DEVELOPMENT OF MATHEMATICAL MODELS OF THERMAL PLASMA PROCESSES

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Abstract: *Application of a mathematical modelling of thermal plasma processes is effectively during development and optimization of electric power equipment as well as electro technological equipment. In the field of electric power industry such devices are: circuit breakers (simulation of arc extinction in the arc chamber); multi-chamber arresters for lightning protection of overhead power lines (simulation of arc discharge in a chamber of the arrester), and others. In the field of electro technological equipment such devices are: DC (and AC) arc plasma torches for air-plasma spraying of coating, metal welding and cutting; ICP (inductively coupled) plasma torches for nanomaterials production, fine powder treatment, plasma-chemical technologies and others. The article describes the main stages of the development of mathematical models: a study of the features of the physical process that allows us to formulate the basic assumptions of the model (stationary or non-stationary process, 2D or 3D geometry, laminar or turbulent flows and others); construction of the computational domain and of the mesh; setting the boundary conditions. Examples of results of calculations are shown. Recommendations on the use of specialized software are presented.*

Keywords: MATHEMATICAL MODELING, PLASMA PROCESSES, ELECTRO TECHNOLOGICAL EQUIPMENT

1. Introduction

In the field of electric power industry the operation of such electrical apparatuses as automatic switches, arresters, etc. is connected with an extinction of electric arc. For example, the use of multi-chamber arresters with electrodes placed into a chamber made of dielectric material is a promising way to protect overhead transmission lines from lightning overvoltages. When lightning current goes through the arrester, electric arcs appear in discharge chambers and they form the plasma jets from chambers.

In the field of electro technological equipment processes based on the use of arc plasma torch and radio-frequency (RF) inductively coupled plasma (ICP) torch are widely used. These are processes such as air-plasma spraying of coating, welding and cutting of metals, treatment of fine powder with various purposes, plasma-chemical technologies, etc.

Thus, during the development and optimization of electric power equipment and electro technological one the main subject of research are thermal plasma processes which are characterized by plasma parameters such as temperature and velocity as well as their variation in time.

To achieve this goal it is necessary to identify qualitative and quantitative relationships between the efficiency of the process (it can be an extinction of electric arc with minimal time or, conversely, generation of stable electric arc) on the one hand, and the geometry of the device and its operation parameters on the other hand. To determine those relationships it is necessary to carry out a large amount of experimental research which requires large time and material costs. Another way of obtaining that information is mathematical modeling of thermal plasma processes in arc and RF plasma torches.

2. Mathematical model

At present time a large number of mathematical models of plasma processes have been developed including a disturbance of thermal equilibrium, a plasma turbulence, etc.

The basic equations in a simplified model of plasma (it is assumed that plasma is in a state of local thermodynamic equilibrium, it is laminar and optically thin), express the fundamental conservation laws (of energy, momentum and mass), and for the elementary volume are written as follows [1]:

- energy equation:

$$\nabla\cdot\left(\rho\vec{\upsilon}h\right)=\sigma E^2-u_{rad}-\nabla\cdot\left(-\frac{\lambda}{c_p}\nabla h\right) \qquad (1)$$

- motion equation:

$$\nabla\cdot\left(\rho\vec{\upsilon}\vec{\upsilon}\right)=-\nabla p+\vec{F}_B+\rho\vec{g}+\nabla\cdot\left(\mu\nabla\vec{\upsilon}\right) \qquad (2)$$

- continuity equation:

$$\nabla\cdot\left(\rho\vec{\upsilon}\right)=0\,. \qquad (3)$$

Equations (1) – (3) include:

- plasma parameters such as enthalpy h that related to temperature T; velocity υ; pressure p;

- thermophysical plasma properties such as density ρ; thermal conductivity λ; specific heat c_p; viscosity μ; electrical conductivity σ; specific radiation power u_{rad};

- electromagnetic values such as electric field intensity E; electromagnetic force $\vec{F}_B=\vec{J}\times\vec{B}$.

