Comparison of the classical integral model with Eddington approximation and Helmholtz equation based models for photoionization produced by non-thermal gas discharges in air

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This paper presents extensions of computationally efficient models of photoionization produced by non-thermal gas discharges in air based on the Eddington approximation to the radiative transfer equation proposed recently by Ségur et al. [2006], and on the effective representation of the classic integral model for photoionization in air developed by Zheleznyak et al. [1982] by a set of three Helmholtz differential equations proposed recently by Luque et al. [2007]. The validity of the developed models is demonstrated by performing direct comparisons of the results from these models and results obtained from the classic integral model. Specific validation comparisons are presented for a set of artificial sources of photoionizing radiation with different Gaussian dimensions, and for a realistic problem involving development of a double-headed streamer at ground pressure.

1. Introduction

The filamentary streamer discharges at atmospheric pressure have received renewed attention in recent years due to their ability to enhance the reactivity of gas flows for various applications [1, and references therein]. On the other hand, about a decade ago large-scale electrical discharges were discovered in the Earth's atmosphere above large thunderstorms, which are now commonly referred to as sprites. It is interesting to note that the decametre filamentary structures observed in sprites are the same as streamer discharges at atmospheric pressure only scaled by reduced air density at higher altitudes [2, and references therein].

In streamer modeling, the accurate and efficient evaluation of the effects of photoionization remains one of the most challenging tasks. In this work, we discuss several models based on differential equation approach currently proposed in the literature for the calculation of the photoionization term [3,4], and we develop improved models based on the same principles by more accurately accounting for the spectral dependence of the photoionization.

2. Model formulation

2.1. Classical integral model for photoionization in air

In the widely used model derived by Zheleznyak et al. [5] for photoionization in air, the photoionization rate at point of observation $\vec{r}$ due to source points emitting photoionizing UV photons at $\vec{r}\,'$ is

$$S_{\mathrm{ph}}(\vec{r}) = \iiint_{V'} \frac{I(\vec{r}\,')g(R)}{4\pi R^2} dV' \qquad (1)$$

where $R=|\vec{r}-\vec{r}\,'|$. In this model, to simplify calculations, the production of photons I in (1) is assumed to be proportional to the ionization production rate S_i. Zheleznyak et al. proposed a simple analytical expression for the function $g(R)$ with coefficients derived from the comparison with experiments [6,7]. This model agrees well with results of more recent experiments [8, and references therein]. The calculation of the photoionization source term with equation (1) at a given point of the volume studied requires a quadrature over the complete volume of the discharge. Therefore, the calculation of the photoionization source term in streamer discharges is computationally expensive.

2.2. Helmholtz models for photoionization in air

Luque et al. [4] have recently proposed a novel approach allowing to effectively replace the calculation of the integral (1) of the classic photoionization model with a solution of a set of Helmholtz differential equations. The two-exponential fit provided in [4] has been applied to low pressure experimental data of Penney and Hummert [6]. In this work, we propose to work directly on the function $g(R)/R$ derived by Zheleznyak et al. and to fit this function with a sum of two and three exponents. The two-exponential fit was performed for the range $1<p_{O2}R<60$ Torr cm (where p_{O2} is partial pressure of O_2 in air), which directly corresponds to the $p_{O2}R$ range shown in Figure 3 of [5]. The three-exponential fit was performed for the range $1 < p_{O2}R < 150$ Torr cm. The function $g(R)/p_{O2}$ is shown in Figure 1, with the two fits. For $p_{O2}R>1$ Torr cm, we note that with a three-exponential fit, the agreement with Zheleznyak model is generally improved in comparison with the two-exponential case, but it is very difficult to fit this function even with three exponents at $p_{O2}R<1$ Torr cm.

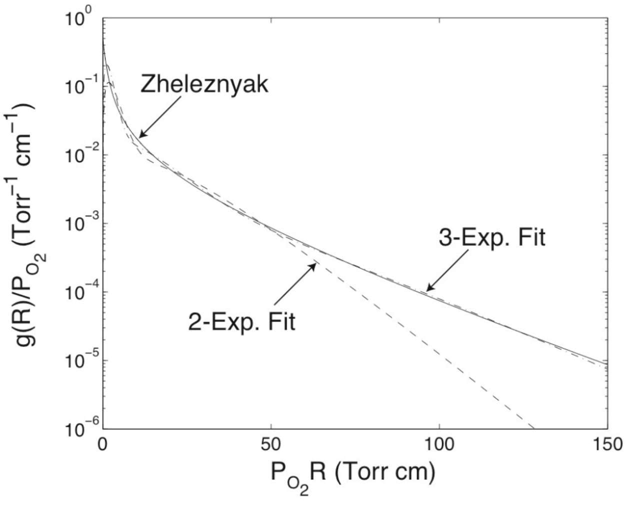

Figure 1 : Solid line: The $g(R)/p_{O2}$ function from the model of Zheleznyak et al. [5]. Dashed line: Two-exponential fit. Dot-dashed line: Three-exponential fit.

