2011 GEC Plasma Data Exchange Project

Comparisons of sets of electron-neutral scattering cross sections and calculated swarm parameters in Argon

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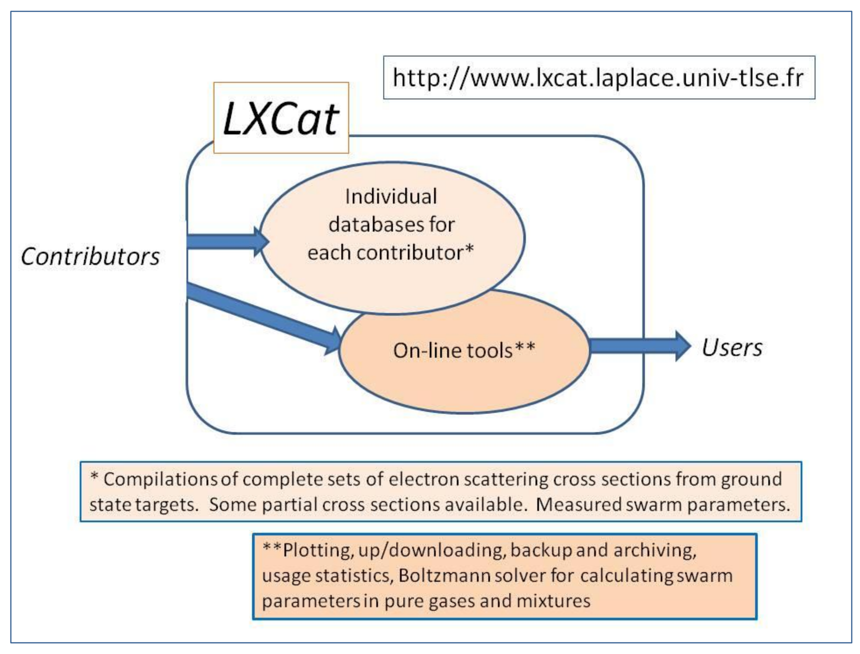
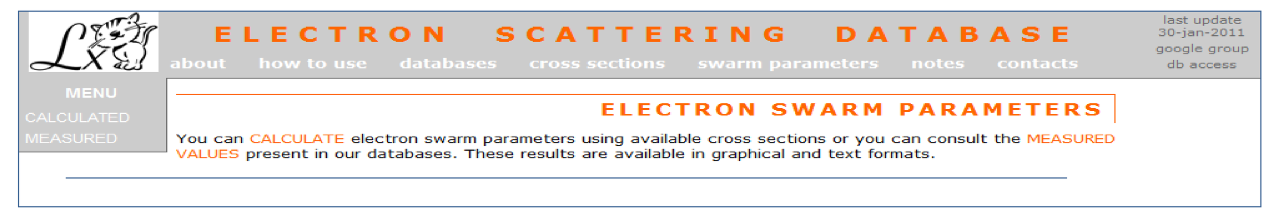
Extensive data are available in the literature for cross sections for electron-neutral scattering from argon and for swarm parameters in argon and argon-containing gas mixtures. Seven independently compiled sets of cross sections in argon are presently available on the LXCat website, including one set of data derived from theory. The recent theoretical elastic momentum transfer cross section is in excellent agreement with recent results from a swarm analysis. The purpose of this communication is to show intercomparisons of swarm parameters calculated using these different sets. For the most part and within the accuracy required for plasma modeling, calculated swarm parameters using the different cross section sets agree with experiment and among themselves. Swarm parameters calculated using classic 2-term Boltzmann solvers are in good agreement with those from Monte Carlo simulations except for the diffusion coefficients, where the 2-term approximation overestimates the values by about 30% in the 5 to 100 Td range. The cross section sets and measured swarm parameters used in this work are available on-line at www.lxcat.laplace.univ-tlse.fr.





"Complete" set of electron-neutral scattering cross sections

"Complete" => elastic momentum transfer, total inelastics, total ionization. In most cases, no other information about the angular scattering is needed.

Boltzmann solver => eedf

Boltzmann equation solvers : "Two-term" expansion is commonly used. More accurate techniques include multi-term solvers or Monte Carlo simulations. See below for some comparisons.

