QUICK GUIDE

PHOTOPiC

PHOTO-ionization Parameter Calculator

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Contents

Chapter 1

Introduction

1.1 WHAT IS PHOTOPIC

PHOTOPiC is a software developed in Python, devoted to calculate photo-ionization parameters that can be used for numerical simulation of plasma discharges. A database consisting N2, O2, CO2, H2O are incorporated and will be extended in future updates. The function of PHOTOPiC include:

(1) Identify the dominate specie that is responsible for photo-ionization;

(2) Calculate photo-ionization functions for all the gases in the mixture;

(3) Fitting for factors of high efficient photo-ionization models;

The algorithms in this software is mainly based on the theoretical work of Dr. Sergey Pancheshnyi [1]. Papers using this software are listed in the Appendix.

1.2 MANUAL STRUCTURE

This manual is devoted to introduce the usage and basic algorithm of PHOTOPiC.

Chapter 2 is a step-by-step tutorial. Users will learn how to use this software to produce the photo–ionization functions for specific gases or gas mixtures, and how to put them in their plasma models.

Chapter 3 introduces the physical parameters and data that are used. Users will learn how to organize their own physical parameters for specific usages.

Chapter 4 briefly reviews the mathematical model incorporated in the software.

Chapter 5 shows the benchmark cases.

Chapter 2

A quick start

2.1 STEP I: SPECIFY GASES

The software starts with the gas specification page. One has to select the gases to be studied, and define the percentage in %. The sum of the percentage should be 100, otherwise you will not be able to proceed.

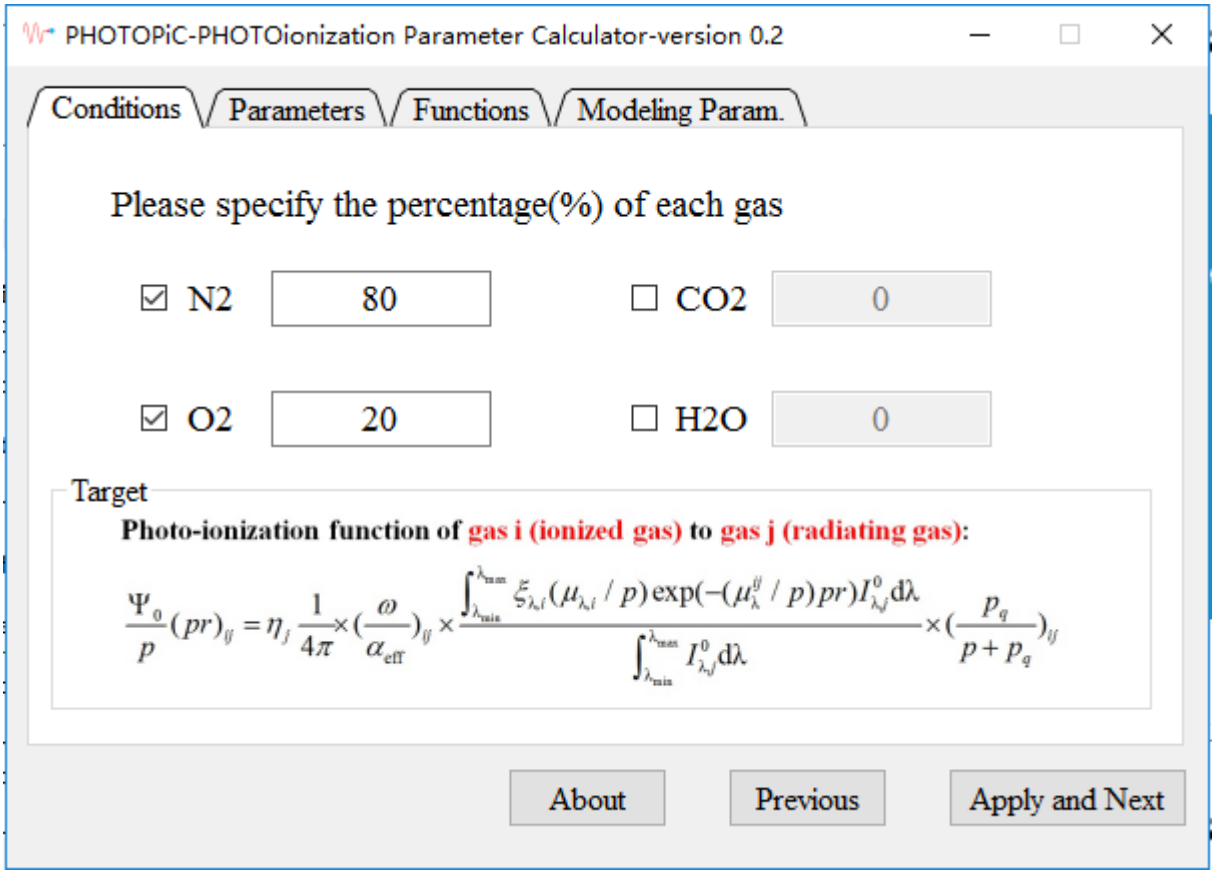

Figure 2.1: Specify a gas and corresponding percentage in Page 1

Figure 2.1 shows the default setting. One can click the “apply and next” button after filling all the ticked boxes.

You can tick as many gases as you want, but more gas species correspond to longer calculation time. If the percentage is 0, please just do not tick this gas to avoid additional calculation time.

Click “Apply and Next” to proceed to next page.

2.2 STEP II: LOAD/SET PHYSICAL PARAMETERS

In this page you can set the condition and physical parameters required for photo-ionization function calculation. Those include:

(1) Temperature (K), Pr (the product of pressure and radius) and pressure (Torr).