2.3. Eddington models for photoionization in air

In [3], the photoionization source term $S_{\text{ph}}(\vec{r})$ is calculated using direct numerical solutions of the first order (Eddington) and the third order (called SP3 in [3]) approximations of the radiative transfer equation. Ségur et al. [3] introduce a simple monochromatic approach (we refer to it as one-group method in the following) and derive the physical parameters required for applying this method to calculate $S_{\text{ph}}(\vec{r})$ for non-thermal gas discharges in air at atmospheric pressure by making the model results as consistent as possible with the classical Zheleznyak model. In order to achieve a better agreement with the Zheleznyak model for the Eddington and SP3 approximations, we consider N_g effective monochromatic radiative transfer equations. To use this approach in air, we have compared the photoionization source term given by this approach and the one derived from the Zheleznyak integral model. Both approaches are in excellent agreement, if the function $g(R)/p_{O2}$ is represented by a sum of three exponents (i.e., $N_g=3$).

Figure 2 shows the function $g(R)/p_{O2}$, the three-exponential fit derived in this paper and the one-exponential fit proposed in [3] for the range $1 < p_{O2}R < 150$ Torr cm. It appears that the three-exponential fit allows to have an excellent agreement with the function $g(R)/p_{O2}$, which is much better than the one-exponential fit, in particular for large $p_{O2}R$ values. It is interesting to note that, in the $p_{O2}R$ range shown in Figure 2 the fit obtained using a three-group method is generally more accurate than the one obtained using a three-exponential Helmholtz model (Figure 1).

Finally, using the first order Eddington approximation of the radiative transfer equation, we obtain a set of three elliptic equations which can be solved to derive the photoionization source term. In this work, we will present only results for the first order Eddington model. Discussions and results for the SP3 approximation are given in [9].

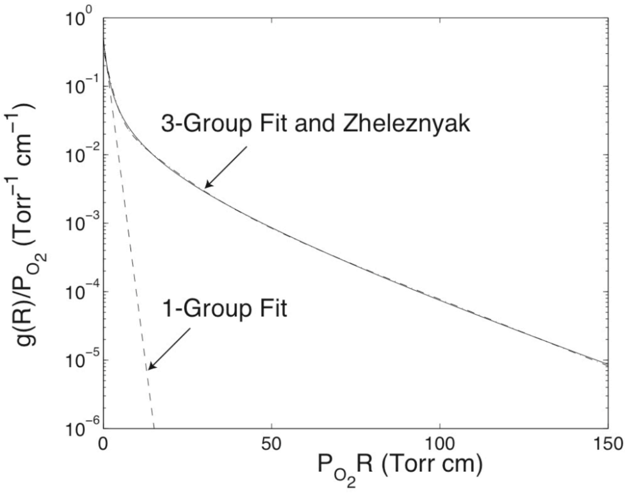

Figure 2 : Solid line: The $g(R)/p_{O2}$ function from the model of Zheleznyak [5]. Dashed line: One-exponential fit given in [3]. Dot-dashed line: Three-exponential fit.

2.4. Streamer equations

The most common and effective model to study the dynamics of streamers is based on the following drift-diffusion equations for electrons, positive and negative ions (identified below with subscripts 'e', and 'p' and 'n', respectively) coupled with the Poisson's equation [10]:

$$\frac{\partial n_e}{\partial t} + \vec{\nabla}\cdot n_e\vec{v_e} - \vec{\nabla}\cdot(\overline{\overline{D}}_e\cdot\vec{\nabla}n_e) = S_{\text{ph}} + S_e^+ - S_e^-$$

$$\frac{\partial n_p}{\partial t} = S_{\text{ph}} + S_p^+ - S_p^-$$

$$\frac{\partial n_n}{\partial t} = S_n^+ - S_n^-$$

$$\nabla^2 V = -\frac{q_e}{\epsilon_0}(n_p - n_n - n_e)$$

where n_i is the number density of species i, V is the potential, $\vec{v_e}=-\mu_e\vec{E}$ ($\vec{E}$ being the electric field) is the drift velocity of electrons, $\overline{\overline{D}}_e$ and μ_e are the diffusion tensor and the absolute value of mobility of electrons, respectively, q_e is the absolute value of electron charge, and ε_0 is permittivity of free space.