Since plasma exists in an electromagnetic field the system of equations (1) – (3) is supplemented by Maxwell's system of electromagnetic equations:

$$\begin{cases}\nabla\times\vec{E}=-\dfrac{\partial\vec{B}}{\partial t}, & \nabla\cdot\vec{E}=\dfrac{\rho_{el}}{\varepsilon_0},\\ \nabla\times\vec{H}=\vec{J}, & \nabla\cdot\vec{B}=0,\end{cases}$$

where $\vec{E}$ и $\vec{H}$ are electric and magnetic field intensities; $\vec{B}$ is magnetic induction; $\vec{J}$ is current density; ρ_{el} is volume density of electrical charge; ε_0 is electric constant.

For thermal plasma processes the Maxwell's system of equations reduces to equations for the scalar (φ) and vector ($\vec{A}$) potentials:

$$\begin{aligned}&\nabla\cdot\left(\sigma\,\nabla\varphi\right)=0,\\ &\sigma\frac{\partial\vec{A}}{\partial t}+\frac{1}{\mu_0}\nabla\cdot\vec{A}=\vec{J},\end{aligned} \qquad (4)$$

where $\vec{J}=\sigma\left(-\nabla\varphi+\vec{\upsilon}\times\vec{B}\right)$, $\vec{B}=\nabla\times\vec{A}$.

Thus, equations (1) – (4) represent a system of equations that need to be solved simultaneously to obtain the distributions of the required quantities – plasma parameters, namely, temperature, velocity, pressure, electromagnetic quantities. The region of existence of the plasma is taken as a computational domain.

Boundary conditions for each required quantity are set at each boundary of the computational domain on the basis of the simplest physical considerations.

As already mentioned the system (1) – (4) includes thermophysical properties of plasma. For the main gases used in plasma processes the dependence of these properties on temperature (usually at atmospheric pressure) is given in the scientific literature [2-4]. The difficulty in solving system (1) – (4) lies in the fact that the temperature in the plasma torches varies in the range 300–20000 K, and with this temperature change the properties of the plasma vary by several orders of magnitude.

There are many software packages that allow modeling thermal plasma processes. The most famous commercial programs are ANSYS (CFX, Fluent), Comsol Multiphysics. The indisputable advantages of these programs are: the breadth of application (from the aerospace design to the biomedical application), relative simplicity (most of the functions and equations are already written, one just need to learn how to use them correctly) and high workflow productivity (a competent specialist can create a working model within a few hours).

In addition, usually it is possible to improve existing models with own code. For example, in the ANSYS Fluent software package it is possible to add user defined functions (UDF) written in the C programming language. This allows you to focus on a detailed description and investigation of the specific features of thermal plasma processes, while using ready-made procedures for those parts of the calculation that are common to other standard models (for example, using standard methods for solving systems of linear algebraic equations).

Examples of the application of various software products for the calculation of thermal plasma processes are presented below.

3. *Modeling of thermal plasma processes in an arc plasma torch for spraying in Comsol Multiphuysics*

A two-dimensional axis-symmetrical mathematical model of the plasma torch has been studied. The torch geometry corresponding to the real experimental set-up is presented in Fig. 1. The mesh is shown in Fig. 2. The mesh for calculation consists of 5098 elements.

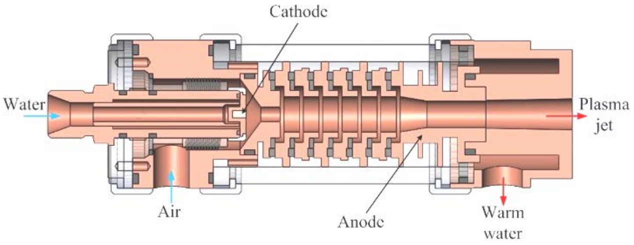

Fig. 1 *Design of DC plasma torch with inter-electrode sections*

Fig. 2 *Mesh for calculation*

Two models have been implemented in the software Comsol Multiphysics [5]: laminar plasma flow model and turbulent plasma flow model (SST-model).

