Numerical Modeling of Pulse-Periodic Nanosecond Discharges

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Abstract. The first results of the numerical simulation of the Pulse-Periodic Nanosecond discharge in pin-to-pin configuration in 2D approximation of the full self-consist system of Navier-Stocks equation for real thermo-chemically non-equilibrium gases, drift-diffusion approximation of the low temperature plasma evolution in external electric and magnetic field and, alternative – arc (spark) discharge model of high-density energy input discharge. The intuitive criteria of the alternative discharge models re-switch are proposed and tested. The pin-to-pin the pulse-periodic nanosecond 5-MHz discharge has been considered for 1 microsecond interval. It was found that rather strong longitudinal non-uniformities of main physical parameters are created at the first corona stage of the interelectrode conducting channel. These nonuniformities reveal long-lived features that have define strong effect on the discharge performance.

1. Introduction

Pulsed electric discharges of various types are widely used as initiating and controlling means in a variety of thermochemical processes; they create rapid local heating of the working mixture to the required temperatures (such as, for example, spark plugs in internal combustion engines) or non-equilibrium production of chemically active radicals, triggering chemical ignition reactions. Even though this kind of technology has been successfully used for many decades, modern environmental restrictions force us to look for ways to optimize electric discharge initiation, mainly in order to reduce the production of various harmful impurities.

Spatial and temporal multiscale is a significant obstacle in attempts to clarify the entire sequence of the process. This work is aimed at developing an approach to obtain quantitative characteristics of both the gas-discharge (fast) stage and the subsequent thermochemical kinetics and gas-dynamic stages. At the same time, it is necessary to control processes with characteristic time from subnanoseconds to units of milliseconds. At this initial stage of the approach development to obtaining the integral characteristics necessary for the practice of the initiation process under consideration by igniting the fuel-air mixture by one or another electric discharge method, we will consider as an objective function obtaining data for the conditions of the process, which we considered earlier [1,2]. Accordingly, the developed numerical model consists of components of the PlasmAero package [3] and is based on the experience of its usage for plasma aerodynamics [4,5,6,7,8]. The main components were previously tested on available experimental data. There was achieved an acceptable qualitative and, to a large extent, quantitative agreement of the calculation and the experiment with a high-voltage nanosecond pin-to-plane discharge on a 16 mm interelectrode gap described in [9]. The stage-by-stage
2. Problem Formulation

An axisymmetric pulse-periodic nanosecond discharge between two coaxial conical electrodes in air is considered at atmospheric pressure and temperature. Figure 1 schematically shows the calculated domain, which is a meridional section with a radius of 0.7 mm and a longitudinal dimension of 2.4 mm. In this section there are symmetrically arranged cylindrical electrodes with a radius of 0.25 mm and conical tips. The 75 μm long equipotential current collecting electrode sections are adjacent to the top of the cones. The distance between the vertices of the conical electrodes is 1 mm.

The discharge is initialized and maintained by a pulse-periodic voltage applied to the electrodes. The pulse shape qualitatively approximates the pulse shapes in experiments [9-11] by a linear function modulated by exponential decay:

\[ V(t) = V_0 \frac{t}{t_0} \exp\left(-\frac{t}{t_0}\right), \]

where \( V_0 \) is the amplitude and \( t_0 \) is the rise time. In this work, as a rule, values of 6 kV and 1 ns were used, respectively.
Numerical modeling is performed using PlasmAero package for self-consistent solution of the equations: (1) Navier-Stokes for real chemically nonequilibrium air; electric discharge models in (2) diffusion-drift or, alternativity, (3) magnetogasdynamic (arc) approximations; (4) 11-component kinetic model of ionized air in the strong electric field. Radiative energy transfer was taken into account in the framework of the effective emissivity model. The system of equations, the system of boundary conditions, specific details of physical-chemical processes in the air in the presence of strong electric fields (up to several hundreds of Td) are described in detail in our previous publications [1-8].

