the iterations (corrector step), that is:

\[
\nabla \nu^c = 0.
\]

And the equation for correcting the velocity field will look like this:

\[
\nu^c - \nu^p = \frac{1}{\Delta t} \nabla p^c.
\]

We apply the divergence operator to both sides of equation (4), considering condition (3). As a result, we obtain the Poisson equation for pressure:

\[
p^c = \frac{\Delta t}{\rho} \nabla \nu^p,
\]

or in the projection form:

\[
\frac{\partial^2 p^c}{\partial x^2} + \frac{\partial^2 p^c}{\partial y^2} + \frac{\partial^2 p^c}{\partial z^2} = \rho \frac{\Delta t}{\rho} \left( \frac{\partial \nu^p}{\partial x} + \frac{\partial \nu^p}{\partial y} + \frac{\partial \nu^p}{\partial z} \right)
\]

The stages of pressure correction and velocity fields correction are usually repeated until the velocity field remains unchanged (with a given accuracy). Heat transfer in the molten pool is provided by diffusion and convection:

\[
\frac{\partial T}{\partial t} + v_x \frac{\partial T}{\partial x} + v_y \frac{\partial T}{\partial y} + v_z \frac{\partial T}{\partial z} = \frac{\lambda}{\rho c} \left( \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + q_v
\]

where \(\lambda\) is the thermal conductivity, \(W m^{-1} K^{-1}\), \(c\) is specific heat, \(J kg^{-1} K^{-1}\); \(q_v\) is a heat source distribution function, \(W m^{-3}\). Attention should be paid to the effect of electron backscattering (see Section 3), it is convenient to represent the heating source as a volume-distributed function that does not affect zero in those cubic cells in which electrons lose their energy. It should also be noted that if a metal is in the solid phase in the considered control volume, then the velocity \(v\) can be taken equal to zero, or equal to the speed of movement of the part, filler wire, etc.

Now it is necessary to describe the method for modeling the molten pool free surface movement. The forces acting on the free surface are given in equation (1) as their volumetric equivalents, such approach is widely used in practice [13–15]. Most often, to refer the considered control volume to an element of the free surface, the condition of a nonzero gradient of the \(L\) function is taken \((\nabla L \neq 0)\). The volume fraction transfer is described by the equation:
\[
\frac{\partial L}{\partial t} + v_x \frac{\partial L}{\partial x} + v_y \frac{\partial L}{\partial y} + v_z \frac{\partial L}{\partial z} = 0.
\]  

(8)

Since the function changes continuously only in the range from 0 to 1, then in order to correctly solve the transport equation, it is necessary to use proven methods described in the literature [13].

3. Description of the Model: Surface Forces and Electrons Scattering

To calculate the surface tension forces, we use the technique developed by Brackbill et al. [16], in which the surface curvature is calculated through the divergence and the "smoothed" field \( \nabla L \) (denoted by the tilde sign):

\[
\mathbf{f}_{st} = \sigma \cdot \left( -\nabla \frac{\nabla L}{|\nabla L|} \right) \cdot \nabla \tilde{L},
\]

(9)

where \( \sigma \) is the surface tension, N/m. Figure 2 illustrates how the direction and magnitude of the surface tension force are determined depending on surface curvature.

![Image of Figure 2](image-url)

**Figure 2.** Determination of volumetric equivalents of surface tension forces.

The vapor pressure is calculated at the liquid surface in accordance with the reference data [17]. We can write:

\[
\mathbf{f}_{rec} = -\nabla p \big|_{(x,y,z) \in I}
\]

(10)

When using the VOF method, expression (10) is conveniently applied in the following form:

\[
\mathbf{f}_{rec} = |\nabla p| \frac{\nabla L}{|\nabla L|}
\]

(11)

In order to correctly determine the volumetric distribution of a heat source \( q(x, y, z) \), it is necessary to take into account the backscattering of electrons. The relevance of this problem is confirmed by a number of works published in recent years [6, 18, 19]. In this paper it is proposed to use the Monte Carlo method for Lagrangian particles moving in stationary Euler cells, taking into account stochastic electron scattering processes. To compose an economical algorithm, it is convenient to use the well-known model of single elastic scattering [21]. When using this model, the trajectory of each electron is calculated separately.

