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MATHEMATICAL MODEL AND NUMERICAL SOLUTION OF THE PROCESS OF HEATING AND MELTING OF A TRAVELING CYLINDER FED INTO A ROCKET CHAMBER

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ABSTRACT

The present work deals with analysis of a necessity to develop a metallization tool. Application of and fundamental requirements to the future product (portability, independence and easy operation) were determined. A small-size rocket chamber was taken as a basis for the metallizer design. A wire-shaped coating material is expected to be constantly fed inside the chamber. A mathematical model reflecting the behavior of the key process of the device namely the coating material heating and melting was elaborated. A two-phase Stefan problem with the established phase boundary was defined. A numerical solution of the problem was found by means of a finite volume method. The approaches used for software implementation of this method were described. There was developed an original program with the aid of which correctness of the problem statement as well as the solution stability within the wide range of initial conditions were ascertained. Accuracy and convergence of numerical approach were proved. This development effort will allow carrying out a modeling experiment, evaluating the metallizer performance at the design stage, determining the most efficient modes of its operation and assisting in designing of a gas-dynamic duct in the rocket chamber.

Keywords: rocket chamber, metallizer, Stefan problem, numerical solution, computation algorithm.

1. INTRODUCTION

12% of all fabricated metal in the world is being lost due to corrosion and wear. Corrosion is the reason of premature failure of such large-sized facilities as bridges, power transmission poles, exhaust towers and chimney shafts of gas compressor units, marine vessels. Their protection requires mobile and completely autonomous plants for applying coating in the most cases made from aluminum. A lot of the facilities are located in hardly accessible and non-industrialized regions of the Russian Federation. Areas of the treated surfaces amount to square kilometers.

Coating with fine condensed particles is performed by thermal spraying methods which involve heating and melting of the sprayed material by any heating source and its following acceleration by gas flow. The sprayed material is delivered to the base surface in a dispersed state in the form of fine melted or plasticized particles which impact the surface, become deformed and through hardening superimpose one upon another thus forming the coating.

The plasma spraying method [2, 3, 4] became the most widespread among the existing ways of thermal spraying [1]. The coating material melts at time of passing between the electrodes. The temperature inside the flow may reach 16000K which is useful for applying refractory [5, 6] heat-protective coatings [7, 8]. However for aluminum such temperature is excessive and may result in overheating and evaporation of a significant part of the material.

Other method named as high velocity air fuel (HVAF) [1] is based on use of the principle of chemical reaction between an oxidizing agent and fuel in the thruster chambers. Fuel combustion takes place inside a limited space at the pressure which is in large excess over the atmospheric. Thereby a supersonic gas flow as to its concentration and energy power is much more in demand as compared to traditional heat sources [9]. Use of air as an oxidizing agent allows working at the flow temperatures of about 2000K and avoiding overheating of the molten coating material. The velocity of the combustion products due to passing through a small critical section almost reaches the sound speed. It is possible for them to remove the achieved molten material from the melting zone and to deliver it to a workpiece surface in a split second.

By the efforts of the Chair of Materials Machine Working of Samara State Aerospace University there was designed [10], manufactured and tested [11] a metallizer using a gaseous fuel oxidant system: propane and air. The device is designed for use on surface. Coating material: wire-shaped aluminum. This solution is based on experience and structural designs used for construction of thrusters [10]. The wire is being fed to the critical section zone where the working medium heat transfer is at the maximum (Figure-1). The zone may be represented as a finite-size cylinder moving progressively inside the medium which ensures convective and radiant heat transfer. Given constant feeding speed the volume of wire fed inside the chamber and the volume of the melted material become equal. Thus we obtain a two-phase Stefan problem with the established phase boundary. It is advisable that the phase boundary would not exceed the limits of the high-energy critical section zone. Mathematical simulation of the melting material formation process will allow determining the principal parameters influencing the metallizer performance.

