Mathematical modeling the process of wire surfacing by the smoothed particle hydrodynamics method

R P Davlyatshin¹, R M Gerasimov¹, Y V Bayandin², G L Permyakov¹, D N Trushnikov¹

¹ Perm National Research Polytechnic University, Komsomolsky prospect, 29, Perm, 614990, Russian Federation
² Institute of Continuous Media Mechanics UB RAS, ul. Academ. Koroleva, 1, Perm, 614013, Russian Federation

E-mail: romadavly@gmail.com

Abstract. We discuss issues the process of layer-by-layer synthesis of metal products by wire surfacing. A mathematical model of the process has been developed and implemented. The model allows one to calculate the volumetric distributions of temperatures, melt flow rates, pressures, components of heat fluxes density, the shape and dimensions of the molten bath, the shape of the free surface of the molten metal, the shape and dimensions of the weld bead. For this purpose, the main physical processes that affect the formation of the metal product were considered, namely: melting and crystallization of the metal, surface tension, the Marangoni effect and the heat source features. The smoothed particle method was used to implement this model. A number of numerical experiments were carried out using the developed model. Firstly, the model parameters for steel and titanium were identified and verified. After that, calculations were carried out to verify the model itself using the obtained roller geometry. The numerical solution for the deposition of one layer was compared with the full-scale experiment. The error was no more than 5% in any direction. Thus, the efficiency and correctness of the constructed model is shown.

1. Introduction

Additive manufacturing or layer-by-layer synthesis technologies are considered to be breakthrough developments of this century and represent the processes of combining material to create a modelled object layer by layer. In this case, the use of wire materials allows to avoid a number of problems related to low productivity of existing methods, high cost of equipment used, limited types of materials used, due to the traditional use of powder systems as a material for additive formation of products. The use of an electron beam for melting additive wire proves to be a very productive solution for a number of promising materials, in particular, titanium and other chemically active metals and their alloys [1-3].

However, such method of metal products manufacturing has a number of disadvantages. The key one is the difficulty of setting the surfacing parameters, namely the path and speed of wire feed, as well as the heat source power [4, 5]. Incorrect setting of these parameters may lead to melting or even collapse of the walls of the future product, resulting in increased scrap and, as a consequence, to higher costs and slower production process. Existing methods for optimization of heat source power parameters often do not consider changes in geometry in real time, have low performance and are mainly used for SLS (Selective Laser Sintering)
Meshfree methods, for example, the method of Smoothed Particle Hydrodynamics (SPH) have been increasingly used recently to solve these problems. However, they are aimed either at modeling laser sintering processes, or do not consider surface effects, or the task is set in 2D [9-12].

Thus, it is necessary to create a mathematical model that would make it possible to determine the volumetric temperature distributions, melt flow rates, pressures, components of heat flux density, the shape and size of the molten bath, the shape and size of the free surface of the molten metal, the shape and size of the molten bead using more efficient meshless methods.

2. Mathematical model

To solve the problem, the following system of hypotheses were accepted:

- the heat source power, the feed rates of the substrate $V_s$ and the wire $V_w$ are constant in the simulated process;
- the ambient temperature is constant;
- substrate and wire material have the same chemical composition;
- metal melt is considered an incompressible Newtonian fluid;
- physical parameters of metal melt (density, viscosity, thermal conductivity, etc.) do not depend on temperature;
- latent heat of fusion and crystallization is not considered;
- the two-phase zone of the melt is specified by the condition of the liquidus-solidus transition by the melting temperature;
- the heat source is specified in the surface layer of particles;
- the heat source has the form of a normal distribution;
- the surface tension force, the Marangoni force and the vapor pressure acting on the metal melt are considered.

The variable parameters are:

- heat source power;
- heat source energy flux distribution;
- initial sample temperature (300 K);
- dependence of the thermophysical characteristics of the material on temperature;
- phase transition characteristics;
- substrate feed speed $V_s$;
- wire feed speed $V_w$.