The electron enters the target material at point \( P_0 \) (Figure 3). Let us assume that the first act of elastic scattering occurs at the point \( P_1 \) (before this act, the electron passed the path \( s_0 \)). In the model of single elastic scattering, it is also assumed that only such interactions lead to the deviation of particles from the initial trajectory. The electron will deflect through a solid angle \( \phi_1 \) and rotate through an azimuthal angle \( \psi_1 \), after which it will cover the path \( s_1 \) determined by the free path at given energy and given parameters of the material. After that, the electron will be at point \( P_2 \), at which elastic scattering will occur again (deflection by an angle \( \phi_2 \) and rotation by an angle \( \psi_2 \)), after which the electron will pass the path \( s_2 \) and end up at point \( P_3 \). The calculations are repeated until the electron loses almost all of its energy – it becomes part of the electron gas or leaves the material and scatters back.
The model assumes that in the process of motion, the electron will continuously lose energy, which is determined by the stopping power of the particle:

$$\frac{dE}{ds} = -2\pi e^2 N \frac{Z \cdot p}{A \cdot E} \ln \left( \frac{1.166E}{J} \right),$$

where $E$ is the electron energy, keV; $s$ is the electron path, cm; $e$ is the electron charge, C; $N$ is Avogadro’s number, $N = 6.022 \times 10^{23}$, mol$^{-1}$; other parameters relate to the material: $Z$ is atomic number; $A$ is atomic weight, g/mol, $J$ is ionization potential, keV, defined as:

$$J = (9.76Z + 58.5Z^{0.19}) \times 10^{-3}.$$

The elastic scattering cross-section is calculated based on the expression:

$$\sigma_E = 5.21 \cdot 10^{-21} \frac{Z^2}{E^2} \cdot \frac{4\pi}{\alpha (1 + \alpha)} \left( \frac{E + m_0c_0^2}{E + 2m_0c_0^2} \right)^2,$$

where $m_0$ is the electron rest mass, kg; $c_0$ is speed of light, m/s ($m_0c_0^2 = 511$ keV). If we substitute the value of $E$ in keV in this expression, the value of $\sigma_E$ will be in cm$^2$. The screening parameter $\alpha$ is determined by the Bishop formula ($E$ is also substituted in keV):

$$\alpha = 3.4 \cdot 10^{-3} \frac{Z^{0.67}}{E}.$$

Electron mean free path between elastic scattering events can be written as

$$\lambda_E = \frac{A \cdot \rho \cdot \sigma_E}{N}.$$

The actual value of the electron path is determined based on the random variable:

$$s_E = -\lambda_E \cdot \ln R_1.$$

Finally, we must define expressions for calculating the solid angle $\phi$ and azimuthal angle $\psi$. They are also taken from specialized literature [20, 24]:

$$\cos \phi = 1 - \frac{2\alpha R_2}{1 + \alpha - R_2},$$

$$\psi = 2\pi R_3.$$
In the last three expressions, $R_1$, $R_2$, and $R_3$ are independent random numbers generated by the program in the ranges from 0 to 1.

Comparison of experimental and theoretical studies [22–24] showed that the stopping power is practically independent of the aggregate state of substances, but is determined, first of all, by the medium density and the characteristics of the scattering centers. In a published study of the electron beam melting process of metal powders [6], the absorption of electrons is considered regardless of material phase. In this paper, the dependence of the transport characteristics of electrons on temperature and, consequently, the state of a substance is specified implicitly through the density and a one-component model of a scattering medium is used (for example, for steel is used an iron).

Let us consider the issue of visualizing the surface of a steam-gas channel. The model described above uses the visualization technology of the SLIC type (Simple Line Interface Calculation), described in the literature [14] and illustrated in Figure 4 (a). SLIC technology uses orthogonal planes to display partially fluid control volumes, but if you want to get a continuous line (or family of lines), you need to do some transformations. In Figure 4 (b), the weighting function $L$ is displayed in shades of color (the lighter the shade, the smaller the $L$ value in the cell). The $L$ values are shown in Figure 4 (a and b) by the numbers inscribed in the cells.

Next, we need to build a mesh with a smaller step (for example, 4 times smaller than the initial one, $M = 4$, $N = 4$, see Figure 4 (c), and smooth the distribution of the function $L$. To implement the smoothing algorithm, the Gaussian transform was used:

$$L_{x,y}^* = \sum_{X=x-\frac{M}{2}}^{x+\frac{M}{2}} \sum_{Y=y-\frac{N}{2}}^{y+\frac{N}{2}} L_{X,Y} \frac{e^{-r_{ij}^2}}{\pi \sigma^2}. \tag{20}$$

In the last expression, $L^*$ is the field $L$ smoothed using the Gaussian distribution function, $\sigma$ is the smoothing radius (dispersion), $r_{ij} = ((x - X)^2 + (y - Y)^2)^{0.5}$ is the radius vector between the considered points $i$ and $j$ (Figure 4 (c)).
After performing the smoothing procedure, it is possible to display the locus of points at which the transition of the $L^*$ values through a certain value (for example, 0.5) is carried out, and to obtain the $B_{x,y}$ curve shown in Figure 4 (d).

