# THE ROLE OF ELEMENTARY PROCESSES IN MODELLING NON-EQUILIBRIUM PLASMAS

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ABSTRACT

Numerous plasma chemical processes of great interest from the point of view of industrial exploitation have been discussed in the literature. A successful application of plasma chemical technologies depends in the first place on suitable experimental conditions, which are mostly determined empirically. The effort for an optimization and economical viability can be greatly facilitated by a detailed knowledge and physical insight into the elementary processes taking place in the plasma, which is used as the reacting medium. The task therefore should be to study a sufficiently comprehensive and exact physical model of the plasma.

In this paper the main attention will be devoted to the case of the non-equilibrium plasma in molecular gas discharges at a low pressure and with a small ionization degree. The electric discharge plasma not only has found application in numerous plasma chemical processes, but also it can serve as a good example for an elucidation of the role of elementary processes in plasma modelling. Such a plasma represents a system which is far from a thermodynamic equilibrium. It contains a small fraction of electrons, which are accelerated by the electric field and whose energy is in collisions transferred predominantly to the internal degrees of freedom of the remaining constituents. The energy stored in the internal degrees freedom, i.e. in the vibrationally or electronically excited molecules or radicals, or in the form of dissociated atoms may then serve for an activation of the reactans, by which the chemical equilibrium is shifted towards a higher reaction yield. The electron gas in the plasma is described by its distribution function, which can be obtained by solving the electron Boltzmann equation. Given a knowledge of the electron distribution the production rates of various interesting excited particle species can be calculated. Then it is possible to formulate a set of non-linear balance (Pauli) equations, from which the concentrations of the pertinent species in a steady state discharge can be determined.

The basic step in the modelling is thus the evaluation of the electron distribution function. In our paper several examples of the electron distribution calculated from the two-term expansion of the Boltzmann equation are presented, mainly for

the case of $O_2$ and $N_2$ and the solution methods are briefly described.

Futhermore, the influence of the vibrational level population is demonstrated on the example of $N_2$ by inclusion of the superelastic collisions. The results of similar calculations of the electron distribution in a turbulent electric field relevant for the electron beam discharges with plasma chemistry applications are also mentioned. The form of the electron distribution is in the non-equilibrium state shaped by the energy dependence of the electron-neutral impact crosssections and it must be determined for each case individually.

The second step of the discharge modelling is the formulation and solution of the balance equations for the particle species considered. These are essentially the (time independent) continuity equations with the right-hand-side given by various production and loss processes involving either the collision integrals over the electron distribution function (if the particles are produced or destroyed by electrons) or the integrals over a Maxwell distribution (in case of heavy particle collisions). The lateral diffusion loss term is usually replaced by an effective (wall) life-time resulting from a spatial averaging of the particle densities. This step of discharge modelling is again illustrated on the example of an $O_2$ discharge. A number of elementary processes have been taken into account including reactions involving the atomic negative ions $O^-$. The interaction of the discharge particles with the solid surface (tube wall) was accounted for in the oxygen atom and molecular metastable effective life-times by assuming different values for the atomic wall recombination and wall deactivation coefficients. The spatial averaging to eliminate the spatial dependence of the densities is, however, somewhat vague, because the radial dependence of the densities must be guessed. A deeper physical insight may be gained by a direct solution of the balance equations with the radial terms retained, where the wall phenomenae are included by means of an appropriate boundary condition.

The possibility to separate the calculation in the two subsequent steps is based on the assumption that the unknown particle densities do not entre the electron Boltzmann equation. This is not always the case. If the vibrational level population (of the electron ground state) plays a significant role in the formation of the electron distribution, then a simultaneous solution is rendered necessary. The first step in this direction has been recently undertaken for $O_2$, where the time dependent problem was solved with the simultaneous evaluation of the electron distribution function in each step.

The discharge modelling enables us to asses the role various elementary processes in different discharge regimes under non-equilibrium conditions, to estimate the active particle concentration, which are often inaccessible by a direct measurement, and thus to optimize the external parameters for maximum yields in plasma chemical applications.