(2) Photo-ionization cross sections, photo-absorption cross sections, spectrums, λ_{min}, λ_{max}, scale factor $wvsa$ and quenching factor Π.

The meanings and usage of above factors will be introduced in following chapters.

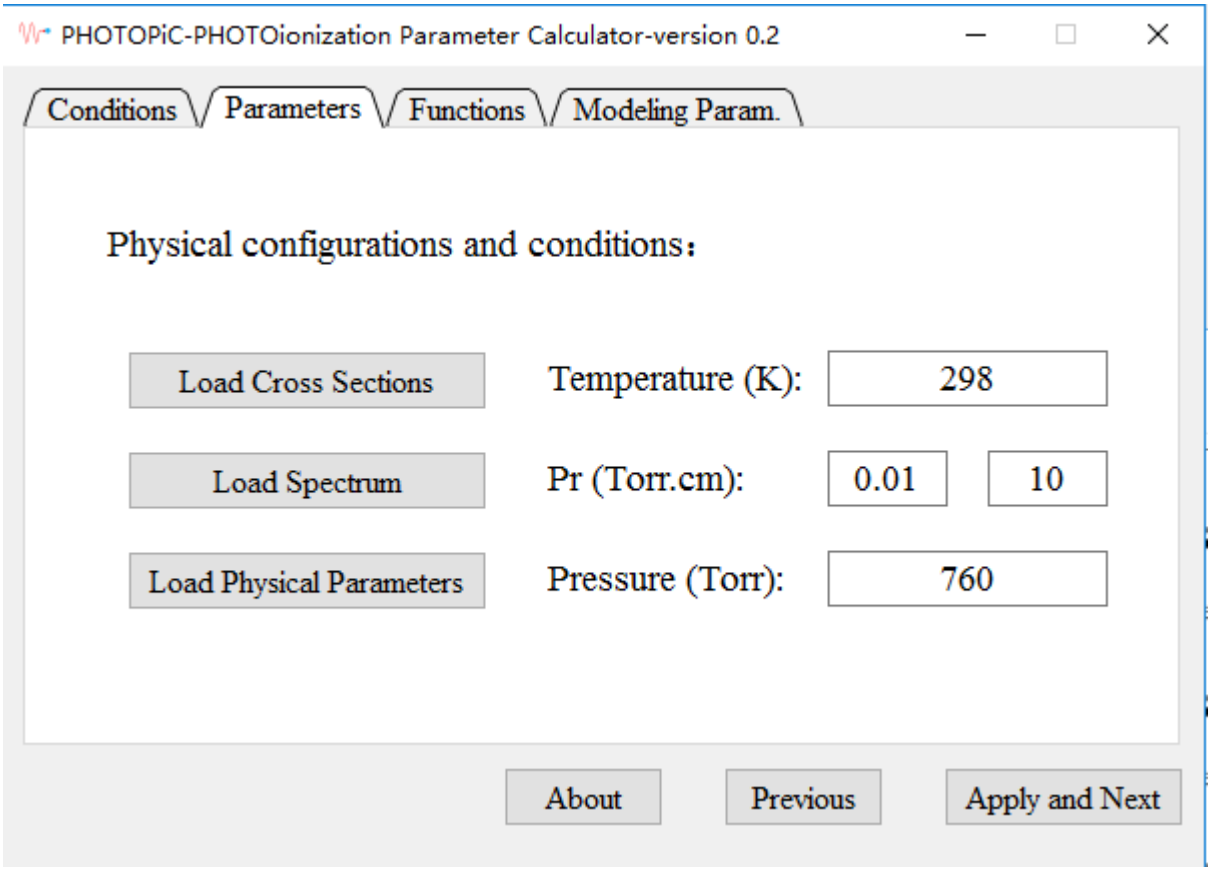

Figure 2.2: Label-1 specify a gas and corresponding percentage

By default, users just have to change the parameters in (1), while for parameters in (2), we have already organized 3 database files with the software release.

When you proceed into page 2, the PHOTOPiC will automatically load the 3 database files called Xsecs.dat, Spectrum.dat and Phys.dat in the same folder. If the files are absent, you will receive a warning message and have to click the 3 buttons shown in Figure 2.2 to specify the location of the files by yourself.

Specifying the data in this page, and then click “Apply and Next” to proceed to next page.

2.3 STEP III: CALCULATE AND PLOT RESULTS

In this page you will be able to calculate the photo-ionization function of each gas ionized by the radiation from another gas. The results can be plotted in this page, too. The photo–ionization function reads[1]:

$$\frac{\Phi_0}{p}(pr)_{ij} = \eta_j \frac{1}{4\pi} \times (\frac{\omega}{\alpha_{eff}})_{ij} \times (\frac{\int_{\lambda_{min}}^{\lambda_{max}} \xi_{\lambda,i}(\mu_{\lambda,i}/p) exp(-(\mu_\lambda^{ij}/p)pr) I_{\lambda,j}^0 d\lambda}{\int_{\lambda_{min}}^{\lambda_{max}} I_{\lambda,j}^0 d\lambda}) \times (\frac{p_q}{p+p_q})_{ij} \quad (2.1)$$

