Numerical simulation of argon flow structure in plasma vortex reactor

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Abstract. Numerical simulation of the turbulent three-dimensional swirling flow in experimentally tested plasma vortex reactor were carried out to ascertain that earlier limited modelling properly represents flow phenomena and to provide further insights into use of such apparatus. Exact experimental geometry, electrode location that maximizes energy utilization in accordance with previous research, model heat source, and reduced mixture composition (pure Ar) were used. A qualitative agreement between the results of the calculations and the experimental data for pure argon has been obtained. Structure of counterflow zone, crucial for energy extraction, and corresponding temperature field are presented.

1. Introduction

Recently, the problem of creating efficient energy sources has become increasingly noticeable. One of the most promising technologies is the use of plasma vortex reactors (PVRs), which can be both heat and hydrogen source.

Based on the experimental works [1-5] PVR was designed and elaborated. The hydrogen and heat production in the developed setup are based on the hydration reaction of erosion cathode clusters or metal nanopowder introduced into the reaction zone by water vapor, stimulated by plasma formations in a swirling flow. The scheme of this reactor and experimental data are given in [6]. As a working gas, a mixture of argon and water vapor was used. Vortex flow is used for the separation of light hydrogen on the reactor axis, the stability of an electric discharge and the thermal insulation of the walls from the hot plasma flow. It was shown that there is a long recirculation zone located between the anode and the swirler. Measured gas temperature of this heterogeneous plasmoid is about $T = 2000 \div 5000$ K.

The self-consistent simulation of the flow structure is complicated and requires joint modeling of the gas-dynamic and discharge subsystems. Therefore in [7], as a starting step, a simulation of the three-dimensional unsteady viscous turbulent vortex flow of pure argon in a model duct is carried out for different configurations of electrode system. The spatial distributions of the power of the source were chosen phenomenologically with the use of the data [6]. It was verified that the recirculation zone forms in such system and its characteristics strongly depend on the heat source power and the shape of electrodes and their location. The numerical modelling has demonstrated that it is possible to configure electrodes in such a way as to ensure energy transfer mainly downstream from the interelectrode zone.
Otherwise, apparatus suffers from several deficiencies. Among them are a strong overheating of the swirlr and fastener elements and undesirable transfer of hydrogen in upstream direction. It was shown that the optimal electrode configuration may be accomplished by the combination of thin anode and pipe-like cathode through which areas of different pressures are connected. A qualitative agreement between the results of the calculations and the experimental data [6] has been obtained.

However, the assumptions made in [6] limit the use of investigation results only to general demonstration of proposed idea. Therefore, a numerical simulation of the unsteady viscous turbulent swirl argon flow structure in the PVR duct, corresponding to the experimental setup in detail, with an optimal configuration of the electrodes obtained in [6] was carried out here.

2. Mathematical modelling

2.1. Numerical model geometry and governing equations
The schematic duct geometry is sketched in figure 1. Governing parameters for the electrode system are the shape, distance between them and the distance from the nozzle. The heat source is located between cathode (at left) and anode. The outlet of the duct has the form of a convergent nozzle. The nickel anode was thin, the nickel cathode was a hollow thin cylinder. The pipe-like cathode has an external diameter of 20 mm and a thickness of 1 mm. The cathode is located at the outlet of the duct, figure 1. The interelectrode distance is 60 mm remains constant, the length of the quartz glass duct is 407 mm.

![Figure 1](image_url) A schematic diagram of the geometry of experimental setup used for numerical simulation

Standard unsteady Reynolds averaged Navier-Stokes (URANS) equations were used to describe the flow:

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\begin{align*}
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v_i)}{\partial x_i} &= 0, \\
\frac{\partial (\rho v_i v_j)}{\partial x_i} &= -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_i} \left[ \mu \left( \frac{\partial v_i}{\partial x_i} + \frac{\partial v_j}{\partial x_j} - \frac{2}{3} \delta_{ij} \frac{\partial v_k}{\partial x_k} \right) \right] + \frac{\partial}{\partial x_i} \left[ -\rho \overline{v_i v_j} \right], \\
\frac{\partial \rho E}{\partial t} + \frac{\partial \rho (v_i v_j)}{\partial x_i} &= \frac{\partial}{\partial x_i} \left[ (\kappa + \frac{\epsilon \rho c_p}{Pr_T}) \frac{\partial T}{\partial x_i} + \nu \left( \tau_{ij} \right)_{eff} \right] + N(\vec{x}), E = h - \frac{P}{\rho} + \frac{v^2}{2}, P = \rho T, \end{align*}
\]

