57. SIMULATION OF LOW-CURRENT DISCHARGES IN ATMOSPHERIC-PRESSURE AIR

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Abstract. Models of two types of discharges in atmospheric-pressure air are developed: stationary low-current arcs and discharges in fast flows of preliminary heated gas. Results of discharge simulation are presented for a wide range of external conditions. Calculated plasma parameters are compared with available experimental data.

1. Introduction

Methods of non-thermal air plasma generation at pressures about atmospheric one have recently received increased attention. Among the sources of such plasma, low-current arcs and discharges in fast flows of preliminary heated gas are considered. In conditions when the gas temperature \( T \) in the discharge core is high enough (for arcs in atmospheric-pressure air, at \( T > 4000 \) K, see below) the plasma state is close to the local thermodynamic equilibrium (LTE). With decrease of the current, the gas temperature decreases, and the deviation of plasma state from the LTE becomes essential. In this work, models of discharges in atmospheric-pressure air are developed, that account for non-equilibrium effects. Results of simulation of two mentioned types of discharge are presented.

2. Stationary low-current arcs

Stationary discharges in air are considered, stabilised by heat conduction to the walls (when convective heat losses are relatively small). Under typical conditions the length of a discharge is much larger than its radius. It allows neglecting the axial transport terms. The discharge is assumed to have an axial symmetry.

As the discharge current decreases, non-equilibrium effects to come into play are a deviation of the electron energy distribution function (EEDF) from the Maxwellian one with the gas temperature \( T \) (more precisely, \( T \) is the translational temperature of neutral particles); a deviation of the vibrational temperature \( T_v \) of \( \text{N}_2 \) molecules from the gas temperature \( T \); effect of diffusion on species densities. Distributions of the gas temperature \( T \) and of the mean vibrational energy \( \langle E_v \rangle \) of nitrogen molecules along the radial coordinate \( r \) are governed by equations

\[
\frac{1}{r} \frac{d}{dr} \left( r \frac{d}{dr} T \right) + \eta_T \sigma E^2 + Q_{VT} = 0
\]

\[
\frac{1}{r} \frac{d}{dr} \left( n_{\text{N}_2} Dr \frac{d}{dr} \langle E_v \rangle \right) + \eta_V \sigma E^2 - Q_{VT} = 0
\]

Here \( \chi \) and \( \sigma \) are the thermal and electrical conductivity coefficients, \( E \) is the electric field, \( n_{\text{N}_2} \) is the number density of nitrogen molecules, \( D \) is the diffusion coefficient for molecules, \( \eta_T \) and \( \eta_V \) are the fractions of energy input transferred to gas heating and to vibrational excitation of \( \text{N}_2 \) molecules. The sum of \( \eta_T \) and \( \eta_V \) is assumed to be equal to unity (fractions of energy input transferred to other degrees of freedom of molecules, such as electronic excitation, etc., are negligible under conditions considered). At currents below 1 A, the gas temperature does not exceed 6000 K and radiation losses may be neglected. The term \( Q_{VT} \) describing the VT relaxation of nitrogen molecules is written in the form

\[
Q_{VT} = n \frac{\varepsilon_v - \varepsilon_v(T)}{\tau_v},
\]

where \( n \) is the gas number density, \( \varepsilon_v(T) \) is the equilibrium value of nitrogen vibrational energy, \( \tau_v \) is the time of VT relaxation. The mean vibrational energy \( \langle E_v \rangle \) is related with the vibrational temperature \( T_v \) as \( \varepsilon_v = E_{\text{N}_2}/[\exp(E_{\text{N}_2}/kT_v) - 1] \), where \( E_{\text{N}_2} \) is the vibrational quantum of \( \text{N}_2 \) molecule.

Radial distributions of the number densities \( n_k \) of plasma components of various kinds \( k \) are governed by the system of diffusion equations

\[
\frac{1}{r} \frac{d}{dr} \left( D_k r \frac{dn_k}{dr} \right) + F_k = 0
\]

Here \( D_k \) is a corresponding diffusion coefficient (the ambipolar diffusion coefficient \( D_a \) is to be taken for electrons), the source term \( F_k \) describes the net rate of generation of species of kind \( k \) in
kinetic processes of ionization, dissociation, recombination, etc.