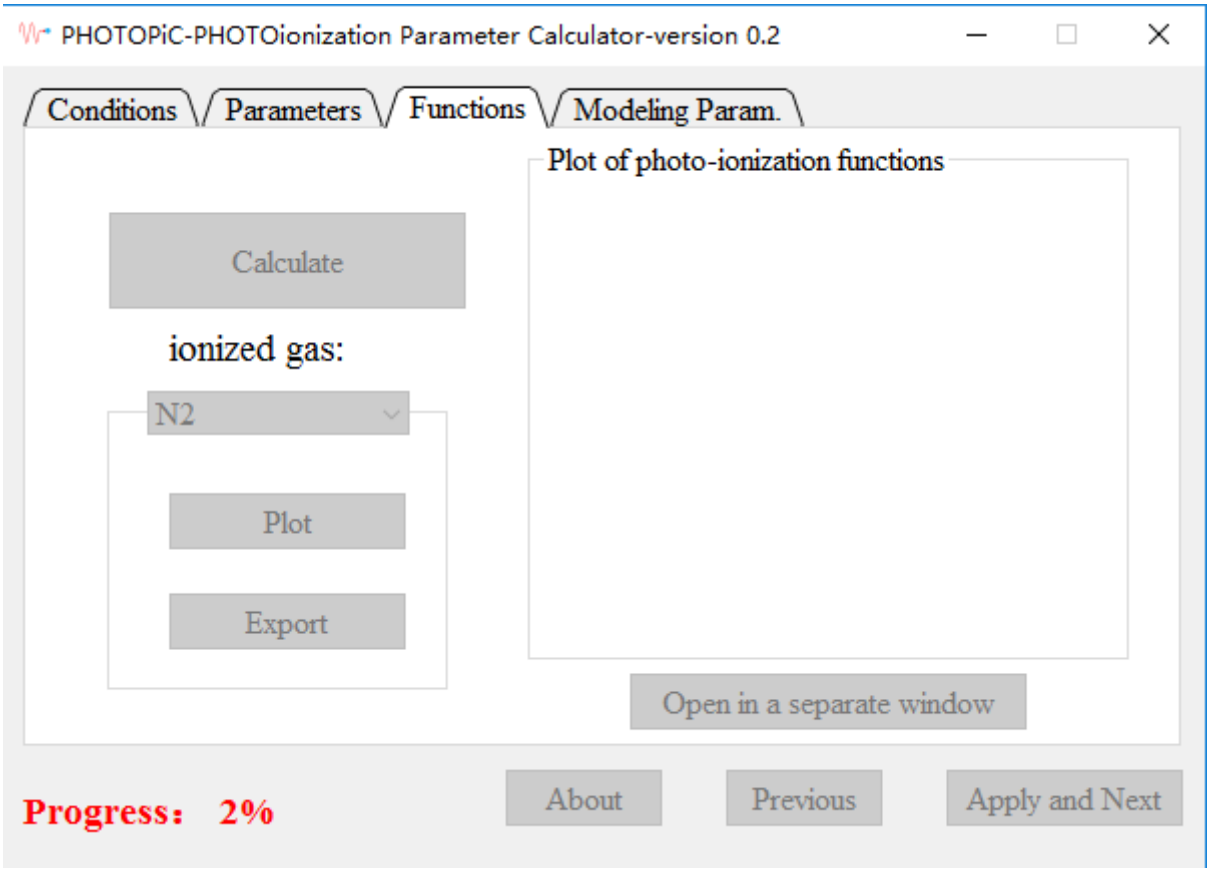

Figure 2.3: Label-1 specify a gas and corresponding percentage

In this page you just have to click the “Calculate” button and wait. When PHOTOPiC is calculating, all the button will be grey, there will be a progress information on the left corner, as shown in Figure 2.3.

If you have clicked “Calculate” before, you will receive a message asking you to confirm that you are going to calculate a new case: this will clean the previous data and plot.

Once the calculation is finished, the grey buttons will turn active (black) again. Then you can plot the results in the window on the right, as shown in Figure 2.4. To achieve that, first select from the list “ionized gas” the target gas specie, and then click the “Plot” button. You will see the photo–ionization functions caused by different source gases in the window on the right. You can then click the “Export” button to save the results on the disk.