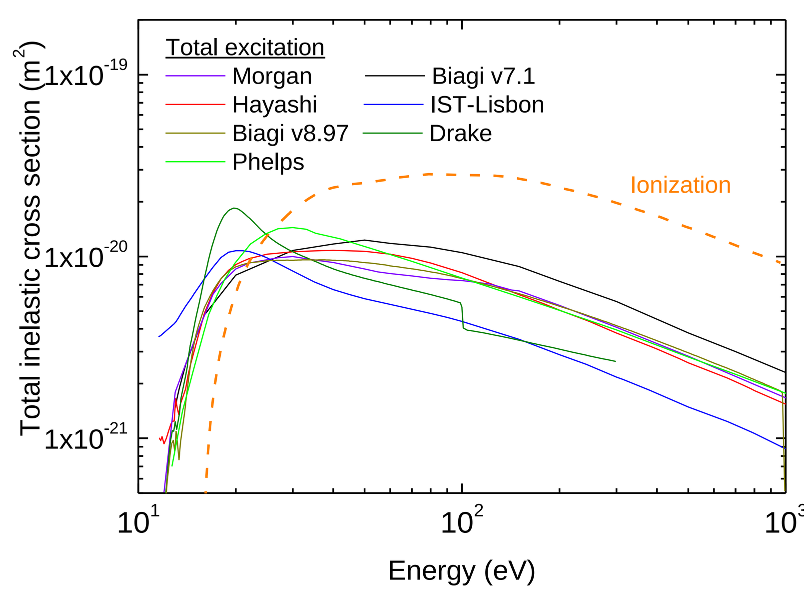
Ensemble averages: "swarm parameters" vs E/N

Data needed for fluid models include electron transport and rate coefficients, determined by experiments or appropriate averages over the calculated electron energy distribution function.

"Complete" sets of cross sections for e + Ar available on LXCat "complete" = elastic momentum transfer + total inelastics + total ionization

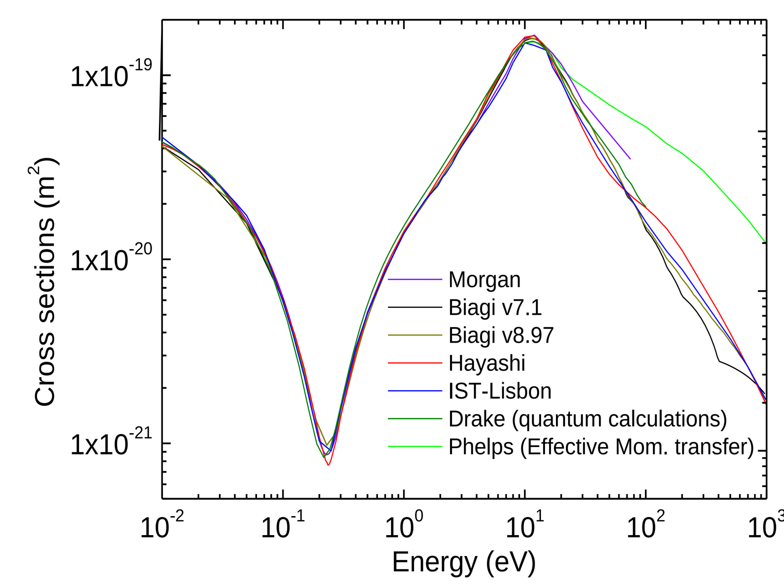
Database	Level of detail for excitation	Comments
Phelps (SIGLO data are from Phelps)	**1 effective excitation level**	For use with a 2-term Boltzmann solver. Originally from Yamabe, Buckman, and Phelps, Phys. Rev. 27, 1345 (1983), revised in 1997
Morgan	**2 levels** **(metastable + resonance)**	For use with a 2-term Boltzmann solver.
Biagi -v7.1	**3 excitation levels** **(S,P & D)**	For use with Monte Carlo or multi-term Boltzmann solver.
Biagi -v8.97	**44 levels**	For use with Monte Carlo or multi-term Boltzmann solver. Resonance regions based on quantum calculations of Zatsarinny and Bartschat
Hayashi	**25 levels**	For use with Monte Carlo or multi-term Boltzmann solvers. See NIFS-DATA-72 2003 report. Note that an informally circulated copy of these data represented incorrectly the elastic momentum transfer cross section. The data in LXCat are correct.
Drake (O Zatsarinny and K Bartschat)	**30 levels**	Results of quantum calculations. Excellent agreement with elastic momentum transfer derived from swarm analyses. From Zatsarinny and Bartschat, J. Phys. B 37 (2004) 4693
IST-Lisbon (L Alves and C Ferreira)	**37 Levels**	For use with a 2-term Boltzmann solver. For detail see poster QRP1.00064, this meeting.

