# Simulation of plasma, chemistry, and flow dynamics in flame-based and plasma-based hydride atomizers

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Atomic absorption and atomic fluorescence spectroscopy are typically employed for extremely sensitive element determination. Hydride generation based on a conversion of analyte from the liquid sample into volatile hydride is a very useful approach since the analyte is introduced to the spectrometer in gaseous form [1]. In this contribution, we focus on hydride atomizers, which aim is to convert an analyte hydride to analyte free atoms. Efficiency of their operation directly impacts the limit of detection of the whole analytical procedure [2]. It has been previously shown [3] that the key chemical specie which enables the process and positively correlates with the efficiency of atomizers is atomic hydrogen, H.

In conventional, flame-based, atomizers, atomic hydrogen is primarily produced in an oxyhydrogen flame retarded by argon gas and it was previously confirmed by a combination of (TA)LIF measurements and numerical simulation that the concentrations of atomic hydrogen e.g. in a miniature diffusion flame atomizer can reach as much as $10^{23}$ $m^{-3}$ [4]. This is several orders of magnitude above typical concentration of analyte supplied to the atomizer.

For the reasons stated above, it shows promise to study low-temperature plasmas as an alternative to flame-based atomizers. Plasma is known to be very efficient in decomposition of molecules while maintaining low temperature of the background gas and it could also act as a potent source of hydrogen radicals.

In this contribution, we present a simulation study which combines 2D or 3D gas flow simulation with global plasma modeling of a DBD atomizer. The simulation data is also compared against (TA)LIF measurements to gain more confidence in the models. The primary aim of the work is to explain certain phenomena which were observed experimentally when developing plasma-based atomizers and also to shed some light on the different chemical dynamics of flame-based and plasma-based atomizers.

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