The S^+ and S^- terms stand for the rates of production and loss of charged particles. The S_{ph} term is the rate of electron-ion pair production due to the photoionization in a gas volume.

3. Results and discussion

3.1. Gaussian photoionization source

In this subsection, a simple model source of photoionizing radiation is used to compare the two and three-exponential Helmholtz, the one and three-group Eddington models with the integral model proposed by Zheleznyak et al. The Gaussian ionization production rate S_i is defined by:

$$S_i(r_s, z_s) = S_{i0} \exp(-(z_s - z_0)^2/\sigma^2 - r_s^2/\sigma^2)$$

where z_0 is the axial position of the source term, σ is the parameter controlling effective spatial width of the source, and $S_{i0}=1.53\times10^{25}$ cm^{-3} s^{-1}. We have performed calculations for different simulation domain sizes [9]. In this report, we present results for $L_d \times R_d=0.2 \times 0.2$ cm. For the source term, we have used σ=0.01 cm, which is comparable to the size of the streamer head at ground pressure. It is assumed that source is positioned in the center of the simulation domain at z_0=0.1 cm. Figures 3, 4 and 5 present axial profiles of the photoionization source term calculated with different models.

Figure 3 shows that the photoionization source term calculated with the 1-Group Eddington model is in good agreement with the Zheleznyak model only in a limited region near the center of the simulation domain. It is important to note that in streamer applications, photoionization is important in regions where $S_{ph}>S_i$. Figure 3 shows that the 3-Group Eddington is much more accurate than the 1-Group model in regions where $S_{ph}>S_i$ and especially close to the boundaries of the computation domain. For a detailed discussion on boundary conditions, we refer to [9].

Figure 4 compares the two and three-exponential Helmholtz models. The results obtained with the three-exponential fit appear to match better with the Zheleznyak integral solution. In particular, the solutions near the center of the simulation domain are significantly improved. This directly relates to a better three-exponential fit at small $p_{O2}R$ values as can be seen in Figure 1.

Figure 5 compares the 3-Group Eddington and the 3-exponential Helmholtz model. We note that both models are in good agreement with the Zheleznyak model.

Finally we have compared the execution times of the different models. All calculations have been carried out with a uniform grid (251 points in both directions) on an Intel Xeon DP 2.8GHz computer.

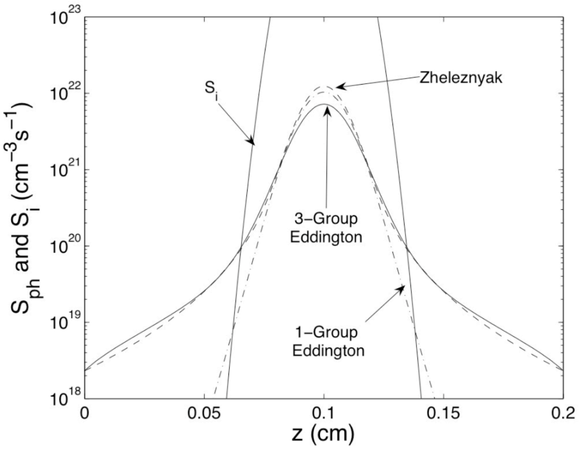

Figure 3 : Axial profiles of the ionization source term and the photoionization source term. Dashed line: integral model derived by Zheleznyak. Dot-dashed line: 1-Group Eddington model. Solid line: 3-Group Eddington model.