Databases containing argon cross sections



Ionization and sum of inelastic cross sections

Ionization cross sections : essentially all from Rapp and Englander-Golder (1965) (except for calculations of Drake)



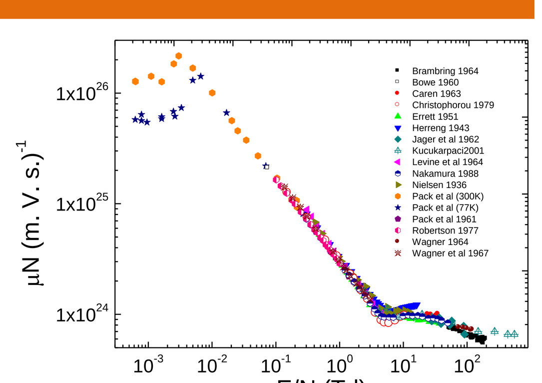
Elastic momentum transfer cross sections

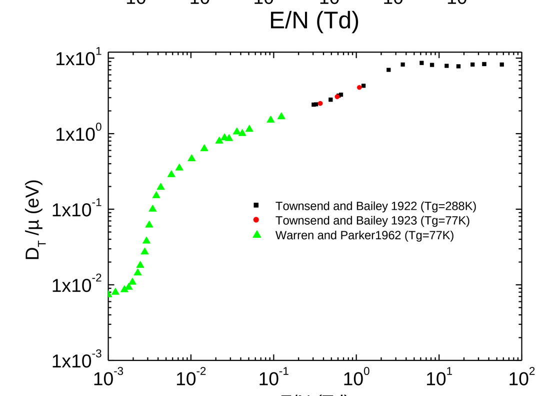
The "effective momentum t ransfer cross section ", useful in a two-term solution of the Boltzmann equation, is the sum of the elastic momentum transfer and the inelastic cross sections.

Experimental databases

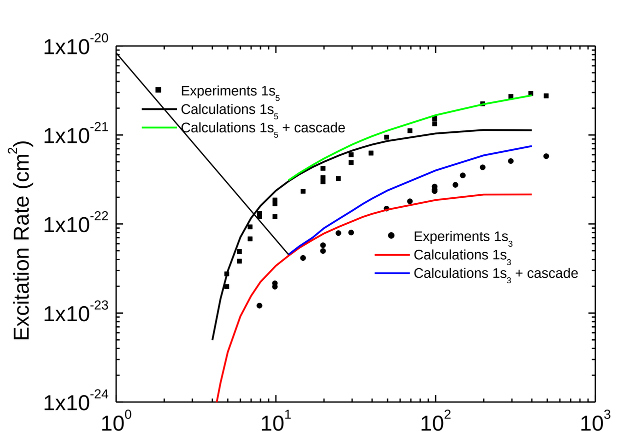
Database	Comments
IST-Lisbon	**Compilation of data used for comparison with calculations.** **See poster QRP1.00064**
De Urquijo	**Pure argon and mixures Ar/C_2F_6, CHF_3**
Dutton-RG	**Rare gas data from J Dutton, "Survey of Electron Swarm Data", J. Phys. Chem. Ref. Data, 4, 577, 1975**
Other-RG	**Rare gas data published later or not appearing in the Dutton review**