where \( \tau_{ij} \) is the deviatoric stress tensor; \( \rho \overline{v_i v_j} \) are the Reynolds stresses which must be modeled to close the set of equations, \( v_i, v_i', \rho, T, P, E \), and \( h \) are the mean and fluctuating velocity components, density, temperature, pressure, total energy, and enthalpy, respectively; \( N \) is the energy source, \( \mu, \mu_t, \mu_{eff} \) are the molecular, turbulent, and effective viscosity coefficients, respectively; \( c_p \) is the molar specific heat capacity at constant pressure; \( \kappa \) is the thermal conductivity coefficient; and \( Pr_T \) is the turbulent Prandtl number.

The model heat source was a homogeneous ellipsoid of revolution located between the anode and the cathode. The small axis of the ellipse equals to 1 cm. In what follows, we investigate the problem for pure Ar close to the experimental conditions [6], corresponding to the total mass flow rate \( m = 1 - 2 \) g/sec, the heat source power \( N = 50 - 100 \) W and the static gas pressure \( P = 10^5 \) Pa.
Initial values of pressure and overall temperature were set to $10^5$ Pa and 300 K, respectively. The initial value of the input velocity is calculated automatically by the mass flow rate, the inlet diameter and the gas density.

The no-slip velocity conditions were imposed along the tube, nozzle, electrode surfaces etc. Outer surfaces of all internal construction elements were kept at ambient temperature of 300 K. For these surfaces we use the “coupled” boundary condition without additional heat generation on the dividing interior wall. All internal boundaries separating the gas flow with electrodes, a glass tube, a nozzle and all internal boundaries between the solid elements of the setup are thermally conductive.

Boundary conditions for the inlet zone are the mass-flow-inlet type. At the duct inlet fixed mass flow rate condition was used. The maximum inlet turbulent intensity is set to 5%. Variation of the inlet turbulent intensity in the range of moderate values of 1-5% did not affect the flow structure discernibly. The boundary conditions for the outlet zone are of the pressure-outlet type with gauge pressure equals to zero. Therefore, at the outlet, we imposed the boundary conditions with the static pressure equal to the atmosphere pressure.

2.2. Numerical procedure
The numerical simulation of the non-stationary 3D turbulent swirling flow was made using the ANSYS FLUENT 15.0 program package, which solves system (1) using the finite volume method. In our simulation, the Spalart-Allmaras model was used. A detailed analysis of the use of the turbulence models in similar problems is given in [8].

For spatial discretization of density, momentum, energy and turbulent quantities, a second-order upwind scheme is applied. The use of higher-order schemes has not changed the flow parameters considerably. The diffusion terms are central-differenced and second-order accurate. We interpolate the pressure values at the faces using the PRESTO! scheme because of the strong swirl nature of the flow.

For transient terms, we used the fully implicit scheme of the second-order accuracy. Different pressure-velocity coupling schemes were tested and gave equal results. So, we used the SIMPLE scheme as the least resource intensive. The convergence was obtained when the residual reached $10^{-6}$ for the energy equation and $10^{-4}$ for the continuity equation, the momentum equation, and the equations for turbulent quantities. The geometric modelling of the setup and the construction of the grid were carried out using the ANSYS Workbench package. The computational grid consisted of about $3\cdot10^6$ hexahedral cells, except for a small region, where the cells were tetrahedral (figure 2). The skewness metric has an average value of 0.16, while the orthogonal quality metric equals 0.94. The grid refinement did not considerably alter the gasdynamic parameters.

![Figure 2](image)

**Figure 2** The horizontal cross sections of grid region with mixed cells structure
Calculations with different values of time step from $1 \cdot 10^{-4}$ sec to $1 \cdot 10^{-6}$ sec were carried out. Finally, the time step was set equal to $5 \cdot 10^{-5}$ sec since using lower values led only to an increase in the computational time.