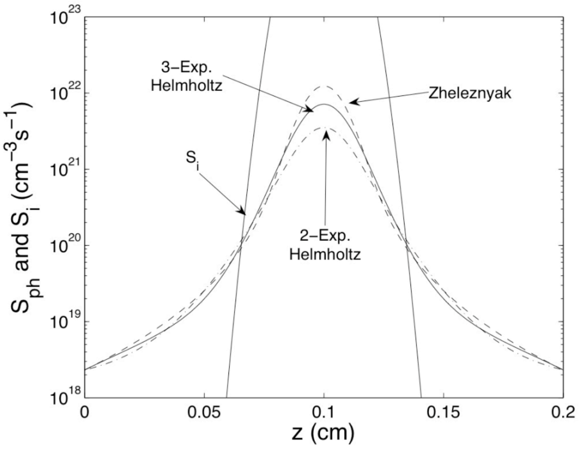

Figure 4 : Axial profiles of the ionization source term and the photoionization source term. Dashed line: integral model derived by Zheleznyak. Dot-dashed line: 2-exponential Helmholtz model. Solid line: 3-exponential Helmholtz model.

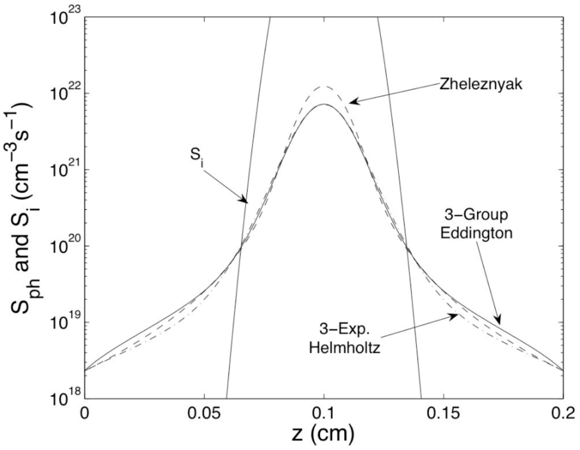

Figure 5: Axial profiles of the ionization source term and the photoionization source term. Dashed line: integral model derived by Zheleznyak. Dot-dashed line: 3-exponential Helmholtz model. Solid line: 3-Group Eddington model.

For the 3-Group Eddington, the computation time was 2.62 s, for the 3-exponential Helmholtz, 3.28s and for the integral method, 3159.36s.

3.2. Double-headed streamers in air

In this section, we report and compare modeling results on a double-headed streamer developing in air at ground pressure (760 Torr) obtained with different photoionization models. The simulation domain is the same as in Figure 4a in [11]. Further details may be found in [9].

In [9] we have shown that an excellent agreement exists between the results obtained with the 3-Group Eddington, 3-exponential Helmholtz models and the Zheleznyak model for both streamer heads. Small differences are observed in the region well ahead of the streamer head, and the differences increase as the streamer advances.

Figure 6 compares the electron number density distribution on the symmetry axis of the computational domain calculated using the one and three-group Eddington model for the photoionization term. The results are shown for the moments of time from t=0 to t=3.5 ns, with a timestep of 0.5 ns.

We note that with the 1-Group Eddington model, the positive (see left side of the figure) and negative (right side) streamers propagate much more slowly. As expected, the influence of the photoionization model is more significant on the positive streamer than on the negative one.

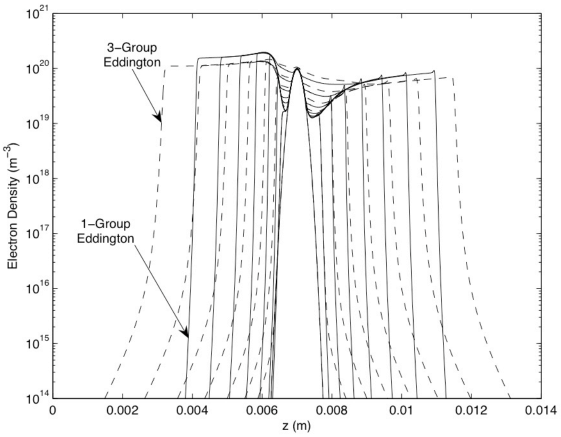

Figure 6: Electron density profiles on the symmetry axis of the computational domain at various moments of time calculated using 1-Group and 3-Group Eddington models for photoionization. Results are shown for the moments of time from t=0 to t=3.5 ns, with a timestep of 0.5 ns.

4. Conclusions

In conclusion, we emphasize that the actual advantage of differential models advanced in this paper in comparison with the integral model lies in the simplicity of implementation of this type of models, and in unquestionable simplicity of extension of these models to complex two- and three-dimensional simulation geometries, involving, for example, propagation of multiple streamer heads in the same simulation domain, and the presence obstacles on the streamer path (i.e., electrodes, dust particles, aerosols, etc) [i.e., 1].

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