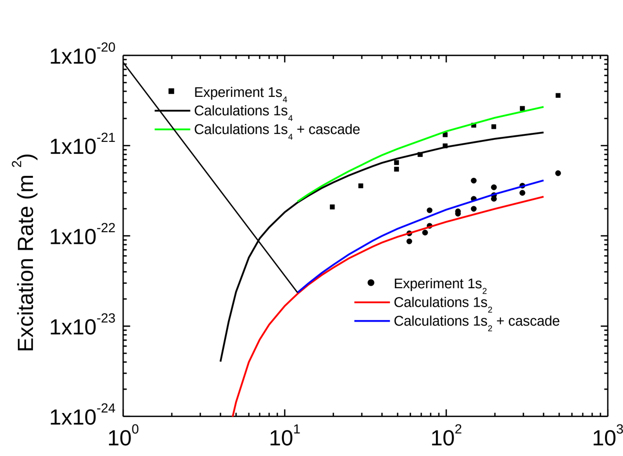
Databases containing experimental results





Excitation rates for selected states, compared to experiment (Tachibana, 1986)





Monte Carlo calculations with Biagi 8.97 cross sections

Remarks on the form of the Boltzmann equation

Boltzmann equation (f is the electron energy distribution function)

$$\frac{\partial f(\vec{r},\vec{v},t)}{\partial t}+\vec{v}\bullet\nabla_r f(\vec{r},\vec{v},t)+\vec{a}\bullet\nabla_v f(\vec{r},\vec{v},t)=C\left[f(\vec{r},\vec{v},t)\right]$$

A complete solution can be obtained with a **Monte Carlo simulation**.
More computationally convenient, is the "**two-term**" expansion which makes several hypotheses , the accuracy of which has been examined in detail previously.

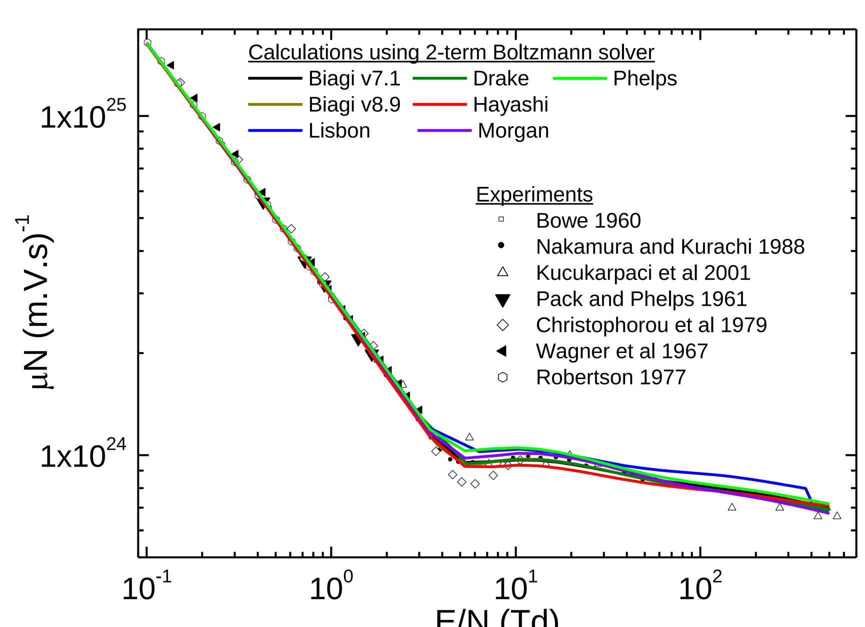
The cross sections enter in the collision operator on the right.
In the two-term approximation, the only cross section information taken into account is the elastic momentum transfer and total cross sections for excitation and ionization (or attachment).