2. MATERIALS AND METHODS

Analytic solution of the Stefan problem in a traditional formulation at the moment has not been yet obtained by anybody. There is a variant of numerical solution of the problem dealing with heating and melting of traveling wire inside the metallizer combustion chamber by the finite volume method [12]. A computational domain is being split to receive a finite volume grid. Here below you can find a derivation of the numerical solution.

Let's formulate a heat-transfer equation for a special case involving a finite-size homogenous fixed cylinder in a cylindrical coordinate system [13]:

$$\frac{\partial T(r,x,\tau)}{\partial \tau} = \alpha_\lambda \left(\begin{array}{l} \frac{\partial^2 T(r,x,\tau)}{\partial r^2} + \\ + \frac{1}{r} \cdot \frac{\partial T(r,x,\tau)}{\partial r} + \\ + \frac{\partial^2 T(r,x,\tau)}{\partial x^2} \end{array} \right), \quad (1)$$

where $\tau > 0$ - an observation period, $0 < r < R$ - the cylinder radius, $0 < x < L$ - the cylinder axis, α_λ - the temperature conductivity coefficient equal to ration between the material heat transfer coefficient λ and its specific heat capacity c_P and density ρ.

$$\alpha_\lambda = \frac{\lambda}{c_P \cdot \rho} \quad (2)$$

Let's transform the equation (1) by plugging in the temperature conductivity coefficient and adding the summand ε_{in} which characterizes the internal heat source:

$$c_P \cdot \rho \cdot \frac{\partial T}{\partial \tau} = \frac{\partial}{\partial r}\left(\lambda \frac{\partial T}{\partial r} \right) + \frac{1}{r} \cdot \left(\lambda \frac{\partial T}{\partial r} \right) + \\ + \frac{\partial}{\partial x}\left(\lambda \frac{\partial T}{\partial x} \right) + \varepsilon_{in} \quad (3)$$

Heat flows inside the material disseminate according to Fourier's law:

$$q_x = \lambda \cdot A_x \cdot \frac{\partial T}{\partial x}, \; q_r = \lambda \cdot A_r \cdot \frac{\partial T}{\partial r}. \quad (4)$$

Let's present the heat flows (4) in the equation (3):

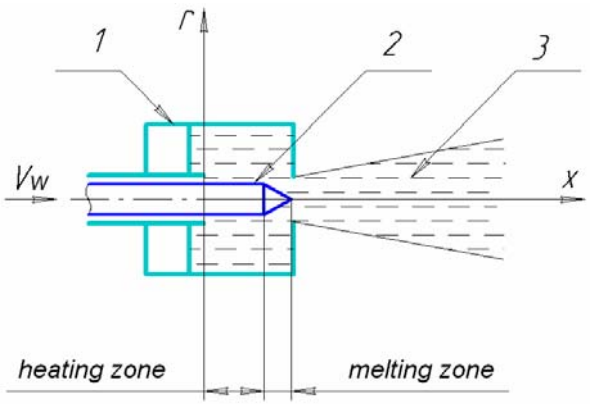
$$c_P \cdot \rho \cdot \frac{\partial T}{\partial \tau} = \frac{1}{A_r} \cdot \frac{\partial q_r}{\partial r} + \frac{1}{A_r} \cdot \frac{q_r}{r} + \\ + \frac{1}{A_x} \cdot \frac{\partial q_x}{\partial x} + \varepsilon_{in} \quad (5)$$

In case of heat conduction simulation for moving medium the heat-transfer equation (1) will be transformed correspondingly. The transition is based on replacement of the partial time derivative $\partial / \partial t$ by the total time derivative [14].

$$\frac{d}{d\tau} = \frac{\partial}{\partial \tau} + V_W \cdot grad, \quad (6)$$

where V_W = local velocity of medium (wire, Figure-1). Direction of movement is aligned with axis x which allows formulating an equation (5) for moving medium as follows:

$$c_P \cdot \rho \cdot \frac{\partial T}{\partial \tau} + c_P \cdot \rho \cdot V_W \cdot \frac{\partial T}{\partial x} = \frac{1}{A_r} \cdot \frac{\partial q_r}{\partial r} + \\ + \frac{1}{A_r} \cdot \frac{q_r}{r} + \frac{1}{A_x} \cdot \frac{\partial q_x}{\partial x} + \varepsilon_{in} \quad (7)$$



1 - metallizer; 2 – wire; 3 - combustion product flow with inclusion of molten material particles.

