Status report on the LXCat project: an open-access, community-wide project on data needed for modeling low-temperature plasmas

L.C. Pitchford[1], on behalf of the LXCat team*

[1]*LAPLACE, University of Toulouse and CNRS, Toulouse, France*

LXCat is a dynamic, open-access website (www.lxcat.net) for exchanging data relevant to modeling low-temperature, weakly-ionized plasmas. LXCat is a community-wide effort; databases belonging to individual contributors are set up and maintained on the LXCat platform and are accessible through the on-line tools. So far, the LXCat project has focused mainly on data relevant to the electron and ion components of the low temperature plasmas and the available data types available on LXCat are discussed in the text below. An on-line Boltzmann solver can be used to calculate electron transport and rate coefficient data in pure gases or gas mixtures for maxwellian or non-maxwellian electron energy distribution functions if the cross section data for the individual components of the gas mixture exist on the site.

1. Introduction

The data needs in modeling low temperature plasmas are extensive. In general, for Monte Carlo Collision models used in PIC (Particle-in-Cell) codes, complete sets of electron- and ion- neutral cross section data are required input data. "Complete" in this sense implies that all major electron and ion momentum and energy loss processes are properly included in the set. Complete sets of electron-neutral cross sections are required for use in Boltzmann solvers to calculate transport coefficients and rate coefficients, which are themselves input data for fluid models of plasmas. Global models of the plasma chemistry require information about rate coefficients for all relevant processes, and collisional-radiative models and models involving plasma surface interactions require yet more detailed input data.

Since the beginning in 2009, the goal of the LXCat project has been to facilitate the collection, evaluation and sharing of data for both modeling and for interpretation of experiments in low temperature plasmas [1]. This presentation will provide a status report and a summary of the data available on LXCat at present.

2. Overview of the structure LXCat platform and on-line tools

The LXCat platform is structured into independently accessible databases set up by individual contributors who are responsible for the contents, and each database is identified a name chosen by the contributor. On-line tools enable importing and exporting data and so setting up a database is an easy task.

Using a series of filters, visitors to the LXCat site can quickly locate data of interest for displaying in graphical form or for downloading in different formats for off-line use. The plotting option is convenient for intercomparisons of data for different processes or of data for the same process but from different databases.

The LXCat site provides automatic back-up of all changes made in the databases. The "time machine" option allows visitors to retrieve data as they existed on the LXCat site at a specific date in the past (after Nov 2013). Thus corrections and new data can be added to the databases while previous versions of the databases remain retrievable. Usage statistics, user guides, unpublished notes, and publications and conference proceedings describing aspects of LXCat are available on the site. A mirror site has been set-up in Eindhoven to assure uninterrupted access to the data.

2. Data types presently available on LXCat

The main emphasis of the project up to now has been on data to describe the electron and ion components of low temperature plasmas. The data types presently available on LXCat are listed in Table I and will be described briefly in the following.

Data for the electrons are primarily in the form of "complete" sets of cross sections for electron scattering from neutral, ground state atoms or molecules, compiled or calculated by different contributors, covering a range of energies from thermal up to about 1 keV. Such cross section data can be used directly in Monte Carlo simulations and Boltzmann equation solvers. Solution of the homogeneous, steady-state Boltzmann equation yields the electron energy distribution function (eedf) vs. reduced electric field strength, E/N, and integrals over the eedf yield electron transport and

rate coefficients. The "complete" sets of cross sections on LXCat are intended to be consistent with measured transport and rate coefficients.

Component	Data types presently available on LXCat
Electrons	Electron-neutral scattering cross sections: - Complete sets - Partial sets
	Differential scattering cross sections
	Measured transport and rate coefficients vs. E/N
	Oscillator strengths
Ions	Ion-neutral interaction potentials
	Ion transport coefficients
	Sets of ion-neutral scattering cross sections

Table I. List of data types presently available on LXCat.

Some of the databases contain "partial cross section" data. By this we mean cross sections for electron-impact excitation to individual states, derived from experiment or from theory without regard to the issue of "completeness". As an example, we mention that ionization cross sections from theory for a number of ground state target species can be found on LXCat.

The cross section data are mainly total cross sections (angle integrated) for inelastic processes and momentum transfer cross sections for the elastic processes. However, a full set of differential scattering data for electron scattering in argon is newly available on LXCat and some experimental data for molecules are also available.

Many experimental data for electron transport and rate coefficients vs. E/N are available on LXCat. These are very useful for testing that various "complete" cross section sets are consistent with experiment. A version of the 2-term Boltzmann solver, BOLSIG+ [2], can be run on-line for calculations and comparisons with these experimental data.

Oscillator strength is a quantity that expresses the probability of absorption or emission of electromagnetic radiation in transitions between energy levels of an atom or molecule. These data, combined with a suitable model such as BEF scaling [2] can be used to infer the energy dependence and magnitude of electron-neutral scattering cross sections for specific processes for energies greater than several times the threshold energy.

A large body of data exists for ion-neutral collisions in the form of interaction potentials, from which ion-neutral cross sections and ion swarm parameters can be determined. The interaction potentials and derived transport coefficients are available on LXCat for a large number of ion-neutral pairs.

Some data sets for ion-neutral collision cross sections are available on LXCat. As mentioned above for the electrons, lacking a full set of DCS data, some assumptions about the anisotropic must be made [3].

4. Conclusions

Evaluation of the data available on LXCat is a key issue. To this end, the LXCat team has been making systematic intercomparisons of electron cross section data and comparisons of calculated and measured transport and rate coefficients. Our evaluations for noble gases have been published [4]. Similar evaluations for simple atmospheric gases were reported at the Gaseous Electronics Conference in 2013 and will soon be submitted for publications. Other evaluations are in progress.

At present about 30 people from over 10 different countries have contributed to this project. New contributors are welcome.

5. References

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*As of March 2015, contributors to the LXCat project include: *Australia:* I Bray, D First, L Campbell, M Brunger & S Buckman; *Canada* : A Stauffer, C Brion; *France :* JP Boeuf, MC Bordage, GJM Hagelaar, LC Pitchford, V Puech; *India* : S Chaudhury, B Chowdhury; *Japan* : Y Itikawa; *Mexico :* J de Urquijo; *The Netherlands* : J van Dijk; *Portugal* : L Alves, V. Guerra; *Russia :* I Kochetov, A Napartovich; *Switzerland :* S Pancheshnyi; *UK :* S Biagi, the Quantemol team; *USA :* K Bartschat, O Zatsarinny, WL Morgan, L Viehland.