Molten metal can be described as a viscous incompressible fluid. The system of equations for describing the motion of a fluid consist of differential: evolution of density $\rho$, velocities $\mathbf{v}$, and specific energy $e$ in the form of balance laws (equations for the balance of mass, momentum, and energy, respectively):

\[
\begin{align*}
\frac{d\rho}{dt} &= -\rho \nabla \cdot \mathbf{v} , \\
\frac{d\mathbf{v}}{dt} &= \frac{1}{\rho} \left( \nabla \cdot \mathbf{\sigma} \right) + \frac{1}{\rho} \mathbf{F} , \\
\frac{de}{dt} &= \frac{1}{\rho} \mathbf{\sigma} : \mathbf{D} - \frac{1}{\rho} \nabla \cdot \mathbf{q}
\end{align*}
\]

where $\mathbf{v}$ – velocity, $\rho$ – density, $\mathbf{\sigma}$ – stress tensor, $\mathbf{q} = -\lambda \nabla T$ – heat flow, $\lambda$ – coefficient of thermal conductivity, $T$ – temperature. The closing physical equation for stresses is represented in the form of a viscous law $\mathbf{\sigma} = -p \mathbf{I} + \mu \mathbf{D}$, where $p$ – pressure, $\mu$ – viscosity, $\mathbf{I}$ – identity tensor. $\mathbf{D}$ – strain rate tensor, $\mathbf{F}$ – applied forces. Surface tension force [13], Marangoni force [14] and the vapor pressure [15] are considered as external forces.
\[ F = F^{st} + F^{tr} + F^{v} = \sigma \kappa \mathbf{n} + \frac{\partial \sigma}{\partial T} \nabla T - PS \mathbf{n}, \]  
(2)

\( \sigma \) – surface tension coefficient, \( \kappa \) – Gaussian curvature, \( P \) – vapor pressure, \( S \) – surface area, \( \mathbf{n} \) – surface normal.

3. Smoothed particle hydrodynamics method

Along with meshed and finite element methods for numerical simulation of motion, deformation and destruction of condensed media, there are, more efficient is some cases and less demanding on computational resources meshfree methods [16]. One of these methods is smoothed particle hydrodynamics method (SPH). It was proposed independently by several authors in 1977 for solving astrophysical problems [17, 18], and then for solving problems of continuum mechanics [19, 20].

A certain set of points, which are called particles or pseudoparticles, is required to describe the state of a continuous medium (liquid, gas or solid) in the SPH method. A completely Lagrangian approach is used to describe the evolution of a medium in SPH. It allows to discretize a given set of equations of continuum mechanics by interpolating properties directly on a discrete set of points distributed over the solution domain without the need to define a spatial mesh. The Lagrangian nature of the method, associated with the absence of a fixed grid, is its main advantage. The difficulties associated with fluid motion and structural problems due to large deformations and free surface are naturally resolved.

The essence of the SPH method is to introduce a discrete analog \( f_i \) of continuous function \( f \) which is characterizing any field variable. Piecewise constant value \( f_i \), determined for each \( i \)-th particle as the sum of \( N \) values \( f_j \) from \( j \)-particles of the environment within a given distance \( h \):

\[ f_i = \sum_{j=1}^{N} m_j \frac{f_j}{\rho_j} W(r_i - r_j) = \sum_{j=1}^{N} m_j \frac{f_j}{\rho_j} W_{ij}, \]  
(3)

where \( m_j \) – mass of \( j \)- particle, \( \rho_j \) – density near \( j \)- particle, \( W \) – smoothing function (kernel).

The coordinate derivatives do not affect the masses of particles \( m_i \) and the values of field quantities \( f_i \). Differentiation occurs only with respect to the weight functions \( W_{ij} \). In this case, a gradient of value \( f_i \) can be represented as follows:

\[ \nabla f_i = \sum_{j=1}^{N} m_j \frac{f_j}{\rho_j} \nabla W(r_i - r_j) = \sum_{j=1}^{N} m_j \frac{f_j}{\rho_j} \nabla W_{ij}. \]  
(4)

