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MATHEMATICAL MODELING OF PARTICLE IMPACT AND SOLIDIFICATION IN A THERMAL SPRAY PROCESS: PARTICLE – SUBSTRATE INTERACTION

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ABSTRACT

In the present paper a mathematical model of creation plasma spray coating with the given properties is developed. The flattening and simultaneous solidification of a liquid particle upon its impingement onto a solid surface has been mathematically described and numerically simulated. Numerical simulation has been accomplished on the basis of the full Navier-Stokes equations in cylindrical co-ordinates. Heat transfer process in particle and substrate has been simulated by 2-D problem heat conduction taking into account hydrodynamic processes into molten particle and forces of pressure. Particle solidification has been described by means of one-dimensional Stefan problem. It was investigated the effects of some important processing parameters such as impact velocity, droplet diameter, pressure and temperature of plasma on the flattening and solidification of a single liquid particle. Calculations computational algorithm on the basis of finite-difference method were created and a complex of applied programs was developed.

1. INTRODUCTION

Working features of plasma coatings to a considerable extent depend on the character and conditions of interaction of particle of spraying powder with substrate [4,10]. A theory of physico-chemical interaction of materials shows that in the process of spraying the features of coatings are defined by tem-

perature, pressure caused by impact, duration of interaction, state and the shape of its surface. The solid substrate and the area of contact are the main parameters needed for estimation of kinetics of chemical interaction between spraying particle and substrate. In view of highly limited duration of interaction of particle with substrate and small their dimensions (not over 200μ) any experimental measurements of contact temperature are extremely difficult. More perspective direction of problem solution is mathematical modeling. One of the most important criteria under creation of mathematical model is the choice of common mathematical base allowing to consider different influences on melt, to describe broad class of problems, and to give an opportunity to investigate different entrance parameters of plasma spraying without significant rebuilding of model as well. Taking into account the complexity of the system of equations we put equations of mass and energy conservation in the base of investigations. Flattening and simultaneous solidification is characterized by fast change of dynamic and thermal states. Previous investigations were limited either by study of simplified models or by solutions of problems modeling separate stages of the process [3,9]. Investigations [7], which were based on description of liquid movement with the aid of main laws of conservation (the Navier-Stokes system of equations for non-compressible liquid), made a significant impact on the semi-empirical models development. Most complete processes of flattening and solidification of particle were presented in recent works of R.H. Rangel [6]. However in existing investigations [2,8] the effects arising under dynamic impingement (especially under large velocities of particles) and the change of density owing to large gradients of pressure are not taken into account. In previous works they used the Oberbek-Bussinesk approximation. The legitimacy of this model under small temperature gradients ($\beta_T|T - T_0| << 1, \beta_T$ is a coefficient of temperature expansion) has not given rise to doubt. The last condition restricts the limits of the model application and it depends on input data of system, in particular on initial particle velocity.

Preliminary analysis [1] of head-on collision with large velocity of droplet has shown that it is necessary to take into account the compressibility of liquid in constitutive equations. The consideration of indicated effects led to necessity of molten particle flattening process description with the aid of viscous compressible liquid conservation laws. Besides, the correct mathematical flattening process description demands the of system complete flattening equations and energy equation, which describe the energy transfer and change of velocity and density. Hence, hydrodynamic problems of such type should be considered together with problems of phase change.

2. MATHEMATICAL MODEL

Schematic presentation of the initial configuration of problem is given in fig.1.

The mathematical model developed in this paper is based on the following assumptions:

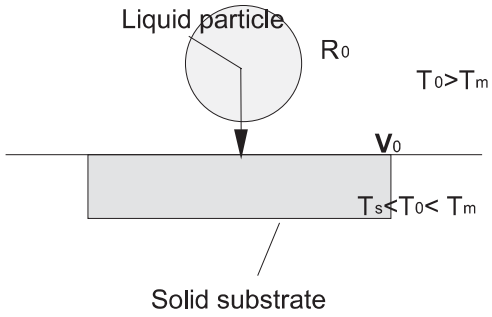

Figure 1. Initial configuration of the problem.

- fluid flow is laminar and compressible,
- axisymmetric system of coordinates is used,
- impingement is perpendicular to the substrate,
- the particle doesn't rotate during the fall,
- in the initial moment the particle is molten,
- one-dimensional heat conduction is assumed for solidification process,
- the contact of the particle with the substrate is ideal,
- the substrate is a cylinder and the initial temperature T is constant,
- the surface of the substrate is smooth.