Figure-1. Basic scheme of wire melting process.

We'll restrict ourselves by analyzing of a quasipermanent stage of wire melting when temperatures distribution inside the material is constant in time, i.e. $\partial T / \partial \tau \to 0$.

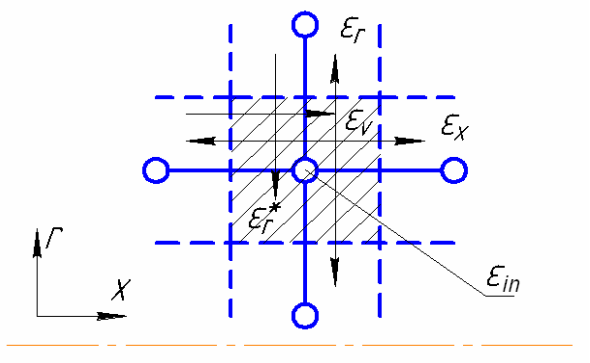
$$c_P \cdot \rho \cdot V_W \cdot \frac{\partial T}{\partial x} = \frac{1}{A_r} \cdot \frac{\partial q_r}{\partial r} + \frac{1}{A_r} \cdot \frac{q_r}{r} + \\ + \frac{1}{A_x} \cdot \frac{\partial q_x}{\partial x} + \varepsilon_{in} \quad (8)$$

Each summand in the equation (8) represents specific energy and the whole equation may be formulated as a specific energy balance equation:

$$\varepsilon_v = \varepsilon_r + \varepsilon_r^* + \varepsilon_x + \varepsilon_{in} \quad (9)$$

Figure-2 shows a scheme of energies dessimination for one final volume (FV).

$\varepsilon_v = \frac{c_P \cdot m \cdot V_W \cdot \frac{\partial T}{\partial x}}{V} = \frac{q_v}{V}$ - amount of heat reaching the final volume with mass m for the period τ due to convective diffusion which proceeds with the velocity V_W relative to the volume V of this finite element.



——— – relations between FV nodes,
- - - - - – FV boundaries.

Figure-2. Scheme of energies dessimination for the final volume.

$\varepsilon_r = \frac{1}{A_r} \cdot \frac{\partial q_r}{\partial r}$, $\left(\varepsilon_x = \frac{1}{A_x} \cdot \frac{\partial q_x}{\partial x} \right)$ – amount of heat passing the distance between the radially (axially) adjacent grid nodes for the time τ relative to the area perpendicular to its dessimination direction A_r.

$\varepsilon_r^* = \frac{1}{A_r} \cdot \frac{q_r}{r}$ - additional amount of heat delivered radially from the cylinder surface to the grid node under concern located at the radius r for the period τ relative to the area perpendicular to its dessimination direction A_r.

The heat source and correspondingly ε_{in} is present only inside the volumes located at the cylinder surface, i.e. coming in contact with ambient environment. The heat flow arriving from outside to the superficial volume is being replaced by the equivalent heat flow generated by the internal heat source located within the same volume [15].