The distributions of the gas temperature for arc current 200 A, laminar and turbulent flow are shown in Figs. 3–4.

Maximal gas temperature is 30 000 K. The shape of the temperature distribution for the model of turbulent flow is confirmed by frame from high-speed shooting – see Fig. 5.

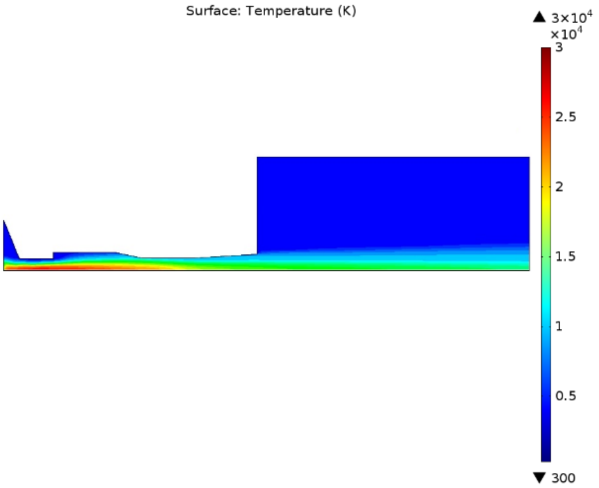

Fig. 3 *Temperature distribution in plasma torch: laminar flow*

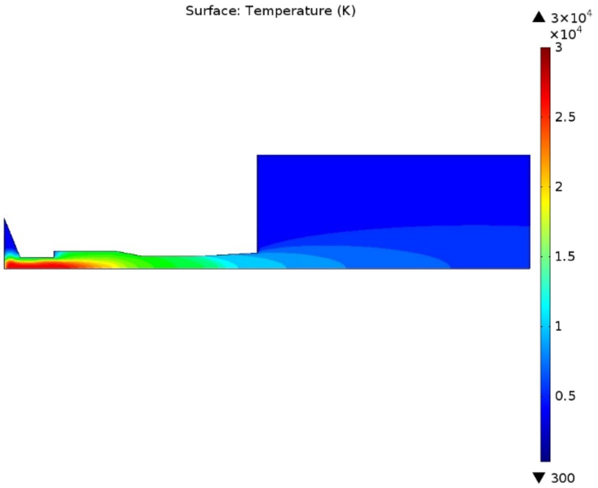

Fig. 4 *Temperature distribution in plasma torch: turbulent flow*

Fig. 5 *Image of plasma jet*

4. *Examples of thermal plasma modeling in ANSYS Fluent*

Discharge chamber of multi-chamber arrester. The multi-chamber arrester consists of a large number of series-connected chambers (Fig. 6), in which electrical breakdown leads to an arc discharge generation [6]. Such discharge is accompanied by erosion of the electrode material and by evaporation of the discharge chamber material. Thus pressure increases in the chamber that leads to appearance of plasma jet from the discharge chamber and to arc extinction.

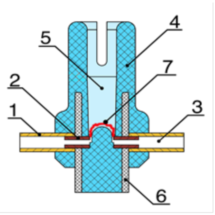

Fig. 6 *Design of discharge chamber of multichamber arrester: 1 – outer tube, 2 – inner tube, 3 – cavity, 4 – silicone rubber, 5 – discharge slot, 6 – fiber-glass plastic sleeve, 7 – arc*

To simulate plasma processes a three-dimensional nonstationary mathematical model was developed with the following features:

- The thermophysical properties of plasma were calculated taking into account an erosion of the electrodes material and an ablation of the discharge chamber walls [7], in the model they are included as dependences on temperature at a constant pressure of 10 atm;

- The case of tungsten electrodes and a silicone rubber chamber (ratio of Si: O: C: H = 1: 1: 2: 6, W: O = 1: 10) was considered;

- Evaporation of the discharge chamber material was taken into account as a source of mass;

- The motion of plasma is turbulent, the SST model was used to simulate turbulence.