When the electron number is changing, we commonly use one of the following :

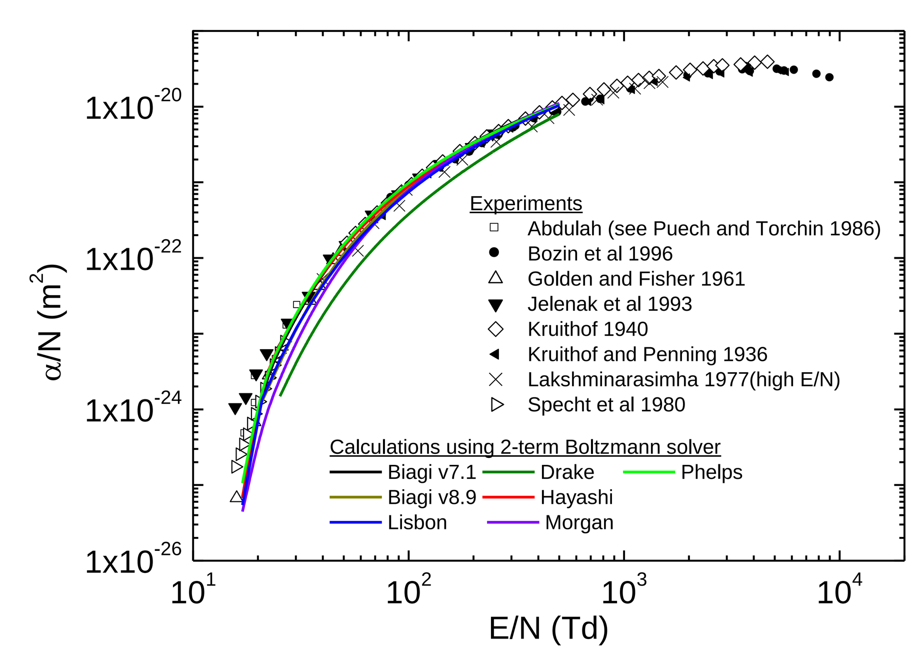
-**Spatial growth model** : time derivative = 0; the exponential growth in electron density with distance from the cathode does not change the shape of f.
Commonly referred to as **SST** for **S**teady-**S**tate **T**ownsend, and corresponding to a particular experimental configuration.
SST has been used in the calculations shown above.

- **Temporal growth model** : spatial gradient = 0; and the time derivative is replace by the product of the ionization frequency and the distribution function.
Commonly referred to as **PT** (**P**ulsed **T**ownsend).

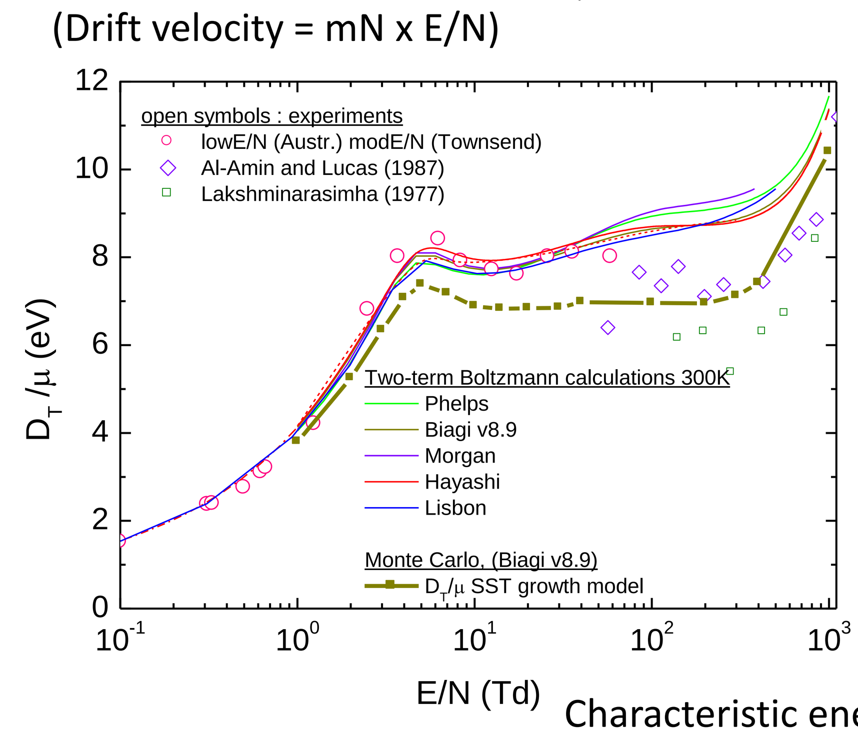
Transport and rate coefficients calculated using LXCat input data and comparisons with experiment

