Sensitivity analysis of an oxygen chemistry model in cold plasma

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This work presents a sensitivity analysis study based on the original Morris method, improved with refinements from different authors. It details the advantages of using such systematic approach for complex models, as well as its adaptation to the oxygen model implemented in the LisbOn KInetics (LoKI) simulation tool. The robustness and applicability of the method are validated, allowing a future generalization to any type of mixtures. Some non-intuitive results are shown, highlighting the interest of using a well-designed sensitivity analysis to study, control and optimize complex systems.

The impact of numerical models is rapidly increasing in numerous fields, e.g. economics, physics, biology, human migrations, etc. As models become more and more complex, their opacity also grows. In the cold plasma community, typical models can have dozens of species and hundreds to thousands different reactions. In these complex non-linear systems, assumptions made 'by hand' about the relative importance of these reactions might prove to be impossible or even lead to important errors. It is then desirable to have an objective procedure measuring the effect of the reactions on the outputs, rather than relying only on one's intuition. *Sensitivity Analysis* (SA) methods were developed to answer this issue: they aim at providing a ranking of the inputs' influence, while keeping a compromise between accuracy and computational cost. Various procedures are described in the literature [1–6] with different reported efficiencies, and the best suited method can vary from one model to another. Nevertheless, in the low-temperature plasma community the application of these methods is relatively recent, as compared for example with the combustion community [7–9].

In this work we perform a sensitivity analysis of the oxygen chemistry in cold plasmas. The reaction scheme includes a total of 51 species and 179 reactions. The equations driving the electron kinetics and the chemistry are solved with the *LisbOn KInetics* (LoKI) simulation tool [10–12], coupling a Boltzmann and a Chemsitry solvers. We followed essentially the Morris approach for the SA, which consists in varying only one input per simulation and measuring the variations in the outputs. As suggested by different authors, we also test different refinements of the original approach, such as the *grouping method*, an improved sampling of the input values, and the influence of two types of distributions for the input values. The number r of simulations required to have meaningful results is investigated as well and can be assessed in figure 1. The ranking obtained *via* the SA method (table 2) is compared with the one presented by Annůsová *et al.* [13] (table 1) for the density variations of atomic ions O(+,gnd). This example illustrates the interest of the SA, as the most influential reactions identified may not involve directly O(+,gnd) and, as such, are not captured by a direct analysis of creation/loss mechanisms.

Table 1: Main creation (top part) / destruction (bottom part) reactions identified by Annušová *et al.* for O(+,gnd).

Creation/Destruction of O(+,gnd) in [13]	**Rank**
e + O(3P) $\rightarrow$ 2e + O(+,gnd)	1
e + O_2(X,v=0) $\rightarrow$ 2e + O(3P) + O(+,gnd)	2
O(+,gnd) + wall $\rightarrow$ O(3P)	1
O(+,gnd) + O_2(X,v=0) $\rightarrow$ O_2+ + O(3P)	2
O(+,gnd) + O(-,gnd) $\rightarrow$ 2O(3P)	3
O(+,gnd) + O_2(a) $\rightarrow$ O_2+ + O(3P)	4

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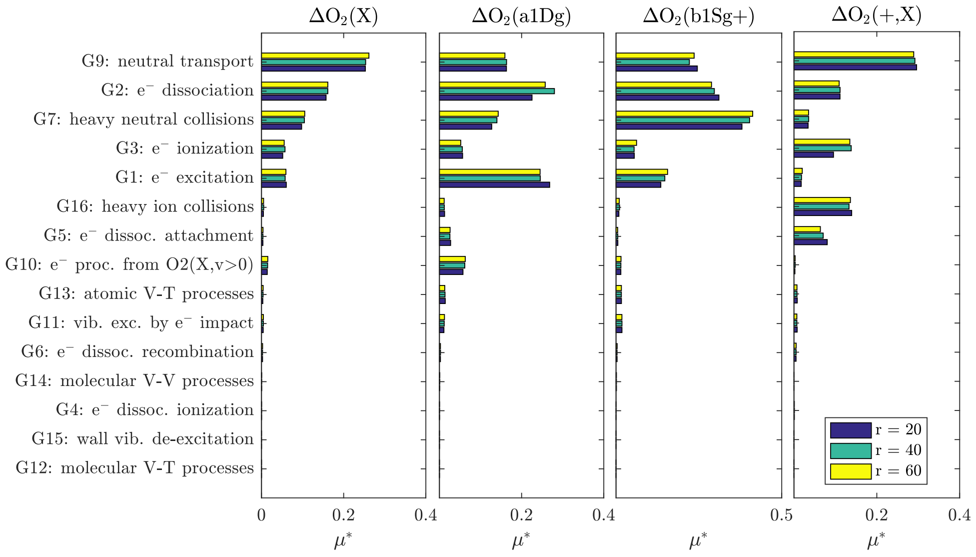

Fig. 1: Example of result from the sensitivity analysis: mean μ^* of the absolute variations in the species densities. The reaction rates varying are grouped into $s_G = 15$ groups. Illustration of the number of Morris trajectories r required to have a consistent ranking.

Table 2: Ranking of the 6 most important processes for O(+,gnd) variations, provided by a full-varying SA (*i.e.* no grouping of reactions).

Variations of O(+,gnd), from the SA	**Rank**	**In [13]**
O_2(+,X) + wall → O_2(X,v=0)	1	No
O(3P) + wall → 0.5O_2(X,v=0)	2	No
e + O_2(X,v=0) → 2e + O_2(+,X)	3	No
e + O(3P) → 2e + O(+,gnd)	4	Yes
O(-,gnd) + O(3P) → O_2(X,v=0) + e	5	No
O(+,gnd) + O_2(X,v=0) → O_2(+,X) + O(3P)	6	Yes

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