One can expect that the diffusion terms in equations (2) and (4) are small in a certain range of discharge currents in atmospheric-pressure air, and balances of vibrational energy $\dot{e}_V$ and of the densities of plasma components may be evaluated, with a sufficient accuracy, in a local approximation. Note that conditions for locality of equations for $e_V$ and for the electron number density $n_e$ are, respectively,

$$L_V << R_{ef}, \quad L_e << R_{ef}.$$  \hspace{1cm} (5)

Here $R_{ef}$ is an effective radius of the discharge which will be defined below, $L_V$ and $L_e$ are diffusion lengths defined as $L_V = (D_W/\nu T)^{1/2}$, $L_e = (D_e/\beta_0 n_e)^{1/2}$, where $\beta_0$ is the electron-ion recombination coefficient (note that $(\beta_0 n_e)^{-1}$ is the electron-ion recombination time).

The locality of equation (2) allows one to rewrite equation (1) as

$$\frac{1}{r} \frac{d}{dr} \left( r \frac{dT}{dr} \right) + \alpha E^2 = 0. \hspace{1cm} (6)$$

The boundary conditions for equation (6) are as follows:

$$\frac{dT}{dr} = 0 \text{ at } r = 0, \quad T = T_w \text{ at } r = R. \hspace{1cm} (7)$$

Here $T_w$ is the wall temperature, $R$ is the tube radius.

In our approach, equation (6) for the gas temperature is the only differential equation of the model. Radial distributions of other parameters (the vibrational temperature of N$_2$ and species densities) are calculated using the local balance equations.

Knowledge of the thermal and electrical conductivity coefficients $\chi$ and $\sigma$ is required for a solution of equation (6). The thermal conductivity coefficient is not affected strongly by non-LTE effects, therefore the LTE $\chi$ values are used in the present calculations.

An effect of deviations from LTE on the electrical conductivity, which is proportional to $n_e$, is much more substantial. A central moment for calculation of $n_e$ is the development of a kinetic model for air plasma. A kinetic scheme used in this work includes processes with participation of N$_2$, O$_2$, N, O, NO, NO$^+$, O$^+$, O$_2^-$, and electrons. (Note that NO$^+$ is the dominating positive ion under conditions considered; all primary ions formed in ionizing collisions of electrons with air components other than NO convert quickly to NO$^+$.) The rate constants of reactions with participation of electrons are taken as functions of the reduced electric field and the vibrational energy of N$_2$ molecules. Such approach is more accurate than the use of expressions for the rate constants as functions of the electron temperature $T_e$, because in weakly ionized plasmas the form of the EEDF may differ substantially from the Maxwellian one.

In summary, the system of equations describing the discharge parameters includes differential equation (6) for the gas temperature, finite (with omitted transport term) equation (2) for nitrogen vibrational energy, a system of finite (with omitted transport terms) equations (4) for densities of each of the plasma components, and the Ohm’s law

$$I = 2pE \int_0^R \gamma(r) r dr \hspace{1cm} (8)$$

where $I$ is the discharge current.

![Fig.1. The reduced electric field at the axis versus the current. Solid lines: non-LTE simulation, dashed lines: LTE simulation.](image)

Calculations have been performed for DC discharges in atmospheric-pressure air in cooled tubes (at $T_{w} = 300$ K) with radii $R = 1$-10 mm, for the current range 0.005-1 A. In figure 1 the values of the reduced electric field at the discharge axis are shown versus the current. The dashed lines represent results obtained in the framework of the LTE model (i.e., with the use of a value of the electrical conductivity corresponding to the LTE at the gas temperature). It is seen that at currents greater than approximately 50 mA results of the non-LTE and LTE models nearly coincide, the reduced electric field increasing with a decrease of $I$. At smaller currents, values of $E/n(0)$ calculated...
with LTE model continue to grow with a decrease of \( I \), while the dependence of the values of \( E/n(0) \) obtained with account of non-LTE effects on the current becomes very weak. Figure 2 shows axial values of the gas temperature \( T \). At low currents (in non-LTE region) the gas temperature is nearly independent of the tube radius. At high currents the smaller is the tube radius \( R \) the larger is the value of \( T \).