Bearing in mind that at this stage, firstly, qualitative estimates of the effects should be obtained, we used robust grids of 200×63, which of course did not provide an adequate description of thin near-electrode layers near the vertices of the conical electrodes. Also in this model, focused on the analysis of relatively long processes (on the scale of nanosecond fronts), there is no accounting for photoionization, which may affect the dynamics of the positive streamer of the first pulse. It should be noted that the initial condition used here and in many of our works earlier with homogeneous background ionization at the level of $N_i = N_e = 10^9$ m$^{-3}$ ensures the initialization of the discharge at the points already when the pick electric field reached 1–2 kV/mm.

The target characteristics of the process under consideration are the evolution of the total currents to the electrodes, the total power and energy released, and the total amount of the active radical (atomic oxygen). In addition, the evolution of the local parameters distributions, in particular, the chemical composition is also of interest.

3. Process description

After the voltage is applied to both electrodes, the development of a capacitive discharge begins, which, as a result of the polarization of the initial extremely weakly ionized medium, quickly (depending on the geometry of the electrodes and the rate of voltage rise) forms near-electrode space charge layers on the equipotential portions of the electrodes. In the considered formulation of numerical simulation, when the voltage across the gap reaches about 2 kV/mm almost simultaneously both on the cathode and anode sides, “breakdown” of the near-electrode layers occurs, and ionization waves begin to form. The main phase of the "streamer" discharge, which takes time from the initial breakdown to the collision of ionization waves, is presented in Figure 2, which shows distributions of potential (level lines) and of the current density (vectors).

The collision of ionization waves under these specific conditions occurs near the maximum of the applied voltage. The interaction of ionization waves creates conditions for the complete closure of the interelectrode gap. Figure 3 shows the beginning of the current pass at this phase of discharge development.

During tens of picoseconds the interelectrode conducting channel formation is completed and the degree of deviation from quasi-neutrality becomes less than one percent, which makes it possible to switch the numerical integration from the drift-diffusion mode to a much more computationally efficient arc mode. Here, as a criterion for changing the model, the intuitive condition of the currents equality at the electrodes obtained by each of these models was used. Figure 4 shows the current and potential evolution of the electrodes at the initial stage of the discharge formation. In the case under consideration the switching between models occurs near the voltage extremum. Hereafter, during the sustaining of the voltage applied (from tens to hundreds of volts), the arc model works in a regular mode. After that the numerical integration time step is regulated by the stability conditions of chemical kinetics and gas dynamics. De facto, this strategy allows us to reduce drastically the time costs of simulation to acceptable level.
Figure 2. Propagation of ionization waves.

Figure 3. Impact of ionization waves.

Figure 5 shows the evolution of currents and voltage during the passage of five pulses of a 5 MHz pulse-periodic discharge. The main result of the discharge operation is represented by the graph in Figure 6: the increase in the amount of dissociated oxygen over time due to energy input.
Figure 4. Evolution of electrode current and potential during 1st voltage pulse.

Figure 5. Cathode current and potential during full simulation time.
4. Discussion

The first stage of modeling the discharge channel formation is essentially a way to set up the initial conditions for the subsequent stages of determining the long-term characteristics changes in the state of the working medium by an electric discharge based on the quasi-neutral plasma model. It should be noted that one of this work motivations was to study the fuel-air mixture activation by the capacitive discharge influence, which is characterized by a significantly lower level of energy input. In this regard the considered configuration meets to a greater extent the operating conditions of an automotive spark plug [10], in which the main energy supply occurs precisely at the electrode spark discharge stage. The peculiarity of the formulation given here can be seen from the graphs presented in Figure 6 and with the selected first pulse initial time interval in Figure 7. The plot shows that the radical production practically stops by the third nanosecond, although the power supply capacity is still significant. Also it can be seen that the contributions of capacitive and spark (arc) discharges are close to each other in the main part of the radical production time interval (< 3 ns). At the same time, the ongoing energy supply from the spark discharge does not give a significant result.

