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One-dimensional simulation of nitrogen dielectric barrier discharge driven by a quasi-pulsed power source and its comparison with experiments

K.-W. Cheng^a, C.-T. Hung^a, M.-H. Chiang^a, F.-N. Hwang^b, J.-S. Wu^{a,*}

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ABSTRACT

Parallel-plate nitrogen dielectric barrier discharge (DBD) driven by a quasi-pulsed power source (60 kHz) is simulated using a fully-implicit 1D self-consistent fluid modeling code. Simulated discharged currents of gap distances (0.5, 0.7 and 1.0 mm) agree very well with measured data; while simulated discharged currents of wider gap distance (1.2 mm) fail to reproduce the measured data. It is found that the discharge mode is homogeneous Townsend-like for the former case; while it is filamentary-like for the latter case based on the experimental observation. These findings demonstrate that previous numerical studies showing mode transition by changing the gap distance may require further investigation.

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1. Introduction

Types of non-equilibrium atmospheric-pressure plasma (APP) are generally classified based on the power sources, which may include radio frequency (RF) capacitively coupled discharge, AC dielectric barrier discharge (DBD) and microwave discharge. Among these, nitrogen parallel-plate DBD driven by AC power supply (10–100 kHz) may represent one of the most attractive discharges because of: 1) its easier implementation, 2) low cost of nitrogen, and 3) numerous applications. Nitrogen DBD is much easier to sustain as compared to the air or oxygen since the latter is basically an electronegative discharge, which is comparably difficult to sustain. In addition to experimental diagnostics, the fluid modelling has been proved to be a very useful and cost effective tool in understanding the APP physics and chemistry of nitrogen discharges [1]. There have been relatively few numerical studies using 1D fluid modeling for simulating nitrogen DBD [2,3].

Thus, in this paper we intend to simulate the parallel-plate nitrogen DBD driven by a realistic quasi-pulse voltage waveform (60 kHz), through the use of a one-dimensional fluid modelling code, by focusing on the effect of gap size by comparing with experimental data and to elucidate the underlying physics based on the simulation data.

2. Fluid modeling equations and solution algorithm

In the framework of fluid modeling, we have considered electron continuity equation with drift-diffusion approximation, ion continuity equation with drift-diffusion approximation, neutral species continuity equation, electron energy density equation and Poisson's equation for electrostatic distribution. Details of these equations can be found in [1]. Note we neglect flow convection effects in the present study. Drift and diffusion coefficients and rate constants related to electrons, which are functions of electron temperature [4], are prepared as a lookup table in the computer code. We have applied a fully implicit numerical scheme to solve the finite-difference discretized equations. Detailed description is skipped here and can be found elsewhere [5].

3. Results and discussion

The nitrogen plasma chemistry employed in the present study includes 9 species (electron, N₂, N₂⁺, N₄⁺, N₂($X^1\Sigma_g^+$, v=1-8), $N_2(A^3\Sigma_u^+)$, $N_2(B^3\Pi_g)$, $N_2(C^3\Pi_u)$, $N_2(a'^1\Sigma_u^-)$) and 31 reaction channels. This set of nitrogen plasma chemistry includes direct ionization (1), excitation into excited, metastable and vibration states (5), de-excitation (6), recombination (3), associative ionization (3), light emission from excited, metastable states (4) and excitation into vibration states (10). Note we have ignored the N⁺ and N₃⁺ in the simulation since they have been found to unimportant in nitrogen plasma simulation [2].

Fig. 1 shows that comparison of simulated and measured discharged currents of nitrogen DBD driven by a quasi-pulsed power

^a Department of Mechanical Engineering, National Chiao Tung University, Hsinchu, Taiwan

^b Department of Mathematics, National Central University, Chung-Li, Taiwan

^{*} Corresponding author. Tel.: +886 3 5712121 31693; fax: +886 3 6110023. E-mail address: chongsin@faculty.nctu.edu.tw (J.-S. Wu).