Applying the discretization of the smoothed particle method to (1) and (2) using expressions (3) and (4), we obtain expressions for the \( i \)-th particle:

\[
\begin{align*}
\frac{d\rho_i}{dt} &= -\sum_{j=1}^{N} m_j \mathbf{u}_{ij} \cdot \nabla W_{ij} \\
\frac{d\mathbf{u}_i}{dt} &= -\frac{1}{\rho_i} (\nabla \cdot \mathbf{\kappa}) + \frac{1}{\rho_i} (F_{i,m}^{tr} + F_{i,rr}^{tr} + F_{i}^{v}) + g \\
\frac{d\mathbf{e}_i}{dt} &= -\frac{1}{\rho_i} (\sigma \cdot \mathbf{D}) - \frac{1}{\rho_i} \nabla \cdot \mathbf{e}_i \\
F_{i,m}^{tr} &= \frac{\alpha}{2} \sum_{j=1}^{N} m_j m_k \rho_j \rho_k \left( |\nabla C_i|^2 + |\nabla C_j|^2 \right) \nabla W_{ij} \mathbf{n}_i, \quad \mathbf{n}_i = \frac{\nabla C_i}{|\nabla C_i|}, \quad \nabla C_i = \sum_{j=1}^{N} m_j \nabla W_{ij} \\
F_{i,rr}^{tr} &= \beta (\nabla T_i - \nabla T_j) \cdot \mathbf{n}_i \mathbf{n}_j, \quad \nabla T_i = -\sum_{j=1}^{N} \frac{m_j (T_i - T_j)}{\rho_j} \nabla W_{ij} \\
-\frac{1}{\rho_i} (\nabla \cdot \mathbf{\kappa}) &= -\sum_{j=1}^{N} m_j \left( \frac{p_j}{\rho_j} + \frac{p_j}{\rho_j} \right) \nabla W_{ij} + \sum_{j=1}^{N} m_j \frac{\mu_j + \mu_j + \rho_j}{\rho_j \rho_j} \mathbf{u}_{ij} \cdot \nabla W_{ij}
\end{align*}
\]  
(5)

(6)

(7)

(8)
\[- \frac{1}{\rho_i} (\sigma : D)_i = - \frac{1}{2} \sum_{j=1}^{\infty} m_j \left( \frac{p_i}{\rho_i^2} + \frac{p_j}{\rho_j^2} \right) u_{ij} \cdot \nabla W_{ij}^h - \frac{1}{2} \sum_{j=1}^{\infty} m_j \left( \mu_i + \mu_j \right) \rho_j \frac{r_{ij}}{r_{ij}^2} u_{ij} \cdot \nabla W_{ij}^h \]  
\[ - \frac{1}{\rho_i} \nabla \cdot \mathbf{q}_i = \sum_{j=1}^{\infty} \frac{m_j}{\rho_i \rho_j} \left( \lambda_i + \lambda_j \right) \frac{r_{ij}}{r_{ij}^2} \nabla_{ij} W_{ij}^h \]  

where \( \mathbf{u}_i \) – particle velocity, \( \mathbf{u}_{ij} \) – velocity of particle \( i \) relative to particle \( j \), \( \sigma \) – stress tensor, \( \mathbf{F}^{\sigma} \) – surface tension force, \( \mathbf{F}^{\text{Mar}} \) – Marangoni force, \( \mathbf{F}^{v} \) – vapor pressure force, \( \mathbf{g} \) – acceleration of gravity, \( \rho_i \) – vapor pressure per particle \( i \), \( \mu \) – dynamic viscosity, \( r_{ij} \) – position of particle \( i \) relative to particle \( j \), \( \alpha \) – model coefficient of surface tension force, \( \beta \) – model coefficient of Marangoni force, \( \mathbf{n}_i \) – normal to the surface at the position of the particle \( i \), \( C_i \) – color function, \( \nabla C_i \) – color function gradient, \( V_i \) – particle volume [1/m^3], \( T_i \) – particle temperature.

4. Modeling the process of wire surfacing
A numerical experiment was carried out to simulate the process of wire surfacing using the developed model. The purpose of the simulation was to test the performance and adequacy of the constructed model. The problem of surfacing a wire made of steel on a substrate made of the same material in the jet transfer mode at a low power of the heat source is considered. The geometry of the problem is shown in Fig. 1.

