Fitting of Electron Collision Cross Sections from Swarm Data using a Genetic Algorithm

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Abstract: We study the application of an genetic algorithm to obtain a complete and consistent set of electron collision cross sections (cs) and to estimate their uncertainty. The validity of this method is studied for a model gas using the swarm analysis technique. We find a very good agreement between the model gas transport coefficients and those from the optimized cs set, confirming the suitability of genetic algorithms to this problem.

Keywords: Electron swarm analysis, genetic algorithms, Boltzmann equation

1. Introduction

The electron collision cross sections (cs) are the starting point to describe the behavior of a gas in a plasma. Accurate modeling of a plasma discharge requires a complete (i.e. including all the relevant processes) and consistent (the set of cs accurately reproduce the plasma transport parameters and electron rate coefficients) set of cs. While experimental measurements and theoretical computation provide a starting point to the cs of a gas, the information available is usually incomplete and inconsistent. A third method which complements the above, is based on the measurement of electron swarm transport properties that depend on the gas cs. Ideally, the solution of the inverse problem should provide the cs. While this method allows to obtain complete and consistent cs sets, the solution is not univocal and the fitting process is tedious and time consuming. For these reasons, several authors have tested automated methods for this problem [1-3] with a particular emphasis on neural networks [4-5]. In the present work we follow a different approach, testing a *genetic algorithm* (GA) algorithm [6] to obtain a physically consistent cs set leading to values of transport parameters within the typical experimental uncertainties.

2. Overview

The task is to obtain in an automatic way, a cs set that, when used in a code solving the Boltzmann equation, is able to reproduce the experimental values of the electron transport parameters for a range of E/N values (where E is the module of the electric field and N the gas density). We start with a collection of guess cs sets that will be tested for this purpose and classified according to some selection criteria. The best sets will be selected, modified and used for the next iteration of the algorithm. This process is repeated until a desired convergence (or number of iterations) is obtained.

To test the algorithm, we use a model gas with a small but representative number of cs, described below.

3. The model cross section set

The model gas has 4 cs indicated in Fig 1: a momentum transfer cs with a low-energy minimum simulating the Ramsauer minimum found in some noble gases; a vibrational excitation cs (ε_{th} = 0.3 eV), an electronic excitation cs (ε_{th} = 3 eV) and the ionization cs (ε_{th} = 10 eV). For the shape of the last two cs we adopted the Binary-Encounter-Bethe (BEB) model [7] which has been shown accurate for the ionization of several atoms and molecules.

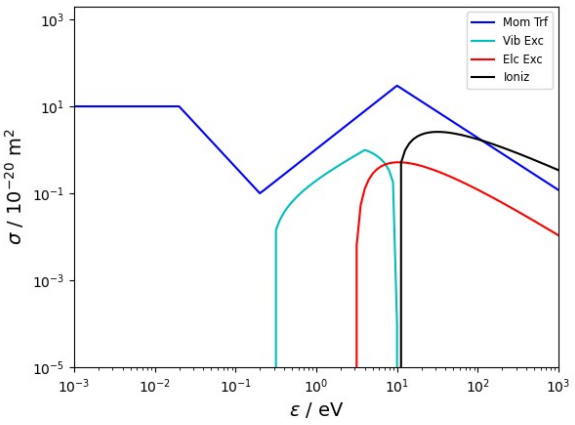

Fig 1: Cross section set used to test the GA algorithm

With this cs set we obtained reference values for transport parameters, simulating those measured in swarm experiments. This parameters include the flux and bulk drift velocity, respectively V_d and W_d, the bulk longitudinal and transverse components of difusion, (D_L, D_T), the effective ionization frequency, υ_{Eff} and the effective Townsend coefficient, α_{Eff}.