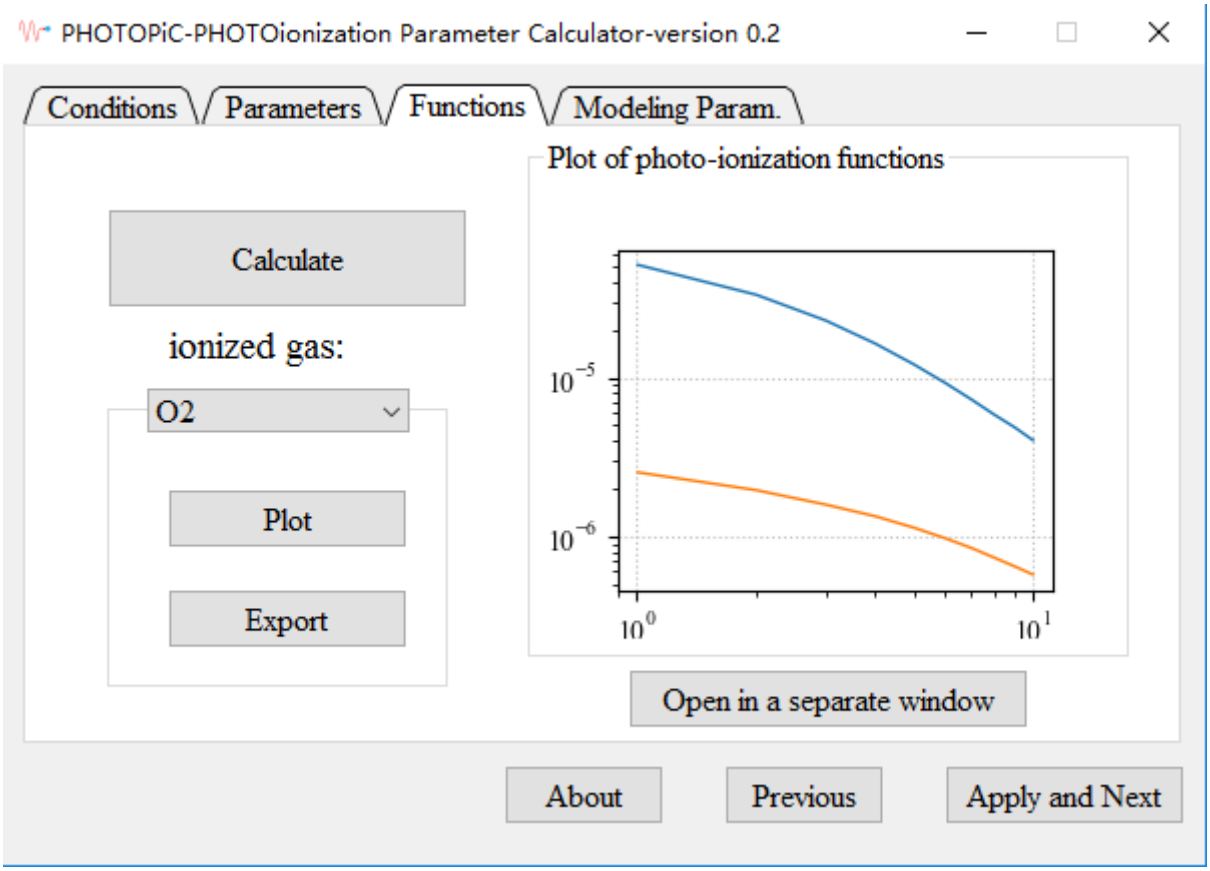

Figure 2.4: Label-1 specify a gas and corresponding percentage

It has to be noted that the right window is quite small to show enough information (legends, et al.). Thus to see more you can click the “Open in a separate window” button, this will allow you to see the results in a full–screen window.

After calculation, you can click “Apply and next” to proceed.

2.4 Step IV: Fitting for plasma models

This page is dedicated for calculating the parameters for specific models that are widely used in plasma modeling (especially streamer discharges). This version incorporates only the

3–terms Helmholtz equations model[2].

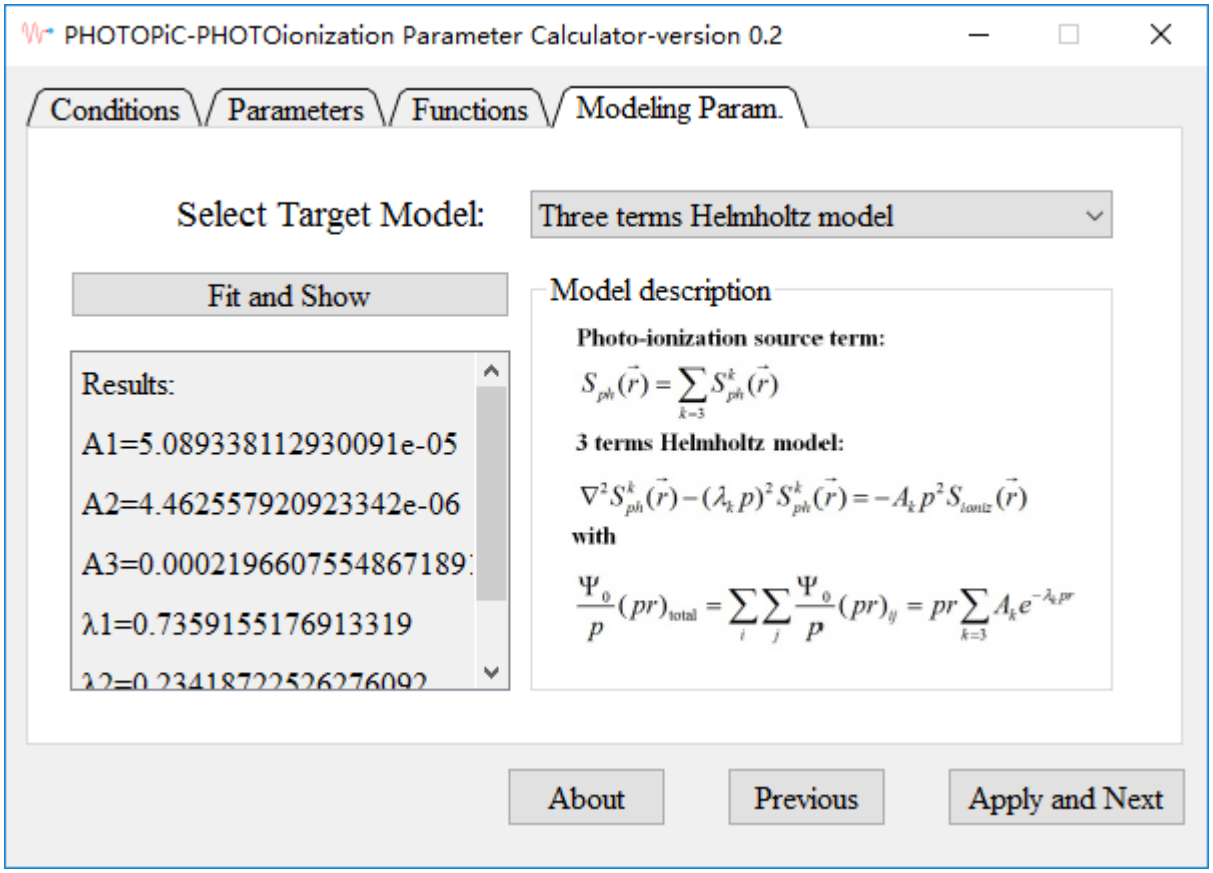

Figure 2.5: Label-1 specify a gas and corresponding percentage

To obtain the parameters, just select the model from the list (see Figure 2.5), the description of the model is shown below the list. Click the “Fit and show” button. The fitting parameters are calculated using the least square method and printed in the window below the button.

