Plasma vs combustion in analytical chemistry: comparing the kinetics of DBD plasma and flame-based atomizers

A. Obrusnik[1], M. Mrkvičková[1], M. Talába[1], J. Kratzer[2], P. Dvořák[1], J. Dědina[2]

[1] *Department of Physical Electronics at Faculty of Science, Masaryk University, Brno, Czechia*
[2] *Institute of Analytical Chemistry of the CAS, v. v. i, Brno, Czechia*

In this contribution, we discuss the reaction kinetics in so-called atomizers, i.e. devices which are used in analytical chemistry to convert molecules of hydride forming elements to free atoms being subsequently detected by atomic absorption or fluorescence spectroscopy. It is known that the atomic hydrogen plays a key role during this process of volatile metal hydrides atomization, and it is produced in conventional atomizers by oxyhydrogen combustion. A logical alternative to the combustion-based atomizers is the DBD plasma, in which the energetic electrons can dissociate the hydrogen molecules directly. We compare the atomic hydrogen production and loss channels in the two respective devices with the help of validated numerical models. We also illustrate the role of advection on the chemistry and atomic hydrogen retaining.

We have previously developed a numerical model which combined a model of the background gas dynamics in full 3D coupled to a 0D kinetics model [1] and was implemented in COMSOL Multiphysics finite-element method package.

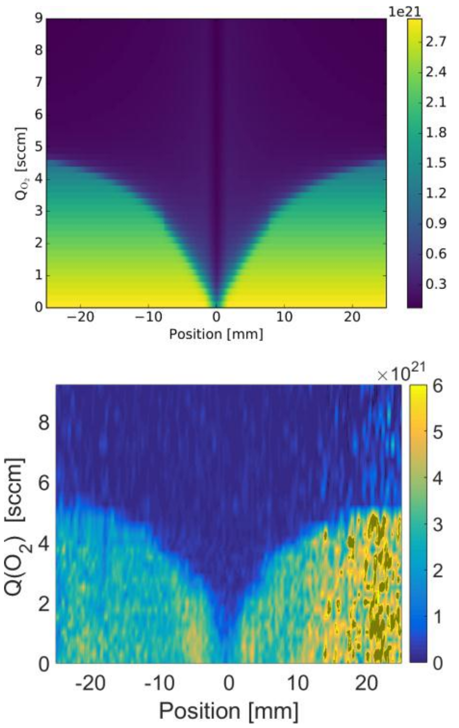

Figure 1: Benchmarking the model with TALIF measurements of atomic hydrogen density for different oxygen admixtures to the plasma.

The gas flow model solves the incompressible Navier-Stokes equation for the mixture of argon, hydrogen and oxygen, and includes diffusion of ambient air into the atomizer (which was, however, previously found to be negligible compared to the impurity of the laboratory gases). By integrating the velocity obtained from the gas dynamics model, we obtain information about spatially resolved gas residence time inside the atomizer which allows us to map the 0D kinetic model onto the 3D gas flow model, on the assumption of neglecting cross-streamline diffusion.

When the model is correlated with TALIF measurements (see figure 1), reasonable agreement is obtained, though it becomes apparent at some conditions [1], that the assumption of negligible cross-streamline diffusion is limiting and the transport of reactive species in this atmospheric-pressure plasma is both advection-driven and diffusion-driven. For this reason, we have begun developing a model which solves the gas flow and kinetics in full 3D geometry and is implemented in the OpenFOAM finite-volume method library which will also be presented and compared to the simpler model.

References

[1] P. Dvořák *et al. Concentration of atomic hydrogen in a dielectric barrier discharge measured by two-photon absorption fluorescence.* Plasma Sources Sci. Technol. **under review**

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