Using the algorithms described above, a computer program was developed.

4. Computational Experiments
At this stage of research, the melting process of a plate made of stainless steel 316L with a thickness of 2 mm was investigated. The temperature dependences of the plate material thermophysical properties, as well as the viscosity and vapor recoil pressure, were taken from the reference literature [17]. The electron beam was modeled by sequentially calculating 800 trajectories, the initial coordinates of which were determined by the equations:

$$
x_n = h \cdot R_x \cdot n^{0.8} \cdot \cos \left( \frac{n}{K} \sqrt{n + 1} \right) + x_{pos},
$$

$$
y_n = h \cdot R_y \cdot n^{0.8} \cdot \sin \left( \frac{n}{K} \sqrt{n + 1} \right) + y_{pos},
$$

where $n$ is the trajectory number, $x_{pos}$ and $y_{pos}$ are the coordinates of the beam center, $R_x$ and $R_y$ are the coefficients required to vary the transverse dimensions of the beam along the $x$ and $y$ axes, and $K$ is the angular step factor.

The results of computational experiments described below were obtained for the following meanings: electron beam power is equal to 960 W, electron energy is equal to 60 keV, and a scanning speed is equal to 125 m/h. For example, the calculation results obtained with the multipliers $R_x = R_y = 0.032$ (Figure 5 (a) – mode 1 and $R_x = R_y = 0.016$ (Figure 5 (b) – mode 2 are shown. The coefficient $K$ was taken equal to 0.2.

![Figure 5](image_url)

**Figure 5.** Distribution of the initial coordinates of electrons in the $xy$ plane for mode 1 (a) and mode 2 (b).

Figures 6 and 7 correspond to different times of the through-fusion channel formation with the electron density distribution corresponding to mode 1. Figure 6 shows the trajectories of backscattered electrons, and the liquid bath surface is displayed using the SLIC algorithm. Figure 7 shows the reconstructed bath surface and temperature distribution. Figures 8 and 9 display the same data obtained for mode 2.

Figures 6 and 8 clearly show that there is a process of electron reflection in the formed penetration channel. Figure 10 shows the time dependences of the penetration depth for both modes. These dependencies were obtained without smoothing, and $H_{\text{max}} = 2$ mm is the plate thickness.
Figure 6. Trajectories of electrons and cross-sections of the pool at different times (mode 1).
Figure 7. Reconstructed molten pool shape (mode 1).
Figure 8. Trajectories of electrons and cross-sections of the pool at different times (mode 2).
Figure 9. Reconstructed molten pool shape (mode 2).

The dependences $H(t)$ have a variable component due to the periodic partial overlap of the penetration channel, which is consistent with generally accepted data and experimental results. It can
also be seen that in mode 2 the through penetration mode starts earlier, since the heat flux density in this mode is higher. These results show that the developed model can be verified and used to study the processes of electron beam welding, melting, and additive manufacturing of products based on the use of powder and wire materials, taking into account the backscattering of electrons and their re-reflection in the penetration channel.

5. Conclusion
A complex mathematical model of the formation of a vapor-gas channel in electron beam welding has been created, based on the numerical solution of the Navier-Stokes equations for a viscous incompressible fluid, the predictor-corrector algorithm for calculating the pressure field satisfying the incompressibility condition, the method of the volume of fluid for studying the behavior of a free the surface of the melt pool, as well as the Monte-Carlo method for studying the processes of scattering and re-scattering of electrons. The model makes it possible to take into account the change in the absorption coefficient of electrons during the formation of a vapor-gas channel and other processes on the free surface.

To effectively solve the problem of reconstructing the shape of the steam-gas channel and the temperature distribution over its surface, the model is supplemented with an algorithm that uses obtaining a continuous distribution of the weight function within the size of one control volume near the free boundary. This is necessary for calculating the geometric location of the level lines points of the steam-gas channel free surface, which allows one to reconstruct the free surface of the molten pool at different points in time.

Analysis of the results of computational experiments showed that under the continuous action of an electron beam, there is a periodic oscillation of the width and depth of the channel associated with its “overlap” by the metal accumulated in the tail part of the pool, which is consistent with the generally known experimental results.

The relevance of using the model for determining the energy efficiency of electron-beam processing (welding, melting, perforation (drilling), additive manufacturing) is shown.

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