$\varepsilon_{in} = \varepsilon_{conv} + \varepsilon_{rad} = \frac{q_\alpha}{V} + \frac{q_P}{V}$ - amount of heat generated by the internal heat source in the final volume for the period τ relative to the volume V of this element. It is formed by the radiant and convective components functioning independently of each other.

$$\varepsilon_{conv} = \frac{\alpha_\alpha \cdot A_\alpha \cdot (T_{env} - T_W)}{V}, \quad (10)$$

where α_α = the heat transfer coefficient, A_α = the area across which heat is transmitted, i.e. area of the final volume contact with ambient environment. T_{env} = the ambient environment temperature, T_W = the wire final volume temperature.

$$\varepsilon_{rad} = \frac{\xi_{add} \cdot C_0 \cdot A_\alpha \cdot \left(\left(\frac{T_{SB}}{100} \right)^4 - \left(\frac{T_W}{100} \right)^4 \right)}{V}, \quad (11)$$

where T_{SB} = the temperature of the body surrounding the wire, C_0 = the coefficient of radiation of an absolutely black body, ξ_{add} = the adducted radiation coefficient for the system of two bodies equivalent to:

$$\xi_{add} = \frac{1}{\frac{1}{\xi_W} + \frac{A_\alpha}{A_{SB}} \cdot \left(\frac{1}{\xi_{CC}} - 1 \right)}, \quad (12)$$

where - ξ_W and ξ_{CC} are the wire and combustion chamber emissivity factors, A_{SB} = the surrounding body (combustion chamber) area.

Heat flows q_x, q_r inside metal disseminate according to Fourier's law:

$$q_x = \lambda \cdot A_x \cdot \frac{\partial T}{\partial x}, \; q_r = \lambda \cdot A_r \cdot \frac{\partial T}{\partial r}. \quad (13)$$

The problem resolves itself into finding out temperature for each grid node. For arriving at the numerical solution it is necessary to replace the temperature partial derivatives at ($i \cdot \Delta x$, $i \cdot \Delta y$) point by means of differential relations using finite differences formulas (equivalently for r):

$$\frac{\partial T_{i,j}}{\partial x} = \frac{T_{i,j} - T_{i-1,j}}{\Delta x} + \xi_1; \quad (14)$$

$$\frac{\partial^2 T_{i,j}}{\partial x^2} = \frac{T_{i-1,j} - T_{i,j}}{\Delta x^2} + \frac{T_{i+1,j} - T_{i,j}}{\Delta x^2} + \xi_2; \quad (15)$$

where ξ_1.. ξ_2 - are residual members tending to zero when Δx and Δr go to zero which may be omitted.

Let's make replacement for the radiant component, approximate variable $T_{i,j}$ raised to the 4th power by means of a piecewise-defined linear function represented as follows: $(T_{i,j})^4 = K^1 \cdot T_{i,j} + K^2$. It is not necessary to make a replacement for the surrounding body temperature since $(T_{SB})^4 = const$.

$$K^1 = \frac{(T_1)^4 - (T_2)^4}{T_1 - T_2}, \quad K^2 = (T_1)^4 - K^1 \cdot T_1 \qquad (16)$$

At low differential temperature T_1–T_2 at the boundaries of the piecewise-defined function approximation error will be equivalently low. After the necessary replacements and insertion of all given relationships into the specific energies balance equation (9) we'll receive the resulting equation (17) for one node of the finite volume grid.

Temperature distribution across the nodes may be determined by solving a set of such equations. Let's use for this aim one of the Gaussian method variations, namely the so called LU-decomposition method. The set is reduced to the following form: $A \cdot X = B$, where A - a square matrix of n-size coefficients, X - a vector of n-size unknowns, B - a vector of n-size right-hand members of equation. Nodes temperatures are unknowns. Vector B includes known boundary conditions and is formed by the members of equations corresponding to the boundary nodes which come in contact with the products of combustion (Figure-3). Matrix A is represented in the form of a product of two triangular matrices of special form $A = L \cdot U$. Matrix transformations require significant time expenditures. Single temperature field computation involves tens of successive iterations for determining the piecewise-defined function coefficients as well as iterations for adjustment the wire feeding speed relying on the fixed position of the melting boundary cone vertex (Figure-1).

