Data Needs for Modeling of Plasma Processing Reactors

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Abstract. We shall provide a survey of the existing data base normalized using the transport data (swarm method). In particular we shall discuss different strategies to use the existing binary collision data in collisional low temperature plasmas. There is a tendency that increases with time to treat the data bases as black boxes which is tantamount to thinking that responsibility for a possible misuse rests with the provider and not the user. At the same time some of the data bases do not provide all the necessary information required to establish the limitations. Most problems in using swarm data in plasma modeling have been summarized in some of our earlier papers. We list the necessary precautions and discuss resulting errors occurring if those are not implemented. First, it is important to have the full list of sources and modifications that have been made from the original sources. For example cascading contribution from higher levels should be considered in electronic excitation cross sections. Second, it is essential to know the range of data used in a swarm analysis. On the other hand, to avoid numerical instability of the codes we need to put some data at energies higher than those that one can accurately probe. That does not mean that we have much to say about cross sections at those, higher energies. Furthermore, if done, the tests of uncertainty are performed by multiplying the entire cross section by a constant factor. The uncertainty, on the other hand increases towards and even more so beyond the range of energies defined by the swarm data. Swarm data may suffer from non-uniqueness. In other words it is possible to reassign the contribution of some processes to other. As a result one may have multiple sets that may provide good fits for general swarm data. Most data bases and sources in general are based on two term approximation for solving the Boltzmann equation (TTA). If used with TTA the cross sections will return the same data (i.e. accurate results) but that does not mean that the same degree of accuracy will be achieved if mixtures are made or if applied in a more accurate numerical scheme such as Monte Carlo simulation (including the PIC MCC codes) or exact solutions to the Boltzmann equation (moment method or direct numerical procedure). It is important to establish which procedure has been used to produce the cross section data and act accordingly. To our knowledge most swarm analysis has been done without differentiation between flux (velocity space) and bulk (real space) transport properties. Transport coefficients imply hydrodynamic approximation which effectively means that the electron energy distribution function (EEDF) is uniform in real space. This assumption is met in the bulk of most plasmas but fails in the regions where fields are variable and there is a strong non-locality. For higher mean energies (beyond 10 eV) it is necessary to include angular dependence of the cross sections especially in the nonhydrodynamic situations. Redistribution of energy in ionization is also a necessary piece of information that affects the outcome of the analysis / modeling very much. Still it is seldom listed in the papers and almost never in data bases. Some of these issues are addressed in presently available data sets but most are not considered and the main goal of our paper is to reestablish rules for swarm based cross section data sets.