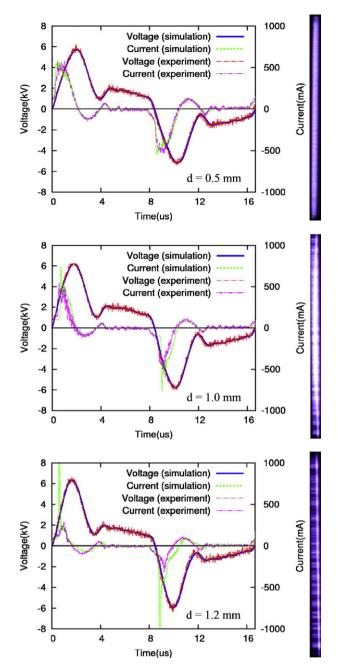


Fig. 1. Comparison of simulated and measured discharged currents along with photo images of discharge at the right.

(60 kHz) for different gap distances (0.5, 0.7, 1.0 and 1.2 mm) along with the experimental photo images (0.2 s exposure time) of discharge on the right. Note the measured relative permittivity and thickness of the ceramic material is 11.63 and 1 mm, respectively. Details of the experiment will be published else in the near future and are skipped here due to the page limit. In general, the simulations agree very well quantitatively with the experimental data for the cases of d = 0.5 and 0.7 mm (not shown), but begin to deviate slightly from the measurements as d = 1.0 mm and exhibit large discrepancy with the measurements as d = 1.2 mm. For the cases of smaller gap (0.5 and 0.7 mm), the simulations demonstrate they are typical homogeneous Townsendlike discharges with much fewer electrons than ions (not shown here). For the d = 1.0 mm case, the discharge begins to be more filamentary-like with high number density of microdischarges. The simulations still agree with the measurements reasonably well. In

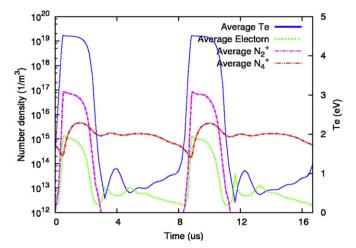


Fig. 2. Spatial-average temporal discharge properties of nitrogen DBD (60 kHz, d = 0.7 mm)

the $d=1.2\,$ mm case, the simulation shows it is a glow-like discharge (quasi-neutral in the bulk) with very high current density during the breakdown phase. However, this is obviously against the measurements. This is attributed to the fact that the discharge has transitioned from Townsend-like to filamentary-like, as shown in the photo images in Fig. 1, which makes the 1D fluid modeling invalid. Note the measure current shows no sign of filamentary-like phenomena, probably because of relatively low number density of the microdischarges. This shows that one has to be very cautious about the use of one-dimensional fluid modeling for simulating parallel-plate nitrogen DBD. To capture the correct physics with a larger gap, one should employ at least two-dimensional fluid modeling, which is currently in progress and will be reported elsewhere in the near future.

Fig. 2 shows the spatial-average temporal discharge properties as d=0.7 mm. Results clearly demonstrate that the total number density of ions (N_2^+ and N_4^+) is always larger than electron number density throughout a cycle. The simulated electric field across the gap is almost linear without any distortion by the charge density at all times during a cycle (not shown here). Both the above two phenomena show that this is a typical Townsend-like discharge. In addition, N_2^+ is found to be most abundant during the breakdown process (same period of those current peaks in Fig. 1), while N_4^+ is found to be dominant after the breakdown caused by the associative ionization of excited/metastable nitrogen species.

4. Conclusion

We have simulated the parallel-plate nitrogen DBD driven by a quasi-pulsed power source (60 kHz) using a self-consistent one-dimensional fluid modeling code. Simulations agree very well with experimental data for smaller gaps ($d=0.5-1.0\,$ mm) (homogeneous Townsend-like), but deviate greatly from the measurements for larger gap ($d=1.2\,$ mm) (filamentary-like). Experimental photo images show that the use of one-dimensional fluid modeling for larger gap is invalid. This shows that 1D fluid modeling of nitrogen needs to be cautious without the validation of experiments.

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