The fitting parameters can be incorporated into your codes or softwares (for example COMSOL cases taking into consideration photo–ionization).

2.5 STEP V: USE THE RESULTS FOR SIMULATIONS

It has to be noted that, PHOTOPiC allows one to calculate multi–component gases, thus the classical Helmholtz equation model proposed in Ref [2] can not be used directly. These parameters should be used in the code or softwares with the equations to be solved in

following style:

$$\nabla^2 S^j(r) - (\lambda_j p)^2 = -A_j p^2 I(r) \tag{2.2}$$

where S^j is the source term of photo-ionization, λ_j and A_j are parameters to fit, I is the ionization source term, p is the pressure. It has to be noted that, p here is ambient pressure, not the partial pressure of oxygen. This allows a more general condition.

Chapter 3

Input data

This chapter provides more information on data preparation for the calculation. Users can edit the database knowing the correct format, change the default gas and calculate for their own data.

3.1 CROSS-SECTIONS

Photo–ionization cross sections and Photo–absorption cross sections are required for each gas. The database of these cross sections for PHOTOPiC is stored in Xsecs.dat file. The template of the database is:

#Gas name
#photo-ionization or photo-absorption
Energy(eV) xsec($\times 10^{-18} m^2$)

for example for N_2, then cross section data reads:

#N2
#photo-ionization
2.370 0.80
2.847 0.96
2.879 0.95
2.952 0.99
3.000 0.61
...
#N2
#photo-absorption
2.370 0.80
2.847 0.96
2.879 0.97

The photo–ionization and absorption cross sections are used to calculate the photo–ionization yield and absorption coefficient. These data are presented and validated in the Appendix II.

3.2 OPTICAL EMISSION SPECTRUM

Optical emission spectrum in as large range as possible for each gas is required. The database of these spectrums is stored in Spectrum.dat file. The data file can be found in existing publications. The template of the database is:

#Gas name
#some comments
Wavelength(nm) strength(a.u.)

for example for N_2, then spectrum data reads:

#N2
#precision 0.5nm, 50–200nm
52.5773 0.01997
52.8522 0.08068
53.1271 0.18684
53.2646 0.23235
53.5395 0.15670
...

3.3 OTHER PHYSICAL PARAMETERS

Some other physical parameters are required. They are used to decide the integration limit of spectrum, the scaling factor relating to the emitting processes and the quenching factors. Usually the users don't have to adjust them. But if users would like to replace with new gases, or to update from latest publications, will have to check carefully these parameters.

(1) One has to decide the upper and lower limit for integration. The lower and upper limit is denoted as "LAMBDA_MIN" and "LAMBDA_MAX".

The upper limit is the maximum wavelength that can ionize gas j, i.e. the ionization threshold of ionized gas, thus there is 4 numbers in "LAMBDA_MAX", corresponding to N_2, O_2, H_2O and CO_2.

The lower limit is decided to ensure there are at least two peaks between "LAMBDA_MIN" and "LAMBDA_MAX" for the emitting gas j. Thus there are n×n (n is the number of species in the database) values to be decided, they are tabulated as a matrix, if i=2, j=3 then "LAMBDA_MIN" value is located at the second row and third column.

(2) The scaling factor does not affect the profile of photo–ionization functions, but will affects the absolute value. It corresponds to the excitation of one system of radiative transitions and is also a matrix denoting the radiation of gas i and ionizing of gas j. This value can be obtained by two steps:

First, find the cross section of corresponding emitting reactions of gas i, σ_{ext}. Divide σ_{ext} by χ (see [1]):

$$\sigma_{ext} = \sigma_{ext}/\chi \tag{3.1}$$

Second, use the scaled cross section σ_{ext} with the cross sections of all species in the mixture at wanted ratio, run BOLSIG+ to get the rate coefficients. Then the scaling factor can be calculated according to:

$$\omega/\alpha_{eff}(E/N) = \frac{k_{exc}(E/N)}{\sum k_{ion}(E/N) - k_{attch}(E/N)} \tag{3.2}$$

(3) Quenching factor. Measurements atelevated pressures show significant deviation from the low-pressure results, which has been attributed to the quenching of radiative states. A pressure correction factor has to be used:

$$\Pi = \frac{p_q}{p + p_q} \tag{3.3}$$

The value of quenching pressure is defined according to stationary kinetics balance of excited radiating species by taking into account radiative decay and quenching. The value can be decided from following formulation:

$$p_q = \frac{k_B T}{\tau_0 k_q} \tag{3.4}$$

where τ_0 is the radiative decay time and k_q is the quenching rate of corresponding emitting species. The uncertainty of k_q leads to some deviations. Typical p_q for pure nitrogen, oxygen and nitrogen in air is 9.8, 30 and 36 pa, respectively. This value is tabulated as a matrix, the quenching factor of excited gas i by gas j is stored in row i and column j of the matrix.

3.4 NOTES

The input data has to be adjusted in case of following cases (or other cases).

(1) Low pressure. In this case just set a huge quenching factor, thus $\Pi \approx 1$.

(2) Compare with some classical formulation. That is to say, if users want to get the photo–ionization function without scaling factors and quenching factors (which is the case in Ref [2] and in many codes), just set the scaling factor as 1.

(3) Replace the gas with another. To achieve this, one can select a gas (for example N_2) and replace the cross–section, the spectrum and other physical data.

Chapter 4

Appendix I: The basic formulation

Important nomenclature:

I_0: spectral density of ionizing radiation.