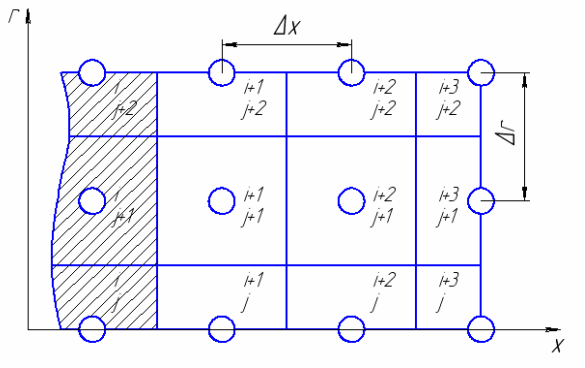


Figure-3. The grid including all of the nine different finite volumes, boundary ones among them.

$$c_P \cdot \rho \cdot V_W \cdot \frac{T_{i,j} - T_{i-1,j}}{\Delta x} = \lambda \frac{T_{i,j-1} - T_{i,j}}{\Delta r^2} +$$
$$+ \lambda \frac{T_{i,j+1} - T_{i,j}}{\Delta r^2} + \frac{\lambda}{r_j} \cdot \frac{T_{i,j+1} - T_{i,j}}{\Delta r} + \lambda \frac{T_{i-1,j} - T_{i,j}}{\Delta x^2} +$$
$$+ \lambda \frac{T_{i+1,j} - T_{i,j}}{\Delta x^2} + \frac{\alpha_\alpha \cdot A_{\alpha,i,j} \cdot (T_{env} - T_{i,j})}{V_{i,j}} + \qquad (17)$$
$$+ \frac{\xi_{add,i,j} \cdot C_0 \cdot A_{\alpha,i,j}}{100^4 \cdot V_{i,j} \cdot c_P \cdot \rho} \cdot (T_{SB})^4 -$$
$$- \frac{\xi_{add,i,j} \cdot C_0 \cdot A_{\alpha,i,j}}{100^4 \cdot V_{i,j} \cdot c_P \cdot \rho} \cdot (K^1 \cdot T_{i,j} + K^2)$$

Simulation of melting is made by elimination of the control volumes from the phase boundary surface. The finite volume temperature exceeding the material melting temperature is taken as an elimination criterion. The grid is being rearranged, matrices are being retransformed and computation is being repeated. In this iterative way the phase boundary line is being adjusted.

It is not possible to perform the above number of repeated mathematical computations manually; this process should be made automatically by means of contemporary programming aids.

3. RESULTS

Via Delphi 7 development environment an original program PLAVCA for theoretical investigations of molten material formation induced by the combustion products flow inside the rocket chamber was developed. The program has simple and user-friendly interface. The user has the opportunity to set all of the problem specifications: geometrical parameters of computational domain, size and number of finite volumes, physical parameters of combustion products flow and of the melting material. Once entered initial conditions may be saved in a file and loaded at time of the following program run. Calculation can be made both for one quasipermanent state of the "rod - working medium" system and for a range of states achieved by changing of one of the problem parameters at a definite interval. Such parameters may include: oxidizing agent excess coefficient, pressure inside the rocket chamber, critical section diameter, rod diameter. The results of computation are represented in the form of temperatures distribution per each iteration and are saved in an Excel file. Besides a file with the principal resulting physical quantities achieved at time of the system equilibrium is also saved.

PLAVCA program is contained in a single plavca.exe file with the size not exceeding 1 Mb. Availability of WINDOWS software and Excel component from Office software package on a personal computer is a prerequisite for the program operation. According to statistical data the mentioned software is installed on 90-95% of computing machines. The processor takes the basic load at time of calculations. The

higher the processor clock rate the greater the computation frequency and the more detailed fragmentation of the computational domain can be set. To start the program run the batch file plavca.exe.