![Graph showing O-production characteristics](image-url)

**Figure 6.** O-Production Characteristics.
Note those chemical transformations (changes in composition) are relatively slow in the considered time range. The initial section of the radical operating time curve significantly lags behind the growth of the energy supply, and, in addition, it can be seen from the graphs in Figure 6 that the amount of radical (as well as the composition of the medium as a whole) practically does not change. This leads to the fact that the subsequent pulse acts to the working media that "remembers" the impact of the previous one. As a result, the electron concentration increases from pulse to pulse and so the conductivity increases, which at the same voltage entails an increase in the power input. This effect is clearly visible in Figure 6, where the power of each pulse increases exponentially. An attempt to "manually" maintain the stability of the calculation by reducing the amplitude of the 4th pulse by 15% proved ineffective - on the 5th pulse, the solution entered the non-physical region due to overheating.

To prevent the occurrence of such problems, it is necessary to carefully describe the internal circuit of the power supply, which, as a rule, in laboratory conditions have limitations on the realized power at a load with a low input impedance.

Note that despite the discharge gap small size, the longitudinal unevenness is remarkably high and can be orders of magnitude. This fact follows from Figure 8 and Figure 9 with the distribution of the composition in the charged and uncharged components of the model air.

Figure 7 O- Production Characteristics at the 1st pulse interval.
Figure 8. Axial distribution of charged particle at time = 200 ns (just before the 2nd Pulse).

Figure 9. Axial distribution of non-charged particle at time = 200 ns (just before the 2nd pulse).
Significant longitudinal distributions inhomogeneities even in the interelectrode gap outside the direct influence zone of near-electrode processes most likely are the influence result of the ionization wave passage in rapidly changing external conditions. Thus we see the need for a neat formation of charged particles initial "seed" distributions to provide pulse discharges deterministic initialization.

Figure 10 shows the molar fraction distributions of the of atomic oxygen and the velocity vector initiated by the energy supply inhomogeneity and, thereby, the inhomogeneity of pressure. Naturally, much longer time intervals are required for the convective transport effects to manifest, the presented result confirms the possibility of significant contribution to the kinetics of targeted chemical transformations. This circumstance is even more noteworthy because the heterogeneity scale of the active radical distribution is large, which is also evident from the above results.

![Figure 10](image)

**Figure 10.** O-Radical Mole Fraction distribution at the latest time moment of this study (~ 800 ns) and Flow Velocity Vector.

5. Conclusion

The paper presents the first results of end-to-end modeling of a multiscale fuel-air mixture activation process by pulsed periodic discharge with a nanosecond voltage rise on coaxial conical electrodes. At a carrier frequency of 5 MHz, the active discharge phase lasts for about 10 ns at the selected pulse shape. The possibility of coordinated usage of alternative gas discharge processes models based on models of pulsed corona and spark (arc) breakdown of the interelectrode gap is demonstrated. The "intuitive" criterion of switching between alternative models used in the work has demonstrated its operability, but still requires strict justification.

At this preliminary stage we used a simplified version of the working medium – an 11-component air model with reduced kinetics based on 103 chemical reactions, including several "field" ones with the reduced field as the main energy argument.

The implemented calculation of the 5-pulse time interval (~ 800 ns) showed the importance of forming a significant inhomogeneity along the discharge gap axis even away from the conical electrodes vertices. Inhomogeneities are very conservative and for this reason have an impact on the consequences of subsequent impulses. In this regard, it does not seem indisputable to create initial conditions based on a "plasma seeds" for the fast initiation of pulsed discharges.

At the next stage, we plan (1) to clarify the criterion for switching between discharge models, (2) to set up numerical experiments with the kinetics of fuel-air mixtures, (3) to continue research with the pulse-periodic corona.
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