The computational domain and the mesh for calculation are shown in Fig. 7.

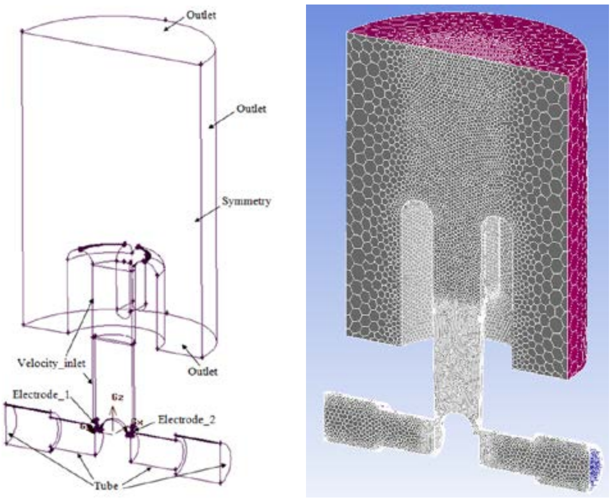

Fig. 7 *The computational domain of discharge chamber and the mesh for calculation*

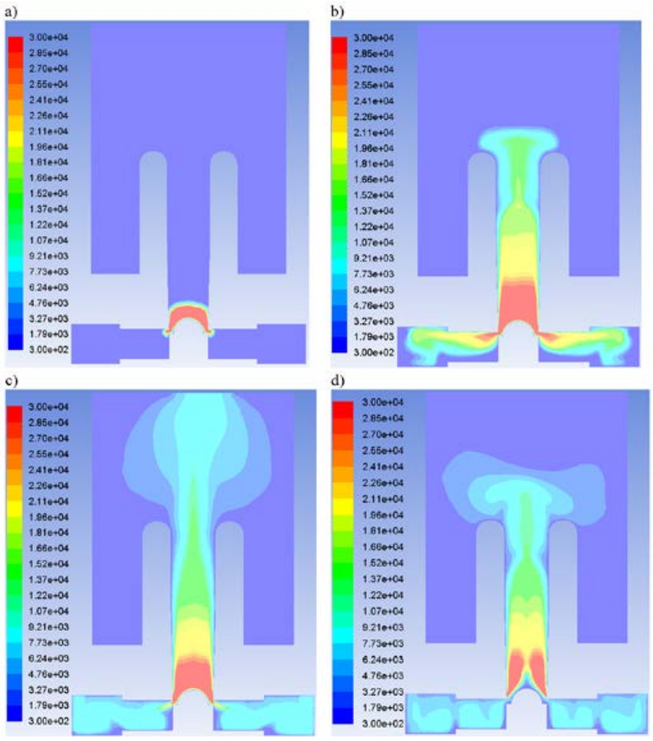

Fig. 8 *Distributions of plasma temperature (T, K)in the discharge chamber at different points of time: a – 2 μs, b – 30 – μs, c – 140 μs, d – 210 μs*

The computational domain includes a space surrounding the outlet of the discharge chamber which allows to calculate a process of formation of plasma jet from the discharge chamber. As a calculation region, it is convenient to take only half the space of the discharge chamber and the surrounding space since this space has a plane of symmetry (this is the plane of Fig. 6).

An electrical potential difference is defined on electrodes surfaces as boundary condition for the electromagnetic problem so that a discharge current through the chamber corresponds to the experimentally obtained dependence at each moment of time.

Results of simulation i.e. distributions of plasma temperature at different points of time are shown in Fig. 8.

Analysis of the simulation results shows that the presence of cavities joined to the main volume of the discharge chamber by small openings leads to the fact that at the initial stage of discharge, when pressure inside the discharge chamber exceeds pressure inside the cavities, plasma begins to spread into these cavities. The pressure inside the cavities is increased as long as it begins to exceed the pressure in the discharge chamber, which is lowered due to propagation of the discharge towards the outlet of the discharge chamber. It occurs in about 140-150 μs after the start of discharge. Thereafter, the gas accumulated in the cavities with lower temperature than the discharge core, begins to move in the opposite direction, i.e. from cavities to the discharge chamber. After 160 μs it leads to cooling of the central part of the discharge, which undoubtedly contributes to the extinction of the electric arc. This conclusion is confirmed by the results of experimental observations.

