

Modeling and sensitivity studies of cc-rf CF₄ plasma

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The aim of this work was to develop a global model describing the bulk plasma of a tetrafluoromethane (CF₄) plasma. A special focus was put on the treatment of higher molecules. We performed energy resolved ion mass spectrometry in a capacitively coupled radio frequency (cc-rf) discharge and compared it to the results of our model. Stability and sensitivity of the model with respect to input data were investigated.

Fluorocarbon plasmas are widely used in plasma surface treatment such as plasma etching, chemical surface modification and thin film deposition [1] [2]. To understand processes in the plasma boundary sheath, as the interaction region between plasma and surface, at first one has to describe the plasma itself. In case of CF₄ we are facing a 'complex' plasma chemistry, e.g. building of higher molecules (C_xF_y) and production of radicals (CF_x). These radicals play an important role in reactive plasma-wall-interaction. Simulation and prediction of properties of CF₄ plasma are quite challenging, especially if one pays attention to the quality of known reaction data (cross sections, reaction rate coefficients, etc.). This is why other plasma simulations often only use a small subset of possible reactions, neglecting especially larger molecules.

We describe the bulk plasma by a global particle balance model in a coupled system of differential equations:

$$\frac{\partial N_i}{\partial t} = - \sum_{i,j} k_{ij} N_i N_j + \sum_{k,l} k_{kl} N_k N_l + Q_{i,feed} - Q_{i,pump} - Q_{i,cs}. \quad (1)$$

All different particles (neutrals, ions, electrons) are created ($k_{k,l}$) and lost ($k_{i,j}$) in a variety of reactions leading to a reaction rate depending on the density of involved particles ($N_{i,j,k,l}$). Stable neutral particles are pumped out of the system ($Q_{i,pump}$) at same rate feed gas is pumped in ($Q_{i,feed}$), so one achieves a constant total pressure. Positive ions are lost from simulation volume by an effective rate ($Q_{i,cs}$) connected to the ion sound speed and the ratio of discharge surface to discharge volume. Hence, one achieves a system of nonlinear partial differential equations describing the temporal development of particle densities, that can be solved very fast using an ODE-solver for stiff problems [3][4].

As an example Figure 1 shows different characteristic temporal development (time scales) of transient and stable particle densities and after nearly 10s the whole system achieves an equilibrium state. In case of neutral species the steady state densities (Tab. 1) are consistent with data from literature [5][6]. CF₄ is still the main species, F₂ as well as C₂F₆ [8] are non-negligible, radicals build a descending order and there is still a lot of atomic fluorine [7] present in the gas phase.

species	CF ₄	CF ₃	CF ₂	CF	F	C	F ₂	C ₂ F ₆	C ₃ F ₈
density [cm ⁻³]	1.07e16	1.05e13	3.13e12	1.12e10	9.42e12	8.54e09	1.45e14	1.33e14	4.33e12

Table 1: Computed neutral densities (50 Pa, 5 sccm CF₄, T_e=2.65 eV)

We performed energy resolved ion mass spectrometry in a capacitively coupled radio frequency discharge. The discharge is ignited between two parallel circular electrodes. The upper electrode is powered at 13.56 MHz over a matching network and the lower one is grounded like the whole chamber. Via an

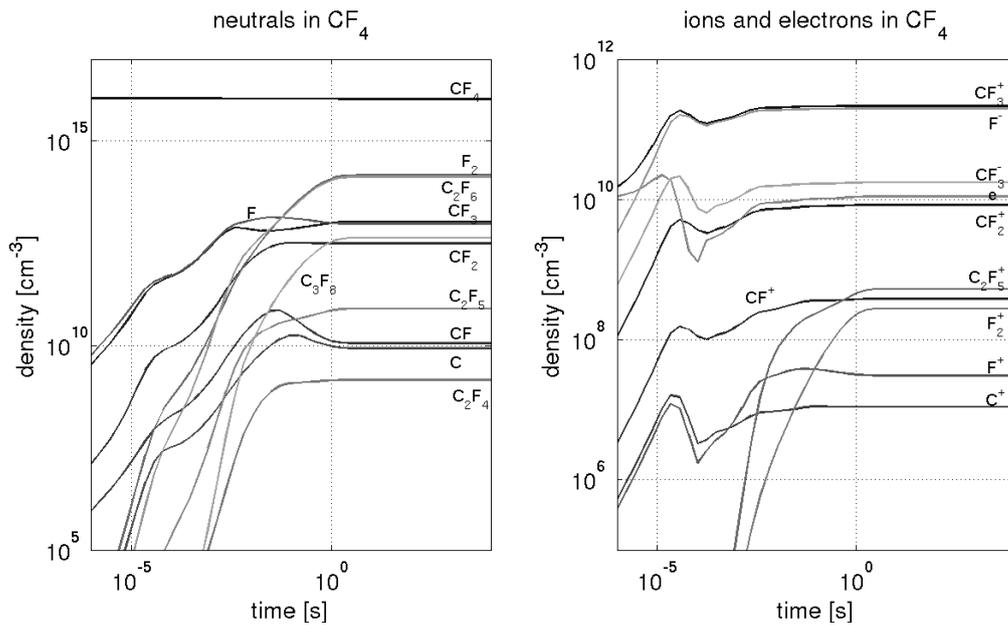


Fig. 1: Solution of a model system (50 Pa, 5 sccm CF_4 , $T_e=2.65\text{eV}$): dependency in time of neutral (left) and electron, positive, negative ion (right) densities.

orifice ($\approx 100\ \mu\text{m}$) in the middle of the grounded electrode ions are transferred into the mass spectrometer. From this setup we gained relative fractions of ionic species, that do not agree well with model predictions. In the measurements CF_3^+ is still the main ion species, but other ion species are much more populated compared to the results of our model. This discrepancy might be caused by interactions of particles in the collisional sheath.

In the used set of reactions, we performed sensitivity studies to gain relevance of different reactions and correlations. Analysis of eigenvalues and eigenvectors of the differential equation system at equilibrium offers the possibility to get information about the importance of species and their interaction among each other. Eigenvalues of such a system show relevant species with great influence on the equilibrium. In steady-state the eigenvectors represent the direct influence of all species on each other. To show the indirect influence of species among each other variations of reaction rates have been applied and their response to the dynamic system is observed. The change of one reaction rate can have a catalytic effect on other species not involved in the primary reaction. The sensitivity studies have proven stability of the model system. A limitation of available data sets with partly estimated values becomes obvious, especially in the density range of smaller radicals and ions.

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