Following the above assumptions, the governing equations for the axisymmetric system of coordinates may be written as follows.

For the description of deforming particle molten material movement let's use full Navier-Stokes system of equations for compressible viscous liquid written in natural variables "velocity-pressure": the mass conservation law

$$\frac{\partial \rho}{\partial t} + \triangle(\rho \cdot \mathbf{V}) = 0, \tag{2.1}$$

the movement quantity conservation law

$$\frac{\partial(\rho \cdot \mathbf{V})}{\partial t} + \triangle(\rho \mathbf{V} \cdot \mathbf{V}) = -\nabla P + \nabla \cdot (\mu \nabla \mathbf{V}) + \mathbf{g}\rho, \tag{2.2}$$

the energy conservation law

$$\frac{\partial(\rho \cdot E)}{\partial t} + \triangle(\rho E \cdot \mathbf{V}) + \nabla(P \cdot \mathbf{V}) = \nabla \cdot (\lambda(T) \nabla T), \tag{2.3}$$

where $E = I + E_{kin}$ is the specific complete energy, $I = c(T)T$ is the specific internal energy of the particle, $E_{kin} = v^2/2$ is the specific kinetic energy

of the particle, λ is the material thermal conductivity, ρ, P, T, μ are density, pressure, temperature and kinematic viscosity of the fluid respectively, and $\rho\mathbf{g}$ represents the body force per unit mass.

To complete the problem formulation of the we should add the state equation $P = f(\rho, T)$.

Under movement of continuous medium the surfaces is called free if surface tensions are balanced at the expense of surroundings pressure. As far as liquid borders upon gas, density of which is small, border "liquid-gas" is a free surface. The shape of the free surface as a rule is unknown beforehand and is defined in the course of problem solution that essentially complicates the numerical algorithm.

In order to define the domain occupied with liquid, i.e. to define a free surface Γ a scalar function F is introduced. It defines the fraction of cell volume occupied with the liquid [7]. It is supposed that $F = 1$ when a cell is fully occupied with the liquid and $F = 0$ in the case of empty cell. The cells with $0 < F < 1$ contain the free surface.

For the function F the following equation is true

$$\frac{\partial F}{\partial t} + (\mathbf{V} \cdot \nabla)F = 0. \tag{2.4}$$

The Laplace conditions are true on the free liquid surface Γ defined with the help of function F

$$(P - P_g)n_r = \sigma'_{rr}n_r + \sigma'_{rz}n_z + \sigma(k_1 + k_2)n_r,$$

$$(P - P_g)n_z = \sigma'_{zz}n_z + \sigma'_{rz}n_r + \sigma(k_1 + k_2)n_z,$$

where P_g is the pressure in the gas surrounding the liquid, P is the liquid pressure on the free surface, σ is the surface tension coefficient, k_1, k_2 are the curvatures of main normal surface sections,n_r, n_z are the projections of a single normal vector to a corresponding coordinate axis, $\sigma'_{zz}, \sigma'_{rr}, \sigma'_{rz}$ are the derivatives of the stress tensor components[5].

The heat exchange conditions are established for the temperature T on a free surface Γ . These conditions reflect the influence of the surrounding temperature on the particle. We use the condition

$$\lambda(T)\frac{\partial T}{\partial n}|_\Gamma = \alpha_T(T - T_g)|_\Gamma,$$

or the condition of heat transfer with radiation

$$\lambda(T)\frac{\partial T}{\partial n}|_\Gamma = \alpha_T(T - T_g)|_\Gamma + \beta\sigma_b(T^4 - T_g^4)|_\Gamma.$$

The coefficient of heat transfer α_T characterizes the heat exchange on outer side of frontier layer and it is defined from the formula $\alpha_T = Nu \cdot \lambda_g/(D_0 \cdot \sqrt{f_n})$,

where f_n is the coefficient of powder shape D_0 is a diameter of a particle, λ_g is the coefficient of heat conductivity of gases mixture (plasma) under temperature T_g) Nu is Nusselt number defined by the modification of Rantz-Marshall formula, and it depends on the temperature in cells of the free surface.