Theoretical justification of the numerical computing method involves acknowledgement of the method compliance with the definite requirements: correctness, accuracy, stability and the method convergence to accurate solution.

A problem is considered to be set properly given that its solution for any values of input data from a definite class is available, unique and stable. The problem of achieving molten material in the rocket chamber was set properly. The quasipermanent stage of wire melting when the desired temperatures distribution in the material is constant with time, i.e. $\partial T / \partial \tau \to 0$, is under consideration. The profiles of the heat flows behavior inside the material were predetermined and the energy source power is known (equations 10, 11). A set of linear algebraic equations is always composed in the way when the number of equations complies with the number of unknowns. It means that the solution is always available and it is unique.

The Numerical solutions of differential equations with partial derivatives usually involve several kinds of errors. The most significant of them is the error of partition or spatial iteration conditioned by application of a finite partition. The lesser the size of the chosen finite volume the closer the numerical results converge to the corresponding accurate values. By enlarging the number of partitions it is possible to achieve more accurate result through increase of time expenditures. Time expenditures for a single solution of an equation set matrix grow hyperbolically with linear increase of the matrix size. On the other hand the numerical method is required to be accurate. This requirement in the model under consideration is achieved by increase of a number of the finite volumes in the computational domain. Accuracy of determination of the wire feeding velocity grows with reduction of an iteration step. Level of detail of the finite volume grid and minimum iteration steps values are limited only by a computer capability. It is necessary to find a good balance between the computation accuracy and time necessary for its achieving. Let's make a series of computations and observe temperature changes in the most heat-stressed grid node in case of increase of the finite volumes quantity (Figure-4).

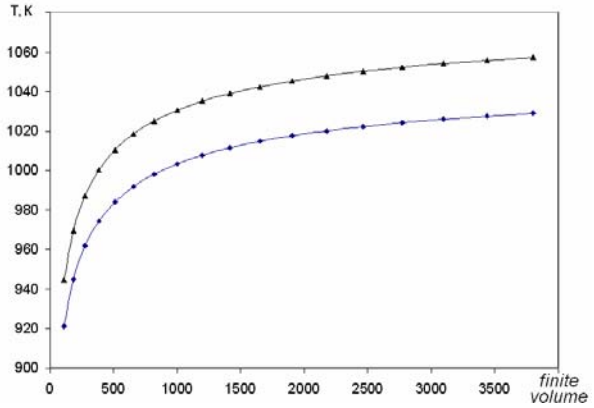


Figure-4. Dependence of temperatures T_{conv} (below) and $T_{conv+rad}$ (above) on the finite volumes number.

The node temperature becomes stable and ceases to depend significantly from the grid detail level. The permissible accuracy may be achieved starting from 2500-3000 finite volumes in a computational domain. Temperature drift to the limit value evidences the numerical method convergence.

Stability of the numerical solution is proved by monotone growth of the graphs on Figure-4. The solution is in permanent dependence on input data and changes proportionally to change of the same. Accumulation of rounding errors in the course of computations could result in the solution instability. But an extended real data type was used for fractional numbers at time of software implementation of the model of achieving molten material in the rocket chamber. The number of significant digits for this type comes up to 20. This allowed excluding the rounding errors influence.

4. DISCUSSIONS

There are other solutions for the quasipermanent Stefan problem. It is used for description of the processed of welding [16], melting and hardening [17] as well as zone melting [18, 19]. The last mentioned process and its mathematical formulation is the most similar to our problem thus let's discuss it in detail. Permanence of the zone melting process behavior is of primary importance for achieving large and high-quality crystals. Figure-5 shows a typical technological workflow of the vertical zone melting of a cylindrical rod. The cylindrical rod is being moved forward near a heat-producing element with the permanent velocity υ_0 which results in formation of a melting zone. In the process of hardening a crystal with higher qualitative characteristics is being created.