Combined plasma torch for nanomaterials production. A combined plasma torch consists of a series-connected a DC arc plasma torch and a RF ICP plasma torch. In this case, plasma jet of the arc plasma torch is fed to the inlet of the RF ICP plasma torch. That design provides an ignition of RF plasma and a reduce the power of the RF discharge. The combined plasma torch was studied for a technology of titanium dioxide nanopowder production.

To simulate the processes in the combined plasma torch and in the reactor a two-dimensional axisymmetric model was developed. The computational domain was divided by a mesh into 300,000 cells. Argon was used as the plasma-forming gas at a pressure of 1 atm.

To select the plasma torch operation mode that provides the evaporation of initial TiO_2 powder a series of calculations was carried out. The power of the arc discharge varied in the range of 10-15 kW, the power of RF discharge was in the range of 20-40 kW, the gas flow rate was in the range of 20-100 slpm, the inductor frequency of 1.76 MHz and 5.28 MHz was used.

Calculations showed that the use of the frequency of 5.28 MHz for such a design is more efficient.

An example of the calculation results is shown in Fig. 9 (arc discharge power is 12 kW, RF discharge power is 20 kW, gas flow rate is 60 slpm).

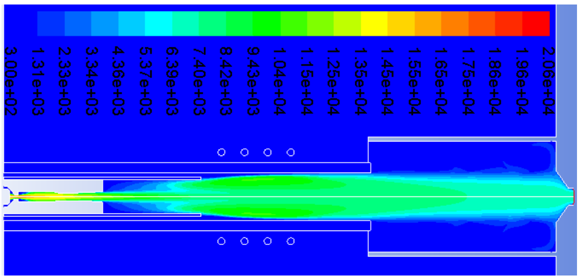

Fig. 9 *Distribution of plasma temperature in the combined plasma torch*

Modeling of a plasma jet loaded with fine powder. The treatment of fine powder (in this case – titanium dioxide powder) in a plasma jet has to simulate using a three-dimensional model. The reason of it is the disturbance of the plasma jet axial symmetry by the lateral feeding of a flow of carrier gas loaded by fine powder.

Initial powder was TiO2 with a mean diameter of 15 μm.

A series of calculations was carried out with the constant start velocity of powder feeding (10 m/s) and different powder feed rate (2–5 kg/h). Also calculations were made for the constant powder feed rate (4 kg / h) and different start velocity (5, 8, 10, 12 and 15 m/s) [8]. These calculations were made in order to find the optimum feed rate and start velocity of titanium dioxide. In those calculations the parameters of plasma jet (temperature and velocity at the inlet of the computational domain – the plasma reactor) correspond to the parameters of plasma jets created by the combined plasma torch.

Calculations showed that without feeding the powder the plasma jet has an axial symmetry which is significantly disturbed when the powder is fed through the feed-through line.

Best results (optimal trajectory of particles and its heating) were obtained at a powder feed rate of 4 kg/h and a start velocity of 10m/s (see Fig. 10).

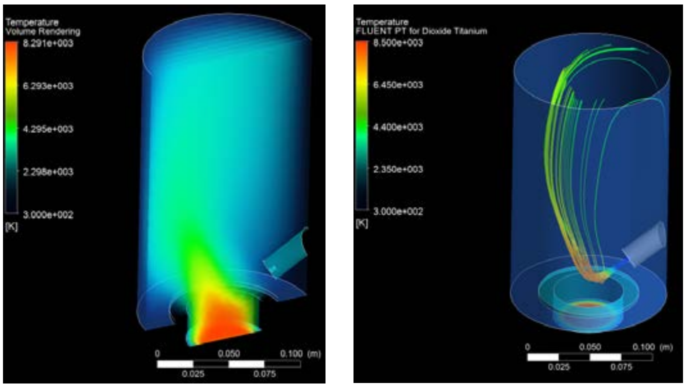

Fig. 10 *Distribution of plasma temperature T, K (left) and trajectory and temperature of TiO2 particles (right) for a powder feed rate of 4 kg h and a start velocity of 10 m/s*