3. Results of numerical simulation

To a great extent, the structure of the flow is determined by the paraxial counterflow zone, typical for strongly swirled flows [8,9]. Formation of recirculation zone is shown in figure 3. Note that figure 4 demonstrates only counterflow regions. During short initial period of time, the zone of the maximum counterflow velocity is concentrated in the region directly behind the cathode. Then it moves quickly enough to the opposite part of the setup ($t = 1$ sec), and completely forms at $t \approx 5$ seconds. After that, no fundamental changes in the shape of the region and velocity values occur. Thus, a quasi-stationary flow velocity field is formed in the duct.

![Image of flow structure](image)

**Figure 3** Counterflow zone structure in a fixed cross section obtained at different time moments. The mass flow rate $m_t = 2$ g/sec, the heat source power $N = 100$ W, the static pure argon pressure $P = 10^5$ Pa

Therefore, a flow structure is characterized by the presence of a long paraxial counterflow zone with relatively low flow velocities. Use of solid electrodes leads to the formation of a counterflow with appreciably large velocity magnitudes, which in turn leads to the formation of a heat flux directed toward the swirler and its heating, as noted in [6].

A similar flow structure was described in [8], where analogous swirler and alike paraxial heat source were used, but in combination with a fully open duct. The numerical simulation is also demonstrated that as well as in [8] that a precessing vortex core (PVC) appears. The obtained PVC is the left-handed co-rotated bending single-vortex structure.

The simulation showed that combination of thin anode and pipe-like cathode leads to desirable flow structure when the pressure gradient along the symmetry axis draws out the hot gas from the interelectrode area. As a result, the formed flow structure leads to the propagation of a heat flux mainly downstream, figure 3. It should be noted that figure 4 demonstrates only regions heated to a temperature above 400 K. Comparison with previous investigation [7] did not reveal fundamental differences in flow structure because of additional heat transfer. Due to heating of electrodes and losses through construction elements, there is decrease in output heat power of up to 20%. Although being significant,
it leads only to some scaling which is manifested through lower flow temperature, at least at stages far from “saturation” when temperature of subsidiary parts becomes steady. Such process of warming-up takes much more time to complete (~30 min, [6]) than typical gasdynamics phenomena so the whole behavior of the reactor can be considered as quasi-stationary.

Thus, the considered localization and form of the electrodes allows to avoid a noticeable heating of the setup structural elements excepting the massive nickel cathode, which is heated to a temperature close to the melting point and, less, the input of the nozzle. It leads to a decrease of PVR coefficient of energy performance (COP) in comparison with the model system [6]. However, the losses in the case considered here are the smallest among the configurations described in [6].

![Figure 4](Image)  
**Figure 4** Gas temperature field at fixed time moment $t = 100$ sec. The conditions correspond to those shown in figure 3

The presented results demonstrate a qualitative agreement with the results of the experimental data. Indeed, the control of the flow mean temperature measured by thermocouple grid TP-K01 and CENTER 304 thermometer showed that the output mean temperature of argon in the presence of two solid electrodes was $T_g \sim 350$ K, whereas in the case of a combination of a thin anode and a hollow cathode located at the duct outlet, it was $T_g \sim 700 - 800$ K. These results are corresponded to the total mass flow rate $m_t = 2$ g/sec, the heat source power $N = 100$ W and the static pure argon pressure $P = 10^5$ Pa, used in numerical simulations.

4. Conclusion  
The numerical modelling has demonstrated that it is possible to configure electrodes in such a way as to ensure energy transfer mainly downstream from the interelectrode zone. It may be accomplished by the pipe-like electrode through which areas of different pressures are connected. Pressure forces draw out the hot gas towards the exit nozzle. Thereby, it can be assumed that the considered setup model is optimal for creating a compact vortex heat generator. A qualitative agreement between the results of the calculations and the experimental data for pure argon [6,7] has been obtained for the exact experimental setup.

However, the construction of effective heat and hydrogen generator remains simulation of the flow and discharge structure for real mixtures of metal, H$_2$O and Ar, taking into account the plasma-chemical kinetics of the discharge mixture components as well as thermal characteristics of the experimental setup. It should be noted in this connection that optimal condition for heat generation and hydrogen generation can differ from each other. Therefore, the next step is the self-consistent simulation of the problem.
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