The process of zone melting of a cylindrical crystalline rod may be represented as an axially symmetric Stefan problem. The problem can be solved numerically by means of the method of additive splitting of singularities [20]. Such statement of the Stefan problem

and its numerical decision are the most proximate to the solution method offered by us.

A portion of the rod $0 \le x_2 \le l_2$ which is affected by the heat source is determined. It is considered that its lateral sides have permanent temperature which is equal to the ambient temperature u_0. On (x_1, x_2) plane the thermal process with phase transition from one aggregate state to another is described by the following nondimensional equations:

$$\frac{1}{x_1}\frac{\partial}{\partial x_1}\left(x_1 k(u)\frac{\partial u}{\partial x_1}\right)+\frac{\partial}{\partial x_2}\left(k(u)\frac{\partial u}{\partial x_2}\right)= = Pec(u)\rho(u)\frac{\partial u}{\partial x_2} \quad (18)$$

$$[u]=0,\ \left[k(u)\frac{\partial u}{\partial N}\right]=PeSt\cos(N,x_2),\ x\in S, \quad (19)$$

where density, heat transfer and heat capacity coefficients are considered to be in a general way dependable on temperature and disconnected at the phase change boundary S, where $u(x)=u^*$. The boundary conditions are set for the lateral sides, upper boundary and axis. The method of additive splitting of singularities described in [20] is used for numerical solution of the problem; quite complex mathematical tools are involved, namely: Kirchhoff transformation, fundamental solution of Laplace equation, fast Fourier transformation [21] and other. Several iteration processes are applied which considerably reduce the computation speed.

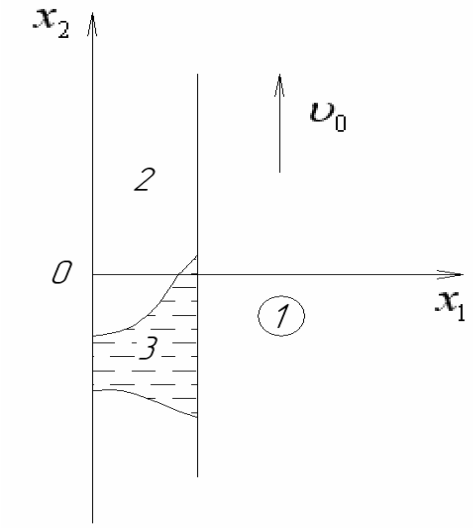


Figure-5. Zone melting scheme:
1 - heat-producing element, 2 - cylindrical rod,
3 - molten zone.

The computations result in achieving the temperatures distribution inside the rode and the phase boundary which depend on the heat source power. The model also allows seeing the effect when the molten material is not formed due to rather high velocity [20].

As compared to the model of wire heating and melting in the thruster chamber this model has a range of disadvantages. It does not take into account radiant heat exchange which has significant effect in the rocket chamber. The formed molten material is not removed thus preventing direct contact between crystalline metal and the heat source. In case of use of a gas generator for metallization the achieved liquid phase will be taken away by the combustion products. But the analyzed model [20] specifically justifies correctness of use of the numerical solution for the problem of the traveling rod melting as well as of use of iterative approach to phase boundary determination.

5. CONCLUSIONS

The software implementation of the numerical solution allows performing the necessary extent of theoretical studies in regard to molten material formation from a rod introduced into a thruster combustion products flow. In case the problem is solved numerically it is important to use detailed grids with high number of nodes. Automation of computations by the way of their programming gives an opportunity to achieve highly reliable results of the theoretical studies and to rely upon good convergence to experimental findings of benchmark tests. It is planned to make adjustments to the mathematical model in the course of theoretical and experimental studies correlation. After that it will be possible to determine efficient operation modes for the metallizer. It is also planned to make calculations for different designs of the device in order to optimize the coating process.

The computation velocity may work as a limiting factor for use of the developed mathematical model and its software implementation. In case of sufficiently detailed wire material splitting into the finite volumes iterative computations time may reach several hours.

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