4. Boltzmann equation and method of solution

To solve the Boltzmann equation for an electron swarm acted by a constant electric field, **E**, we adopted an expansion of the electron velocity distribution function, f(**r**,**v**,t), in the electron density gradients,

$$f(\boldsymbol{r},\boldsymbol{v},t)=\sum_{j=0}^{\infty} F^{(j)}(\boldsymbol{v}) \overset{j}{\odot} (-\nabla)^j n(\boldsymbol{r},t) \qquad (1)$$

where the expansion coefficients $F^{(j)}(\mathbf{v})$ are tensors of order j depending only on $\mathbf{v}$, and $\odot$ indicates a j-fold scalar product. Introducing (1) in the Boltzmann equation we obtain equations for the coefficients $F^{(j)}(\mathbf{v})$ which are solved in a (v,θ) grid using a finite element method [8].
From the above expansion coefficients we obtain two sets of transport coefficients: the *flux* coefficients, neglecting the contribution of non-conservative processes and the *bulk* coefficients including a contribution from ionization and attachment. The later coefficients correspond to those measured in swarm experiments and used in this study.
Further details can be found in [9].

5. The genetic algorithm

While neural networks are inspired by brain processes , in the present work we follow a different paradigm of evolutionary computation inspired by adaptation of populations. These populations evolve through birth and death, variation and selection along consecutive generations.

In our case the population is composed of μ cs sets, each characterized by a vector $\mathbf{k}_\mu$ of control parameters k_1, ..., k_N, The goal of an GA algorithm is to obtain the cs set that optimise a *fitness* function with respect to the set of control parameters.

In most of the algorithm tests, the control parameters, k_i, were scale factors, one for each cs. In later tests the control parameters for the momentum transfer cs also controlled the shape of the cs.

The fitness function is the residual with respect to $\mathbf{k}_s$,

$$F(\boldsymbol{k}_s)=\frac{1}{PM}\sum_{p=1}^{P}\frac{1}{2\,\sigma_p^{\,2}}\sum_{m=1}^{M}\left(\frac{x_{pm}-f_{pm}(\boldsymbol{k}_s)}{x_{pm}}\right)^2 \qquad (2)$$

where P is the number of transport parameters, M the number of E/N values, x_{pm} the reference value of parameter p for E/N value m, $f_{pm}(\boldsymbol{k})$ the corresponding value obtained from the solution of Boltzmann equation and σ_p the uncertainty of parameter p, used to weight the data. We have considered uncertainties of 3% for the bulk drift velocity and of 10% for the other parameters.

The algorithm starts by generating a population of μ cs sets by randomly modifying the control parameters for the model gas cs, within given limits. In most tests we have set 0.25 and 2 as minimum and maximum values for this variation and the population size has varied in the range of $16 \le \mu \le 256$. Each of these cs sets is used to compute the transport parameters at 41 E/N values between 0.1 Td and 1000 Td and the corresponding fitness value, F_s, evaluated. In the next step the best sets are selected and combined through recombination and mutation to produce λ new sets (children). Finally from the joint μ+λ sets, μ are stochastically chosen to constitute a new generation, starting a new cycle. The process is repeated until a termination condition (convergence criteria or maximum number of iterations) is reached.

6. Results

The results obtained in an Intel i7, 8 core processor taking advantage of parallel processing, took, typically, between one and four hours to converge, depending on the number of control parameters.

To facilitate the visualization, the first results were conducted modifying only two cs, the momentum transfer and ionization. Fig 2 shows the pairs of control parameter values for a population of 32 sets, where the red dot corresponds to the set with best fitness and the cross marks the optimum value, while Fig 3 shows the fitness values for each set along the iteration. Note the local minimum corresponding to values close to $\mathbf{k}$ = (1,1).

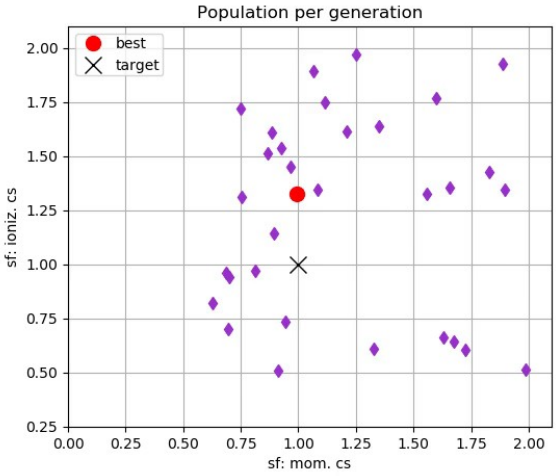

Fig 2: Scale factors for the momentum transfer and ionization cs for the first iteration. As the population evolves the best fit point approaches the target value.