\[
T(r=0), \text{kK}
\]

![Fig.2. The gas temperature at the axis versus the current in arc discharges in air.](image)

\[
R=1\text{mm}, \quad R=3\text{mm}, \quad R=10\text{mm}
\]

\[
I = \pi R_{ef}^2 j(0),
\]

where \( j(0) = \alpha(0) E \) is the current density at the discharge axis. It is seen that \( R_{ef} \) non-monotonously changes with the current and increases with the tube radius. In figure 4 the relation is given between the axial values of the electron number density and of the gas temperature (the latter being dependent on the current, as shown in figure 2). The equilibrium, at the gas temperature, values of \( n_e \) are also shown. Deviations from equilibrium manifest themselves at low enough values of \( T(0) \). The larger is the tube radius, the smaller is the value of \( T(0) \) corresponding to the boundary between the LTE and non-LTE discharge regimes.

\[
\log_{10} n_{e}(r=0), \text{m}^{-3}
\]

![Fig.4. The electron number density at the axis versus the gas temperature at the axis of arc discharges in air. Points: equilibrium \( n_e \) values.](image)

In figure 3 the effective radius of the discharge \( R_{ef} \) is shown, defined according to the expression

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![Fig.3. The effective radius of the discharge versus the current.](image)

The transition from the LTE to the non-LTE plasma state with decrease of the discharge current is related with the change of the ionization mechanism. At high currents, when the gas temperature is rather high, the dominating process of production of electrons is the associative ionization \( N + O \rightarrow NO^+ + e \). Its rate is determined by the value of the gas temperature and does not depend on \( T_e \). With decrease of the current the reduced electric field increases and reaches a value at which the rate of ionization of gas particles by electron impact exceeds the rate of associative ionization. The change of the dominating ionization process marks a transition from LTE to non-LTE plasma state.

The model described above has been developed for discharges in tubes. DC discharges with free boundaries (without walls) have been studied in the available experiments: low-current arc discharges between parallel electrodes, with liquid [1,6], plasma [3] or metal [5] cathodes, and gliding arcs [2,4]. The heat losses were due to convection under conditions of these experiments.
Therefore, a direct comparison of the simulation results with the experimental data is not possible. Still, some common features exist between discharges stabilised by walls and those stabilised by convection. In both cases the discharge volume includes two regions: a central conducting zone (a core) of the radius $R_{cf}$ and an outer region. In both cases the heat transfer from the discharge core to the outer region is due to thermal conduction, and the central part of the discharge may be described by means of the above model. Thus, with a proper choice of the $R_{cf}$ value, the model is applicable to discharges stabilised by convection.

In figure 5 calculated values of the electric field are compared with those measured in [1-6]. (Note that the radius of conducting zone $R_{cf}$ changes in the range 0.2-1 mm under conditions of these experiments, values of the tube radius $R$ corresponding to these $R_{cf}$ data being between 1 and 10 mm, see figure 3). Simulation results obtained using the equilibrium electrical conductivity are also shown. It is seen that the measured values of $E$ agree with the results of non-LTE calculations.