Using the assumption relative to the model of heat process in substrate and the symmetry of the problem let define the temperature field by means of one-dimensional non-stationary quasi-linear equation of heat conductivity

$$\rho_{sub} C_{sub} \frac{\partial T_{sub}}{\partial t} = \nabla \cdot (\lambda_{sub}(T_{sub}) \nabla T_{sub}). \tag{2.5}$$

In practice massive solids are used as a substrate, they are large in comparison with particle dimensions. In order to save a time of calculation it is appropriate to limit the dimensions of computation domain or mesh in substrate. We define the limits from the following condition: a heat introduced in substrate by means of plasma flow through the particle must not exceed the temperature of lower border of calculation domain more than 5% relatively to the initial substrate temperature. Let assume that substrate is a cylinder (fig.2) with a constant initial temperature. The altitude of the cylinder is defined from the condition of non-warming up its lower base, and the upper base is equal to the area of contact of molten particle with substrate. Boundary conditions for hydrodynamic problem should satisfy the following demands: on a solid surface (at initial moment – it is a substrate $z = 0$, at the following moments – it is a border between solid and liquid phases of particle) the condition of slip is established for velocities field, using movement equation we get the condition for pressure $\partial P/\partial z = -1/Fr^2$, hence the condition for the density follows from the state equation as well: on surfaces $r = R_{max}$ and $z = Z_{max}$ the boundary conditions of undisturbed flow are taking place

$$u = 0, \quad v = 0, \quad \frac{\partial \rho}{\partial z}|_{z=Z_{max}} = 0,$$

$$\frac{\partial P}{\partial r}|_{r=R_{max}} = 0, \quad \frac{\partial P}{\partial z}|_{z=Z_{max}} = 0,$$

on symmetry the line $r = 0$ the following conditions are defined

$$\frac{\partial u}{\partial r} = 0, \frac{\partial P}{\partial r} = 0, \lambda(T)\frac{\partial T}{\partial r} = 0,$$

for $z = 0$ (on substrate) the conditions of contact heat transfer are taking place

$$T = T_{sub}, \lambda(T)\frac{\partial T}{\partial z} = \lambda_{sub}(T_{sub})\frac{\partial T_{sub}}{\partial z}.$$

If an oxide pellicle is on the substrate surface, then the first condition must be replaced by

$$\lambda(T)\partial T/\partial z = 1/R(T - T_{sub}),$$

where $R = \delta/\lambda_n$ is the heat resistance, δ, λ_n are the thickness and heat conductivity coefficients on substrate surface respectively. However in a real process of spraying the coatings are sprayed at once after cleaning the surface of substrate, while the thickness of oxidized pellicles is insignificant. Then the influence of pellicles on the contact temperature is not large and it is possible to ignore them. As far as the molten particle drops on a cold substrate and

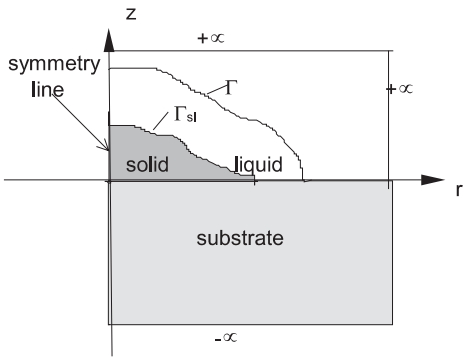

Figure 2. Configuration of problem in arbitrary time moment.

solidifies afterwards, we consider the problem of heat diffusion in the system "particle-substrate" as a problem about crystallization of substance (particle). Let assume that there is no melting, otherwise the heat problem should be defined as a problem of substrate melting introducing additionally equation for front of substrate melting. It follows from the above that the border - line separating molten part of particle from solidified one is not constant and it is defined within the problem solution. On the inter-phase border Γ_{sl} the Stefan condition is satisfied and the condition for temperature on this border

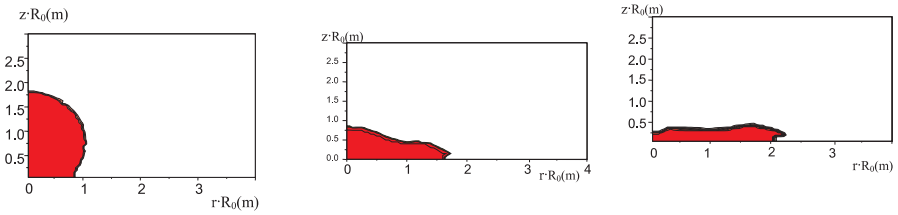

Figure 3. Particle spread dynamics(Al_2O_3).

is given by

$$\lambda(T^s)\frac{\partial T^s}{\partial z} - \lambda(T^l)\frac{\partial T^l}{\partial z} = L_m\rho^s\nu_{sl}, T^s = T^l = T^{sl}.$$

The temperature on the phases partition border is not constant and it must be defined within the process of problem solution $T_{sl} = T_m(P)$. Empiric Johnson formula estimates the change of temperature of melting $\triangle T_{sl}$ causing the change of pressure $\triangle T_{sl} = T_m \triangle P \rho_s/(41.3L_m)$, where L_m is the melting heat, ρ_s is the solid phase density, $\triangle P$ is pressure, change in comparison with the normal pressure; T_m is the melting temperature under normal pressure.

