Insight in the complex argon/humid air plasma chemistry, by means of numerical fluid modeling

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Since experimental diagnostics are expensive, time consuming and only a limited amount of information can be obtained, numerical simulations have proven to be very useful n various research fields, but are still not often performed for devicesused in biomedical applications. With thezero-dimensional (0D) fluid dynamics model GLOBALKIN [1], anextensive reaction chemistry set was developed. Several hundreds of reactions were taken from available literature to describe the kinetics between the included species, given inTable 1. In this way it is possible to identify the relevant species, but also the major formation and destruction pathways. It is important to mention that for a plasma jet device, these pathways will change drastically. Inside the device the chemistry is mainly a noble gas discharge with air impurities, followed by mixing Ar/humid air and finally an afterglow region where noble gas is only present in minute quantities.

In a second stage, once the different pathways are unraveled, it is possible to determine a reduced chemistry set for sophisticated two-dimensional (2D) fluid dynamics modeling. In this way a compromise is made between reaction set accuracy and calculation time. The advantage is that with the 2D fluidcode nonPDPSIM [2] much less assumptions have to be made than that there is associated with zero-dimensional modeling, furthermore additional information is obtained. The latter concerns e.g. self-consistent electric field, fluid dynamics (gas mixing), etc.

Table 1: *Included species for the argon/humid air chemistry set.*

Ground state particles	Excited states	Charged particles
Ar	$Ar(^4S)$, $Ar(^4P)$, Ar_2^* $(a\ ^3\Sigma^+_u)$	e^-, Ar^+, Ar_2^+
N_2, N	$N_2(A\ ^3\Sigma^+_u)$, N_2 $(a'\ ^1\Sigma^-_u)$, $N(^2D)$	N_2^+, N_4^+, N^+
O_2, O_3, O	O_2 $(a\ ^1\Delta_g)$, O_2 $(b\ ^1\Sigma^+_g)$, $O(^1D)$	O_2^+, O^+, O^-, O_2^-
NO, NO_2,N_2O,NO_3,N_2O_5		NO^+, NO_2^+,NO_2^-,NO_3^-
NH, HNO, HNO_2, H_2, H		H^+, H_2^+, H_3^+, H^-, ArH^+
H_2O, H_2O_2, HO_2, OH		H_2O^+, H_3O^+, $H_2O_2^-$, OH^+, OH^-

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