3. Discharges in fast flows of preliminary heated air

In experiment [7] a DC discharge was organised in a fast longitudinal flow, directed from the cathode to the anode, of atmospheric-pressure air preliminarily heated to temperatures $T_0$ in the range 1800-2900 K. In general, an accurate description of such kind of discharge should be based on two-dimensional hydrodynamic simulation. However, estimates show that in conditions [7] (at the residence time of the gas in the discharge region $\tau_{flow} = 7.8 \times 10^{-5}$ s and the radius of the discharge column $R_c = 0.16$ cm) the relations take place

$$(D\tau_{flow})^{1/2} << R_c, \quad (D\tau_{flow})^{1/2} << R_c$$  

It follows from (10) that the heat losses and transport of particles in radial direction may be neglected. The residence time in conditions [7] is of the same order or even smaller than times of establishment of quasi-stationary densities of species, corresponding to the local values of the gas temperature $T$ and the reduced electric field $E/n$. Moreover, at the upper values of the current density $j$ reached in [7] the gas temperature, due to Joule heating, increases with the axial coordinate $x$. Therefore, it is necessary to account for the change of plasma parameters (the electric field, the gas temperature, the mean vibrational energy $\gamma_T$ of nitrogen molecules, the densities of species) with $x$. The distributions of $T$, $\gamma_T$ and number densities $n_k$ of species of various kinds $k$ are governed by the balance equations

$$\rho C_v^* \frac{dT}{dx} = \eta_T \sigma E^2 + Q_{VT}$$  

$$n_{N_2} \frac{d\gamma_T}{dx} = \eta_T \sigma E^2 - Q_{VT}$$  

$$\frac{d[(V - \mu_k) n_k]}{dx} = F_k$$

Here $\rho$ is the gas density, $C_v^*$ is the heat capacity at constant gas pressure, calculated without account of vibrational excitation of $N_2$ molecules, $V = d\tau_{flow}$ is the gas flow velocity ($d$ is the gap length, in conditions [7] equal to 3.5 cm), $\mu_k$ is the mobility of charged species of kind $k$ (with account of sign of the species charge). The system of equations includes also the Ohm’s law

$$j = \rho \eta_T \sigma E$$

where the discharge current density $j$ is taken independent of $x$ (as, according to [7], the radius of discharge column does not change noticeably with $x$).

A kinetic scheme is used the same as for arc discharges (see above). The parameter $\eta_T$ in equation (11) includes both the heating in elastic collisions and due to fast rotational-translational relaxation of $N_2$ and $O_2$ and VT relaxation of oxygen molecules. At values of the reduced electric
field $E/n = 40-60$ Td realised in conditions [7] this parameter may be estimated as $\eta_T \sim 0.03-0.05$ (e.g., [8], figure 5.14). The sum of $\eta_T$ and $\eta_V$ is taken equal to unity.

In most of conditions [7], with the exception of low-current regimes at $T_0 = 2900$ K, the values of $n_e$ inside the discharge column exceed substantially those corresponding to the equilibrium at $T_0$. Hence, an enhancement of $n_e$ takes place in the cathode part of the discharge. Our calculations start at the point $x = 0$ corresponding to the beginning of the discharge column, just after the cathode part of the discharge. Plasma in the column is quasi-neutral, the number density of electrons $n_e$ being nearly equal to the number density of positive ions $n_p$ (in conditions considered the total number density of negative ions is much smaller than that of electrons). From equation (14), with account of the electron mobility dependence of the electric field $|\mu_e| \sim E^\gamma$ (for air $\gamma = 0.2$), one obtains that the product $n_eE^{1-\gamma}$ is independent of $x$. It allows rewriting equation (13) for positive ions as the equation that governs distribution of the electric field along $x$:

$$\frac{dE}{dx} = -\frac{EF_p}{n_p[\gamma \mu_p E + (1-\gamma)F_p]}$$

(15)

(here $\mu_p$ and $F_p$ are the mobility and the source term for positive ions). To obtain the initial condition for equation (15), we assume that the reduced electric field $E/n$ at $x = 0$ has some value $E/n(0) = 100-200$ Td, intermediate between relatively low $E/n$ values (Note that variation of $E/n(0)$ inside this interval influences the calculated discharge parameters only in a very thin region near $x = 0$.) Corresponding $n_e$ value is determined by equation (14). In cases when thus estimated $n_e$ appears to be smaller than that equilibrium at $T_0$, the latter value is used, and corresponding electric field value is calculated using equation (14). Number densities of negative ions are calculated using local balance equations (such approach is justified due to high rates of detachment in conditions considered).