In order to complete the formulation of the heat problem the initial location of front of crystallization Γ_{sl} and the initial distribution of temperature for the particle and substrate are established. At the initial moment the particle is completely melted, i.e. the front of crystallization is absent and Γ_{sl} is the line $z = 0$. At the initial moment the temperature of particle is supposed to be constant and may be larger than the temperature of material melting:

$$T|_{t=0} = T_0 \geq T_m.$$

On the lower border the isothermal condition or boundary condition of the first type with constant initial temperature is established:

$$T_{sub} = T_{sub,0}.$$

3. NUMERICAL ALGORITHM

We solve the problem (2.1) – (2.5) with initial and boundary conditions. The particle velocity at the initial moment and initial radius are chosen as features. The problem is solved by the difference method and we use a splitting of modeling process into elementary physical processes at the iteration level. The field of a particle spreading is covered by the chess mesh. Each cell (i, j) of the

mesh is interpreted as an element of liquid volume, the pressure P, density ρ, temperature T are defined at the center of the cell (i, j), and divergent $D = \nabla \mathbf{V}$ is defined with values of components of velocity vector u, v at semi-integer points $(i \pm 0.5, j)$ and $(i, j \pm 0.5)$, accordingly. The approximation by one-sided differences was carried out in the equations of movement and energy the sign of velocity on the borders of the cell was taken into account. This allowed us to construct conservative schemes and to preserve the transportive feature. The main difficulty is the fact that at any moment the domain of splitting (free surface) is changing and it is defined with the help of volume function. Guiding cosines of curvature to free surface under conditions of heat exchange are calculated approximately as well.

The numerical algorithm is implemented as a complex of applied programs in Fortran.

In fig.3 some results are given for modeling the powder spraying process including spherical particle of oxide of aluminum Al_2O_3. We take the initial velocity $100m/s$, ter pressure $1ATM$, the temperature $2400K$ and the steel substrate of room temperature.

The state equation was defined according [4]:

$$P = \frac{K}{k}((\frac{\rho}{\rho_0})^k - 1) + (\rho T - \rho_0 T_0)\frac{\alpha K}{\rho_0},$$

where k is parameter, $K = E/(3(1-2\mu))$ is the volume module of resilience for isotropic bodies, E is the Jung module, μ is the Puasson coefficient.

The ideas used in this article give us an opportunity to estimate the interaction of particle - substrate in more realistic way and to form the domain of contact at initial stage of impingement. However available data don't allow us to make a complete comparison. It is connected both with the difficulty to define output data for a single particle and to define the values of many thermophysic constant which are not universal and they demand additional specifications connected with their dependence not only on the temperature but also on the pressure. Besides the Fourier law describes the process of heat transfer. The borders of applicability of Fourier law is defined by physical processes, in particular the processes should be slow, and the gradients should be small. These demands are not always satisfied under impingement in domains of high pressures.

The model allows us to calculate at arbitrary moments the fields of temperatures, pressure, the line of solidification. It defines the shape of a free surface (at the end of the process of it is the shape of the solidified surface), and the degree of the melting substrate.

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DALELIŲ POVEIKIO IR KIETĖJIMO PROCESO MATEMATINIS MODELIAVIMAS

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Nagrinėjamas uždavinys yra apie plazminio užpurškimo dangos generavimą. Sudarytas pilnas matematinis modelis, kuriame įvertinami svarbiausi fiziniai procesai. Skaičiavimo eksperimentai atlikti naudojant Navje-Stokso lygtis, užrašytas cilindrinėse koordinatėse. Šiluminiai procesai dalelėse ir pagrindo medžiagoje aprašomi dvimačiu šilumos laidumo uždaviniu, kuriame atsižvelgiama į hidrodinamines ir slėgio jėgas. Dalelių kietėjimo procesas modeliuojamas vienmačiu Stefano tipo uždaviniu. Ištirta įvairių parametrų, tokių kaip dalelių judėjimo greitis, diametras, plazmos temperatūra ir slėgis, įtaka. Uždavinys sprendžiamas baigtinių skirtumų metodu bei aprašytas sudarytų taikomųjų programų paketas.