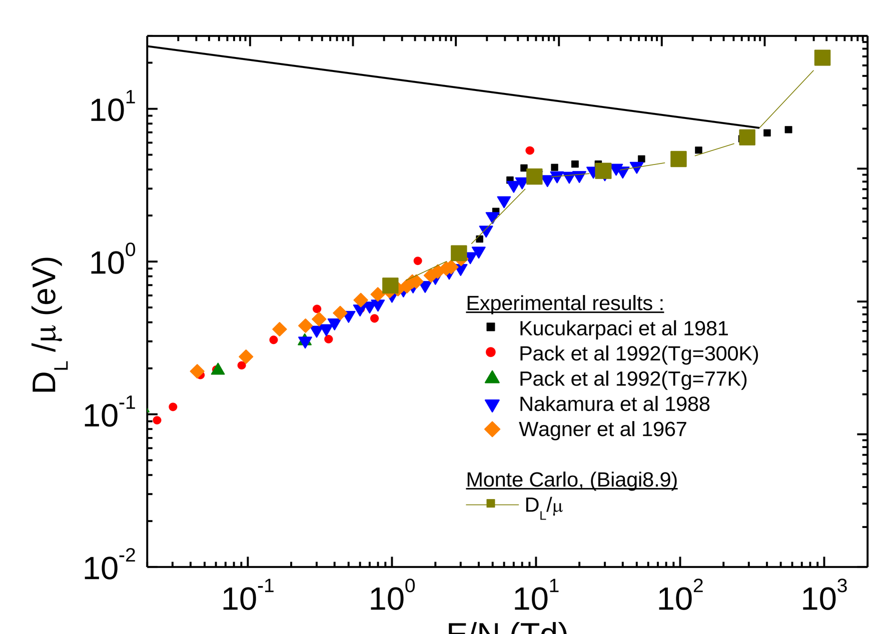


Mobility x neutral gas density **μN vs. E/N**
(Drift velocity = mN x E/N)



Ionization rate coefficient **α/N vs. E/N**



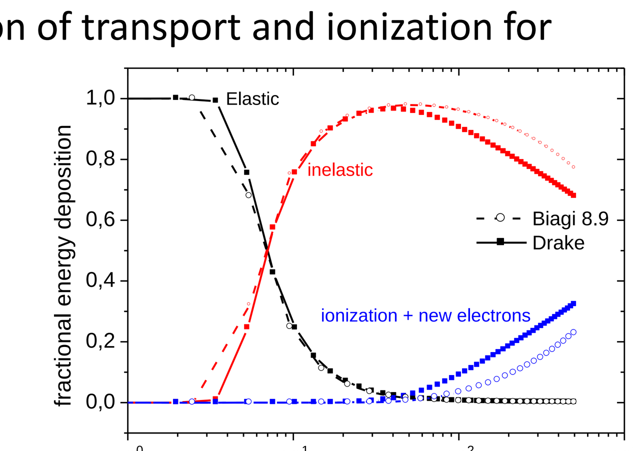


Characteristic energies, **D_T/μ and D_L/μ vs. E/N**

The product of the neutral gas density N and the diffusion coefficient, D_T (transverse) or D_L (longitudinal), is a function of E/N.
The measurable quantities D_T/μ and D_L/μ have units of energy and, while not strictly the average energy, do provide a rough energy scale.

Conclusions

- LXCat provides a convenient means for intercomparisons of cross section data.
- A recently introduced option allows comparison of on-line calculations with data in the experimental databases.
- An option to perform Monte Carlo calculations on-line in LXCat will soon be available.
- The choice of data set will depend on the level of detail needed for the problem being addressed. Collisional radiative modeling will require more detail than, say, calculation of transport and ionization for use in fluid models.
- *Quantum calculations* can provide "complete" sets (!), but they are not yet completely satisfactory.
- The calculated elastic momentum transfer compares very well with swarm derived cross sections, however, the triplet state excitation cross sections seem too high.



Calculated fractional energy deposition in elastic, inelastic and ionization