ω: Townsend coefficient of emitting states.

α_{eff}: Effective Townsend coefficient, defined as $\alpha - \eta$.

μ_λ: absorption coefficient.

ξ_λ: photo-ionization yield.

σ_{ion}: photo-ionization cross section.

σ_{abs}: photo-absorption cross section.

4.1 PHOTO–IONIZATION YIELD AND ABSORPTION COEFFICIENT

The probability of photo-ionization is related to the photo-ionization cross-section, which depends on the energy of the photon and the target being considered. The probability of absorbing radiation is related to the absorption cross-section. The combination of these parameters gives the information of how the photo emission will be absorbed by each species in the system.

For each wavelength of individual gas i, the photo-ionization yield (the probability of ionization of molecules by photon absorption) and absorption coefficient is defined as:

$$\xi_{\lambda,i}(\lambda) = \frac{\sigma_{ion}(\lambda)}{\sigma_{abs}(\lambda)} \tag{4.1}$$

$$\mu_{\lambda,i}(\lambda)/p = \sigma_{abs}(\lambda)\frac{1}{k_B T} \tag{4.2}$$

Above values are essential to calculate the multi–component photo–ionization functions.

4.2 THE MULTI-COMPONENT PHOTO-IONIZATION FUNCTION

The photo-ionization function $\frac{\Phi_0}{p}(pr)$ is necessary for direct numerical simulation of discharges in gas i:

$$\frac{\Phi_0}{p}(pr) = \Pi\frac{1}{4\pi}\cdot\frac{\omega}{\alpha_{eff}}\cdot\frac{\int_{\lambda_{min}}^{\lambda_{max}}\xi_\lambda(\mu_\lambda/p)exp(-(\mu_\lambda/p)pr)I_0 d\lambda}{\int_{\lambda_{min}}^{\lambda_{max}} I_0 d\lambda} \tag{4.3}$$

Above equation is defined for only one specie. For a gas system of n species, there will be $n \times n$ photo-ionization functions. These functions can then be used to analyze the constitute of photo-ionization source. This enables the possibility to find the main contribution and use only one photo-ionization process for 2D simulation when multi-species are studied.

Note that the percent of each specie has to be taken into account to calculate the absorption of radiation by all species. In equation 4.3 the absorption term in $exp(-(\mu_\lambda/p)pr)$, μ_λ is redefined by:

$$\mu_\lambda^{ij} = \sum_j \eta_j \mu_{\lambda,j} \tag{4.4}$$

When the contribution from emission and absorption of every specie are considered, for each species (i) ionized by emission from specie j, the multi–component photo–ionization

function reads:

$$\frac{\Phi_0}{p}(pr)_{ij} = \eta_j \frac{1}{4\pi} \times (\frac{\omega}{\alpha_{eff}})_{ij} \times (\frac{\int_{\lambda_{min}}^{\lambda_{max}} \xi_{\lambda,i}(\mu_{\lambda,i}/p) exp(-(\mu_\lambda^{ij}/p)pr) I_{\lambda,j}^0 d\lambda}{\int_{\lambda_{min}}^{\lambda_{max}} I_{\lambda,j}^0 d\lambda}) \times (\frac{p_q}{p+p_q})_{ij} \quad (4.5)$$

4.3 FITTING PARAMETERS FOR THE HELMHOLTZ MODEL

The Helmholtz photo-ionization model has been used in many teams for its simplicity and continence. But till now there are only fitting parameters for N_2:O_2 mixtures, requiring O_2 being the main part for ionization. The use of this model for other gas mixtures haven't been seen yet. PHOTOPiC allows users to calculate parameters for following 3-term Helmholtz equations:

$$\nabla^2 S^j(r) - (\lambda_j p)^2 = -A_j p^2 I(r) \quad (4.6)$$

where S^j is the source term of photo-ionization, λ_j and A_j are parameters to fit, I is the ionization source term, p is the pressure. It has to be noted that, p here is ambient pressure, not the partial pressure of oxygen. This allows a more general condition.

The parameters follow:

$$\frac{\Phi_0}{p}(pr) = (pr) \sum_j A_j e^{-\lambda_j pr} \quad (4.7)$$

Taking pr as the variables, and knowing the value of $\frac{\Phi_0}{p}(pr)$, the least square method is used to find the 6 parameters. Typically in low temperature plasma streamer stage the gas mixture is not changing dramatically, thus we can use the fitted parameters as constants in the code.

Chapter 5

Appendix II: Benchmarks

This chapter show the calculation results obtained for N_2 and air mixture: the photo-ionization function and the Helmholtz parameters. The calculations are compared mainly with the work presented in paper [1] and [2].

5.1 Validation of photo–ionization functions

The calculated photo–ionization functions are compared with experimental values for pure N_2, O_2 and air. The experimental values have been summarized in paper [1].

Using the default input data, users can obtain results shown in Figure 5.1, or calculate mixtures with other constitution ratios. It has to be noted that, in Ref [1] the quenching factors are not taken account, thus the results obtained by PHOTOPiC has to be multiplied by $(p + p_q)/p_q$.

5.2 Validation of Helmholtz coefficients

The fitting parameters for Helmholtz Photo–ionization model calculated by PHOTOPiC are checked by comparing with results presented in paper [2]. The validation gas mixture is air (the only available benchmark).

The comparison is shown in Figure 5.2. By assuming a Gaussian-distribution ionization source, we can calculate the photo–ionization source required for plasma modeling. Photo–ionization source terms calculated for different scales agree perfectly with existing plication.