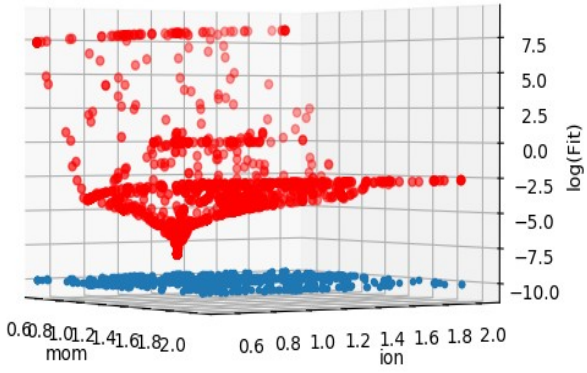

Fig 3: Fitness function values as a function of the population control parameters along the evolution.

With P=4, i.e. all cs were scaled, the convergency time increases but the results are still very good as can be seen in Fig 4 where the values of transport parameter obtained with a cs set with the best fitness value (points) are compared with reference values (lines). The relative errors are below 5%, within the typical values of the experimental uncertainties for these parameters.

Finally, we have repeated the fitting procedure in order to evaluate the distribution of the best control parameters. The results in Fig 5 show a small dispersion around the

optimum value with the exception of the electronic excitation cs, an indication that the transport parameters used are less sensitive to the values of this cross section.

These results allow us to estimate a statistical uncertainty for the cs amplitude.

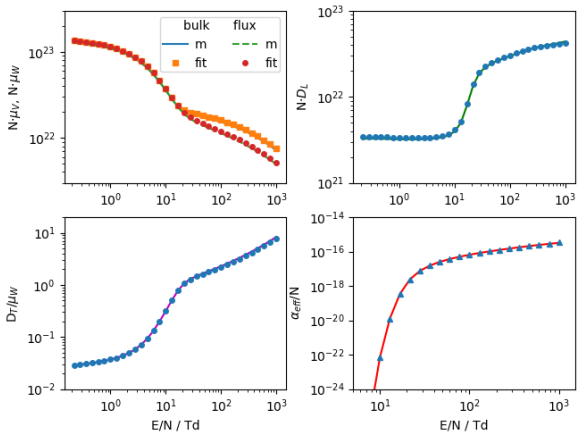

Fig 4: Transport parameters obtained with the model cs and with a best fit set, as a function of the reduced field.

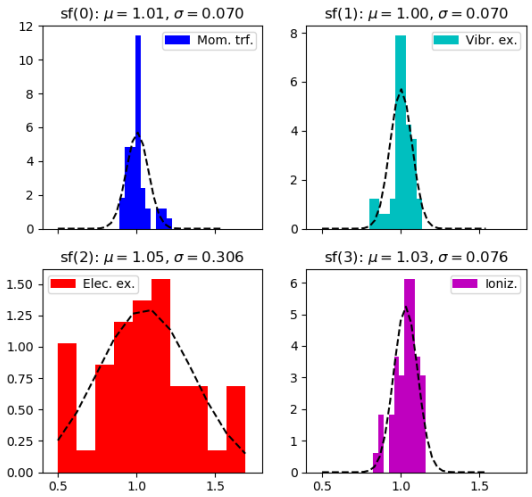

Fig 5: Distribution of control parameters for the four cs obtained in several iterations.

7. Conclusions

A genetic algorithm was successfully used to fit a cs set of a model gas. Although the model gas had a relatively simple set of cs, they include characteristics found in real gases that are challenging for the fitting of cs.

The time required for the computational fitting was much shorter than the time typically required for manual fitting. The estimation of the uncertainty of the cross sections can be useful for further use of the cs, namely in the estimation of rate coefficients for plasma chemistry.

Further work is in progress on more complex cs sets and on real gases.

8. Acknowledments

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