The change of $T$ and $\varepsilon_V$ due to the energy input in the cathode part is neglected, and at $x = 0$ the values of $T$ and $\varepsilon_V$ are taken those determined by preliminary heating: $T(0) = T_0$, $\varepsilon_V(0) = \varepsilon_V(T_0)$. The change of the densities of neutral species in the cathode part is also neglected, their values at $x = 0$ are taken equilibrium at $T_0$.  

![Fig.6. The reduced electric field distribution along the discharge axis at $j = 2$ A/cm$^2$.](image)

![Fig.7. Distributions of the gas and vibrational temperatures along the discharge axis at $j = 2$ A/cm$^2$.](image)

![Fig.8. Distributions of the molar fraction of O atoms along the discharge axis at $j = 2$ A/cm$^2$.](image)
In figures 6-9 axial distributions of plasma parameters are shown, calculated at various values of \( T_0 \) for current density \( j = 2 \) A/cm\(^2\). The reduced electric field \( E/n \) (figure 6) tends to reach, at some distance from the cathode, a value, independent of \( x \), that provides a balance of loss of charged particles due to electron-ion recombination and their production due to ionization of neutral particles by electron impact. Increase of \( T_0 \) results in decrease of \( E/n \). The gas and vibrational temperatures given in figure 7 increase with \( x \). Note that the change of parameter \( \eta_T \) in the range 0.03-0.05 does not influence noticeably the rate of increase of \( T \) with \( x \), because the major source of gas heating is VT relaxation of nitrogen molecules. At large distances from the cathode the values of \( T_V \) are larger at smaller \( T_0 \).

The molar fraction of O atoms shown in figure 8 increases with \( x \), the rate of increase being faster at smaller \( T_0 \). The electron number density (figure 9) increases steeply at small \( x \), in the high-field region, and saturates at the region where the balance of loss and generation of charged particles is reached. The total number density of negative ions decreases with \( x \), due to accumulation of O atoms that effectively destroy negative ions. Note that at \( T_0 = 1800 \) K the process of recombination of negative and positive ions influences substantially the balance of generation and loss of charged particles.

In figure 10 the mean electric field \( \langle E \rangle \), calculated as \( \langle E \rangle = \frac{1}{d} \int_0^d [E(x)] dx \), versus the current density \( j \) is shown, both measured in [7] and obtained by simulation. It is seen that at current densities higher than 0.1 A the calculated electric field agrees with the experiment. At \( j < 0.1 \) A and \( T_0 \leq 2500 \) K, calculated \( \langle E \rangle \) values are nearly independent of \( j \), while the measured field, at 2300 and 2500 K, decreases with \( j \), similarly to the case at 2900 K. At \( T_0 = 2900 \) K the decrease of \( \langle E \rangle \) at low \( j \) is due to relatively high equilibrium electron number density, sufficient to provide required electrical conductivity \( \sigma \) without additional (non-equilibrium) gas ionization by electron impact. (Note that the shift between calculated and measured at 2900 K values of \( \langle E \rangle \) in low current region may be eliminated, if at calculations the value \( T_0=3050\)K is used). However, at temperatures 2300 and 2500 K the equilibrium ionization degree of air is very low, far from being sufficient to provide required \( \sigma \) values at currents 0.01-0.03 A.

A possible cause of the decrease of \( \langle E \rangle \) with \( j \) at \( T_0 = 2300-2500 \) K could be a presence, in experimental conditions [7], of uncontrolled admixtures with low ionization potentials (e.g., vapors of metals). At these temperatures, admixtures could provide electrons at densities substantially higher than those corresponding to the equilibrium ionization degree of pure air. The effect of enhanced, due to admixtures, equilibrium ionization is shown in figure 10, where the results of calculations for \( T_0 = 2300 \) K are presented, obtained in assumption that the equilibrium ionization degree is equal to \( 7 \times 10^{-9} \). It is seen that the use of this assumption allows obtaining \( \langle E \rangle \) values close to those measured in [7].
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References