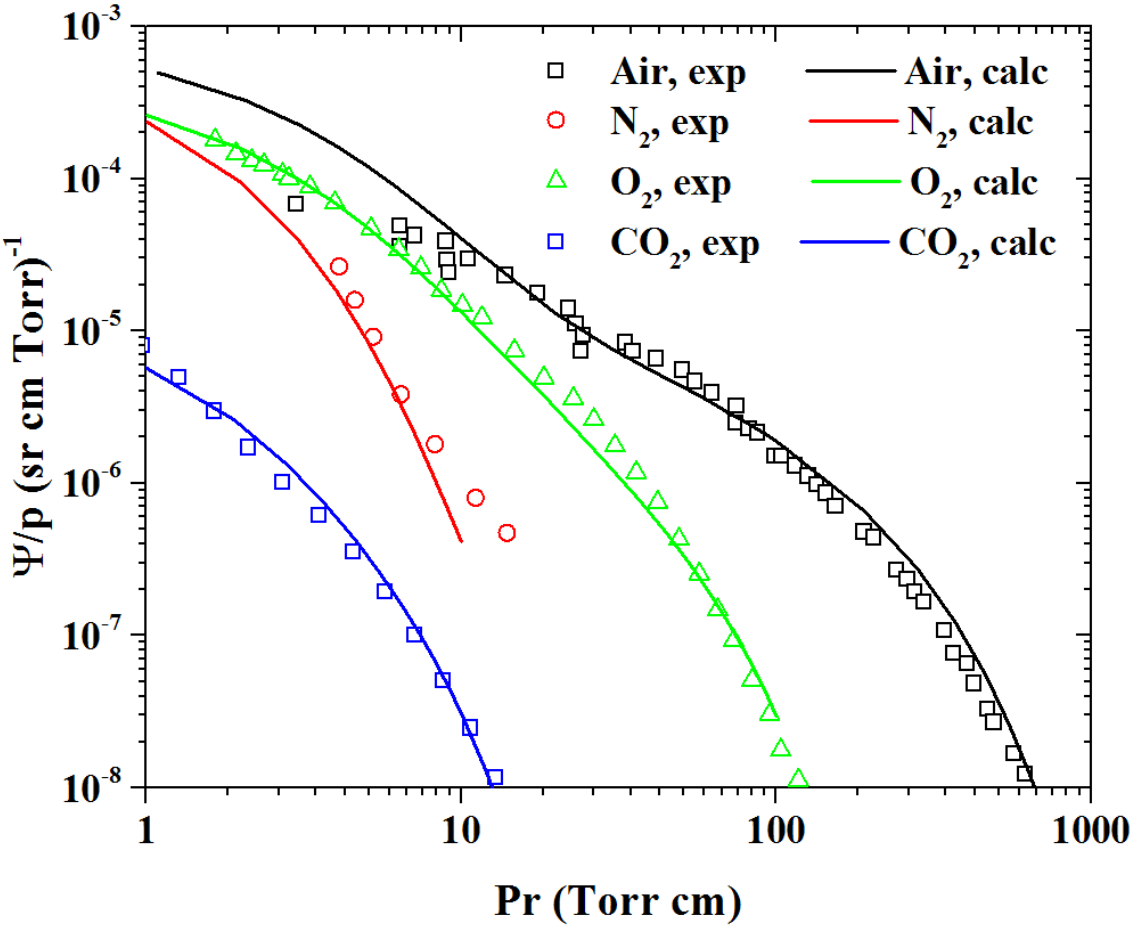

Figure 5.1: Photo–ionization functions calculated by PHOTOPiC and from experimental data presented in Ref [1]. Air data correspond to the work of Penney [3], O_2 data correspond to the work of Przybylski [4], and N_2 data is from the work of Teich [5], CO_2 data is retrieved from Ref [1].