![Figure 1. Geometry of the problem.](image)

Table 1 shows the physical characteristics of steel grade 12X18H10T, required for numerical modeling by the smoothed particle method.

| Property                     | Designation | Value     |
|------------------------------|-------------|-----------|
| Density                      | \( \rho \) [kg·m^-3] | 7890      |
| Melting temperature          | \( \mathbf{T} \) [K]     | 1480      |
| Thermal conductivity         | \( \lambda \) [W/(m×K)] | 42        |
| Thermal capacity             | \( C_v \) [J/(K×kg)]     | 450       |
| Surface tension coefficient  | \( \sigma \) [H/m]       | 1.0       |
| Surface tension gradient coefficient | \( \partial \sigma / \partial T \) [H/(m×K)] | -0.89·10^{-3} |
Figure 2. Numerical simulation results at different time steps: 0.1 sec, 0.3 sec, 0.5 sec, 0.7 sec, 1.0 sec, 1.25 sec.

The numerical simulation parameters are as follows:

| Parameter               | Value         |
|-------------------------|---------------|
| Discretization parameter| 0.1 mm        |
| Time step               | $5 \cdot 10^{-6}$ sec |
| Physical time           | 1.25 sec      |

Preliminary numerical implementations were carried out on an IBM 2x300 sas 15k multiprocessor computer (4xIntel Xeon E7520, 64 GB) using MPI multithreaded computing capabilities in the LAMMPS package.
The following parameters were selected to simulate the surfacing process:

**Table 3. Build-up parameters**

| Property                  | Value         |
|---------------------------|---------------|
| Source power              | 1.5 kW        |
| Substrate displacement speed | 10.0 mm/sec  |
| Wire feed rate            | 38.0 mm/sec   |
| Wire diameter             | 1.2 mm        |
| Substrate size            | 10 x 20 x 5 mm|
| Wire feed angle           | 45°           |

In Fig. 2 shows the typical results of numerical simulation at different times. The presented images demonstrate the process of droplet and bead formation from the moment the power of the heat source is turned on and the wire is fed until a stable mode is established, after which the wire feed is stopped. The color scale displays temperatures from 300 to 1400 degrees Kelvin. The droplet touched the substrate for 0.3 s. The width of the bead increases with the duration of the process, reaching a steady-state value after 0.5 s.

It was revealed that the constructed model can adequately reproduce all the underlying physical processes. And it can be used as a substitute for some natural experiments.

5. Summary and Conclusions

A mathematical model that allows one to describe heat and mass transfer in the process of additive formation of products by fusing wire material with a plasma (electric) arc and concentrated energy sources with an asymmetric wire feed has been described. The developed model includes:

1. unsteady heat transfer equation taking into account the convective contribution;
2. preliminary induction heating by changing the initial temperature, and setting an additional distributed volumetric heat source;
3. unsteady equation of motion of a viscous medium (Navier-Stokes) in the laminar approximation, taking into account the Marangoni effect on the surface of the melt, surface tension and vapor pressure;
4. thermal and hydrodynamic boundary conditions, considering the presence of a free deformable metal-environment interface.

The model allows calculating unsteady volumetric distributions of temperatures, melt flow rates, pressures, the shape and size of the molten pool, the shape of the free surface of the molten metal, the shape and size of the bead being deposited.

The problems of the computational implementation of the developed model in a 3D setting have been solved at this stage. The areas of application of the developed models are determined.

Acknowledgments

The work is supported by the Ministry of Science and Higher Education of the Russian Federation (state assignment No. FSNM-2020-0028), the Ministry of Education and Science of the Perm Territory (agreement S-26/787 of 12/21/2017) and the Russian Foundation for Basic Research (RFBR project No. 18-08-01016A).

References

[1] Lorenz, K.A., Jones, J.B., Wimpenny, D.I., Jackson, M.R. (2015). A review of hybrid manufacturing. *Solid freeform fabrication conference proceedings*, 53, pp.96–108
[2] Stawowy, M., 2018. Comparison of LCAC and PM Mo deposited using Sciaky EBAM™. *International Journal of Refractory Metals and Hard Materials*, 73, pp.162-167.
[3] Tarasov, S., Filippov, A., Savchenko, N., Fortuna, S., Rubtsov, V., Kolubaev, E. and Psakhie, S., 2018. Effect of heat input on phase content, crystalline lattice parameter, and residual strain in wire-feed
electron beam additive manufactured 304 stainless steel. *The International Journal of Advanced Manufacturing Technology*, 99(9-12), pp.2353-2363.