5. Modeling of plasma processes using free software package OpenFOAM

The main disadvantage of commercial software packages is a high price. In addition, the researcher who uses such packages has to "play by someone else's rules", i.e. his capabilities are limited to existing models of the package. For researchers who need to solve non-trivial tasks the commercial packages envisage to create own models but this requires knowledge and programming skills that sharply raises the required skill level of the researcher and reduces the attractiveness of using such packages.

These disadvantages make one pay attention to free software. Currently in the field of free software there are a large number of programs that allow solving numerical simulation problems: Code_Aster, Code-Saturne, OpenFOAM and Elmer. All these software packages have a fairly extensive set of ready-made subroutines, but their main strength lies in a possibility to write own solution for any task.

An example of mathematical modeling of plasma processes using the free software package OpenFOAM is considered.

OpenFOAM (Open source Field Operation And Manipulation CFD ToolBox) is a freely available tool for computational fluid dynamics for operations with scalar, vector, and tensor fields. The basis of the OpenFOAM is a set of libraries that provide tools for solving systems of partial differential equations both in space and in time. The working language of the code is C ++.

OpenFOAM package was applied to calculate a plasma process of TIG welding. In OpenFOAM there is no ready solver for such a task therefore its creation was the first step. As a basis the standard solver *buoyantSimpleFoam* was used, in which the energy equation, the motion equation and the continuity equation are solved together.

The solver *buoyantSimpleFoam* was modified as follows: the equations of the electromagnetic problem were added; the electromagnetic force was taken into account in the motion equation; Joule heating and radiation energy losses was taken into account in the energy equation; nonlinear dependences of thermophysical plasma properties on temperature was introduced into the model; specific for plasma boundary conditions were introduced.

For the calculation the following geometry of the TIG torch was used: the electrode diameter was 3 mm, the internal diameter of the nozzle was 9 mm, the distance from the cathode to the anode (welding parts) was 4 mm. The following operation mode was calculated: arc current was 100 A, argon flow rate was 5 slpm. This mode of operation can be used to weld aluminum plates with thickness of 2–3 mm [9]. The task was solved in a two-dimensional formulation.

The results of the calculation i.e. the distributions of the temperature and the axial velocity of plasma are shown in Fig. 11.

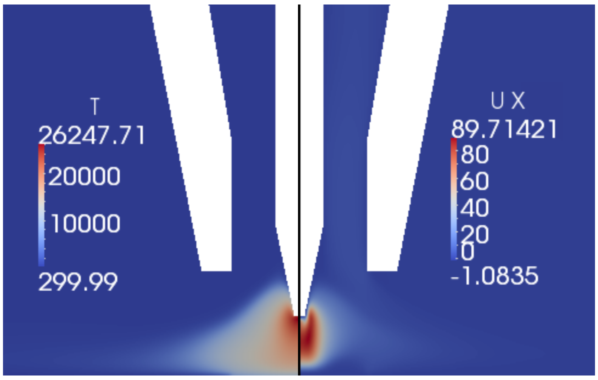

Fig. 11 *Distributions of the temperature (left) and the axial velocity (right) of plasma in TIG torch*

6. Conclusions

Various methods for calculating thermal plasma processes are studied at the Department of Electrical Power Engineering and Equipment of Peter the Great Saint-Petersburg Polytechnic University. The results of the research are used in teaching students, including in the preparation of master's theses.

For complex calculations of thermal plasma processes it is recommended to use specialized software: ANSYS Fluent, Comsol Multiphysics as well as the free software package OpenFOAM. Of course, it is necessary to check the applicability of the built-in models to the plasma conditions and, if necessary, to correct them.

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