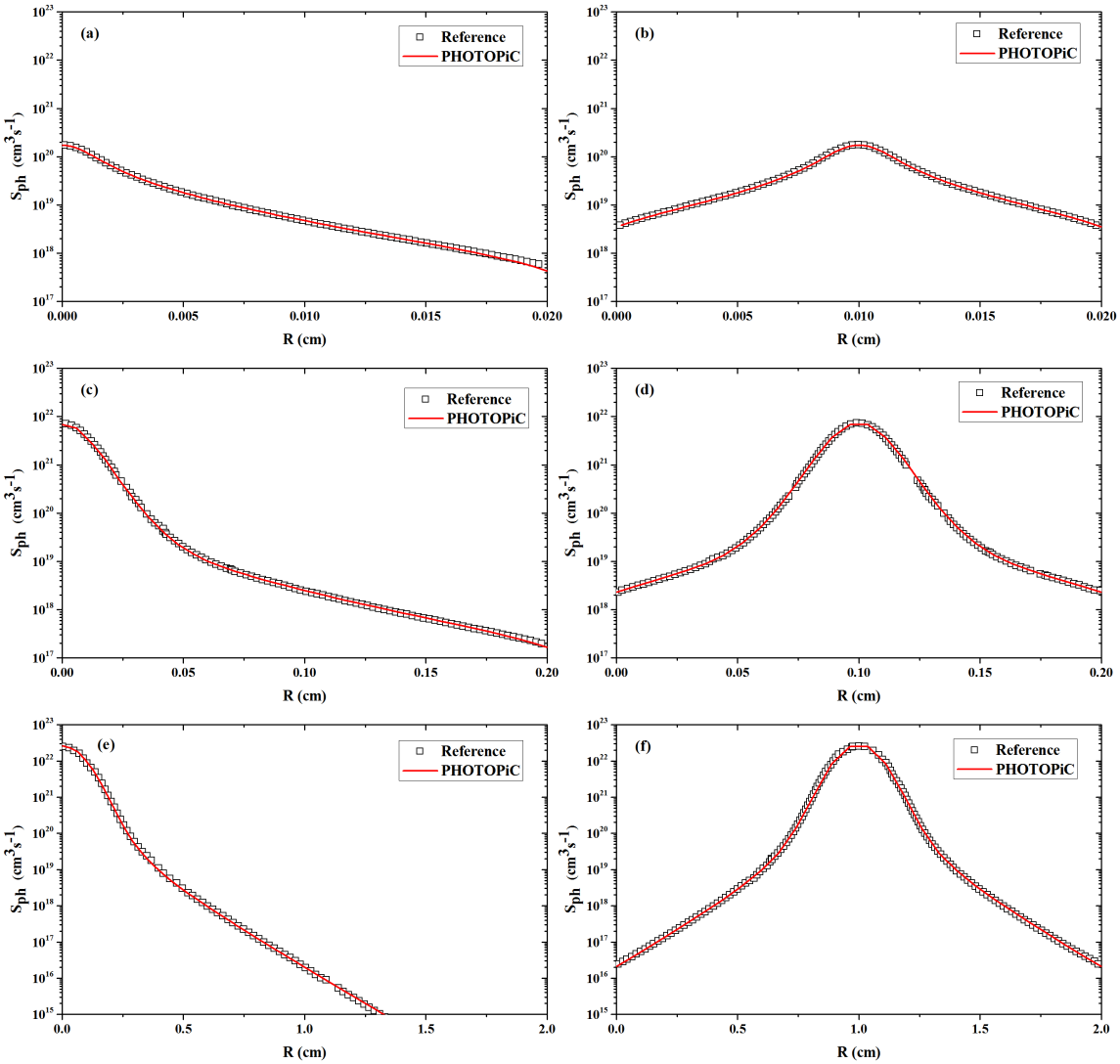

Figure 5.2: Photo–ionization source terms calculated by PHOTOPiC and in Ref [2].

5.3 VALIDATION OF GAS DISCHARGE SIMULATIONS

The fitted parameters are used in a 2D fluid code (PASSKEy code) to reproduce the results of a pin–plane streamer discharge simulation.

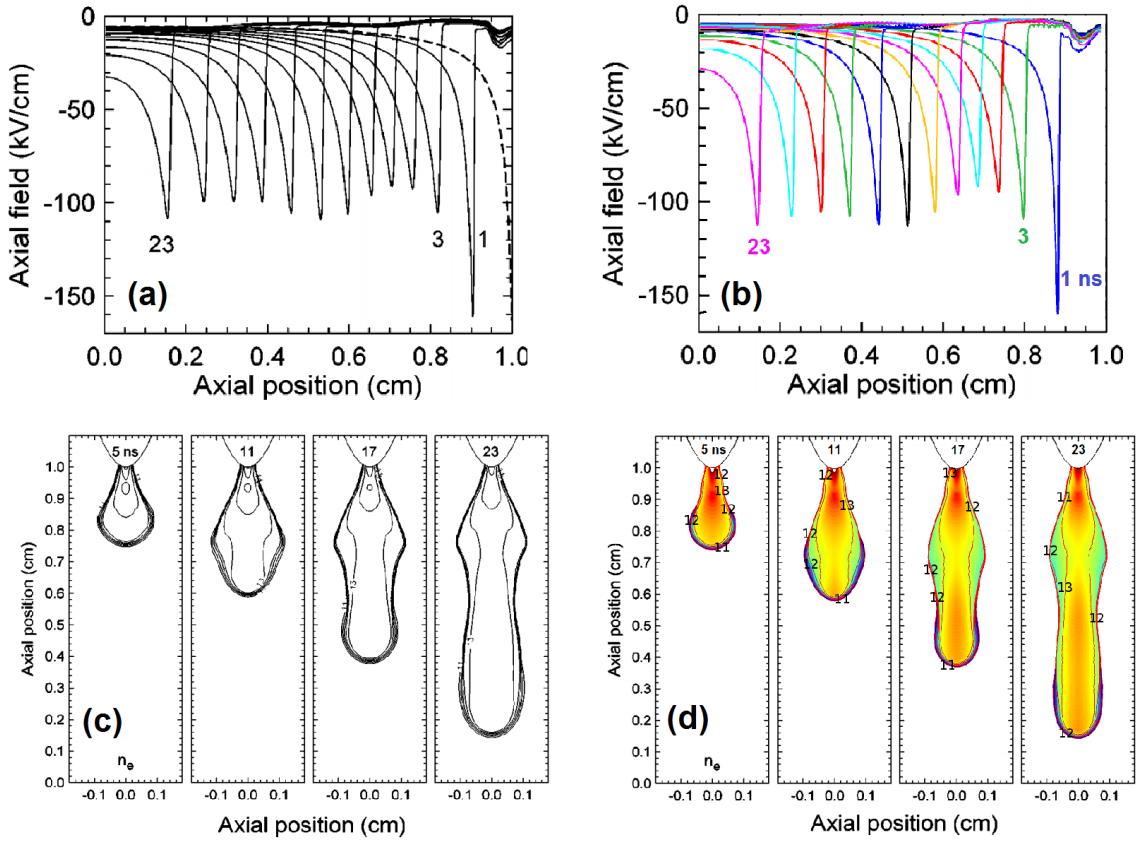

Figure 5.3: The pin–plane discharge benchmark. (a) and (c): the evolution of axial electric field and spatial electron density in Ref [6]; (b) and (d) results calculated by PASSKEy code [7] using the parameters obtained by PHOTOPiC.

The PASSKEy code incorporates the Helmholtz photo–ionization model. Other calculations conducted by PASSKEy code can be found in paper [7, 8].

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