[4] Markl, M. and Körner, C., 2016. Multiscale Modeling of Powder Bed–Based Additive Manufacturing. *Annual Review of Materials Research*, 46(1), pp.93-123.

[5] Mladenov, G., Koleva, E. and Trushnikov, D., 2018. Mathematical modelling for energy beam additive manufacturing. *Journal of Physics: Conference Series*, 1089, p.012001.

[6] Jamshidinia, M., Kong, F. and Kovacevic, R., 2013. Numerical Modeling of Heat Distribution in the Electron Beam Melting® of Ti-6Al-4V. *Journal of Manufacturing Science and Engineering*, 135(6).

[7] Yuan, P. and Gu, D., 2015. Molten pool behaviour and its physical mechanism during selective laser melting of TiC/AlSi10Mg nanocomposites: simulation and experiments. *Journal of Physics D: Applied Physics*, 48(3), p.035303.

[8] Hu, R., Luo, M., Liu, T., Liang, L., Huang, A., Trushnikov, D., Karunakaran, K. and Pang, S., 2019. Thermal fluid dynamics of liquid bridge transfer in laser wire deposition 3D printing. *Science and Technology of Welding and Joining*, 24(5), pp.401-411.

[9] Russell, M., Souto-Iglesias, A. and Zohdi, T., 2018. Numerical simulation of Laser Fusion Additive Manufacturing processes using the SPH method. *Computer Methods in Applied Mechanics and Engineering*, 341, pp.163-187.

[10] Liu, S., Liu, J., Chen, J. and Liu, X., 2019. Influence of surface tension on the molten pool morphology in laser melting. *International Journal of Thermal Sciences*, 146, p.106075.

[11] Shcherbakov, A., Rodyakina, R. and Gaponova, D., 2018. Using of Smoothed Particle Hydrodynamics Method for Constructing a Mathematical Model of Electron-Beam Surfacing Process. *Solid State Phenomena*, 284, pp.523-529.

[12] Trushnikov, D.N., Koleva, E.G., Davlyatshin, R.P., Gerasimov, R.M. and Bayandin, Y.V. (2019). Mathematical modeling of the electron-beam wire deposition additive manufacturing by the smoothed particle hydrodynamics method. *Mechanics of Advanced Materials and Modern Processes*, 5(1).

[13] He, X., Wang, H., Zhang, F., Wang, H., Wang, G. and Zhou, K. (2014). Robust Simulation of Sparsely Sampled Thin Features in SPH-Based Free Surface Flows. *ACM Transactions on Graphics*, 34(1), pp.1–9.

[14] Trautmann, M., Hertel, M., & Füssel, U. (2017). Numerical simulation of TIG weld pool dynamics using smoothed particle hydrodynamics. *International Journal of Heat and Mass Transfer*, 115, pp.842–853.

[15] Alshaer A. W., Rogers B. D., Li L. (2017) Smoothed Particle Hydrodynamics (SPH) modelling of transient heat transfer in pulsed laser ablation of Al and associated free-surface problems. *Computational Materials Science*, 127, pp.161–179.

[16] Liu, G.R. (2009). Meshfree Methods. CRC Press.

[17] Gingold, R.A. and Monaghan, J.J. (1977). Smoothed particle hydrodynamics: theory and application to non-spherical stars. *Monthly Notices of the Royal Astronomical Society*, 181(3), pp.375–389.

[18] Lucy, L.B. (1977). A numerical approach to the testing of the fission hypothesis. *The Astronomical Journal*, 82, p.1013.

[19] Libersky, L.D. and Petschek, A.G. (n.d.). Smooth particle hydrodynamics with strength of materials. *Advances in the Free-Lagrange Method Including Contributions on Adaptive Gridding and the Smooth Particle Hydrodynamics Method*, pp.248–257.

[20] Libersky, L.D., Petschek, A.G., Carney, T.C., Hipp, J.R. and Allahdadi, F.A. (1993). High Strain Lagrangian Hydrodynamics. *Journal of Computational Physics*, 109(1), pp.67–75.