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Knowledge-based probabilistic representations of branching ratios in chemical networks: dissociative recombinations in Titan's ionosphere

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Abstract

Experimental data about branching ratios of dissociative recombination of polyatomic ions with electrons is presently the unique information source available to modelers of natural or laboratory chemical plasmas. Yet, because of limitations in the measurement techniques, data for many ions are incomplete. In particular, the repartition of hydrogen atoms amongst the fragments of hydrocarbons ions is often not available. A consequence is that implementation of DR processes in chemical models is difficult, and many models ignore priceless data. Although partial, this information deserves to be considered in detailed chemical models of ionized media. However, the nominal approach of chemistry modeling is not able to cope consistently with partial data. A probabilistic approach, encompassing plausible cases in conformance with experimental data, is necessary to deal with this situation.

1. Method

We propose a novel probabilistic approach based on Dirichlet-type distributions, which enables modelers to fully account for the available knowledge. Distributions of the Dirichlet family are generic tools for sum-to-one variables, easy to implement in a Monte Carlo uncertainty propagation framework, which enable a versatile treatment of the available data about branching ratios. We have shown that they enable to unlock the modeling of complex chemical networks involving partially known dissociative recombination products. The representation of uncertain branching ratios proposed in this work is compact, self-contained and suited for implementation in kinetics databases.

2. Application

As an application, we show how the full scheme affects dramatically the production rate of radicals in a Titan ionospheric chemistry model, when compared with the "standard" H-loss mechanism implemented by default in all recent models.

When compared to the H-loss mechanism, the Dirichlet modeling provides a spectacular enrichment in the chemodiversity and in the production rates of highly reactive neutral radicals (See Fig. 1). Where the H-loss scenario, forming mainly stable neutral species, can be considered as damping the reactivity of neutral species, the full model can be seen as boosting this reactivity, and contributing to molecular growth through radical chemistry. The effect of these radicals on the chemistry of neutral species has now to be quantified by implementation in a ion-neutral coupled model (work in progress).

3. Conclusion

Despite the large uncertainties, DR should not be used as an adjustment variable to compensate for deficiencies in the models. The vast amount of previously discarded information that can now be accounted for through our Nested Dirichlet approach will certainly help to achieve this.

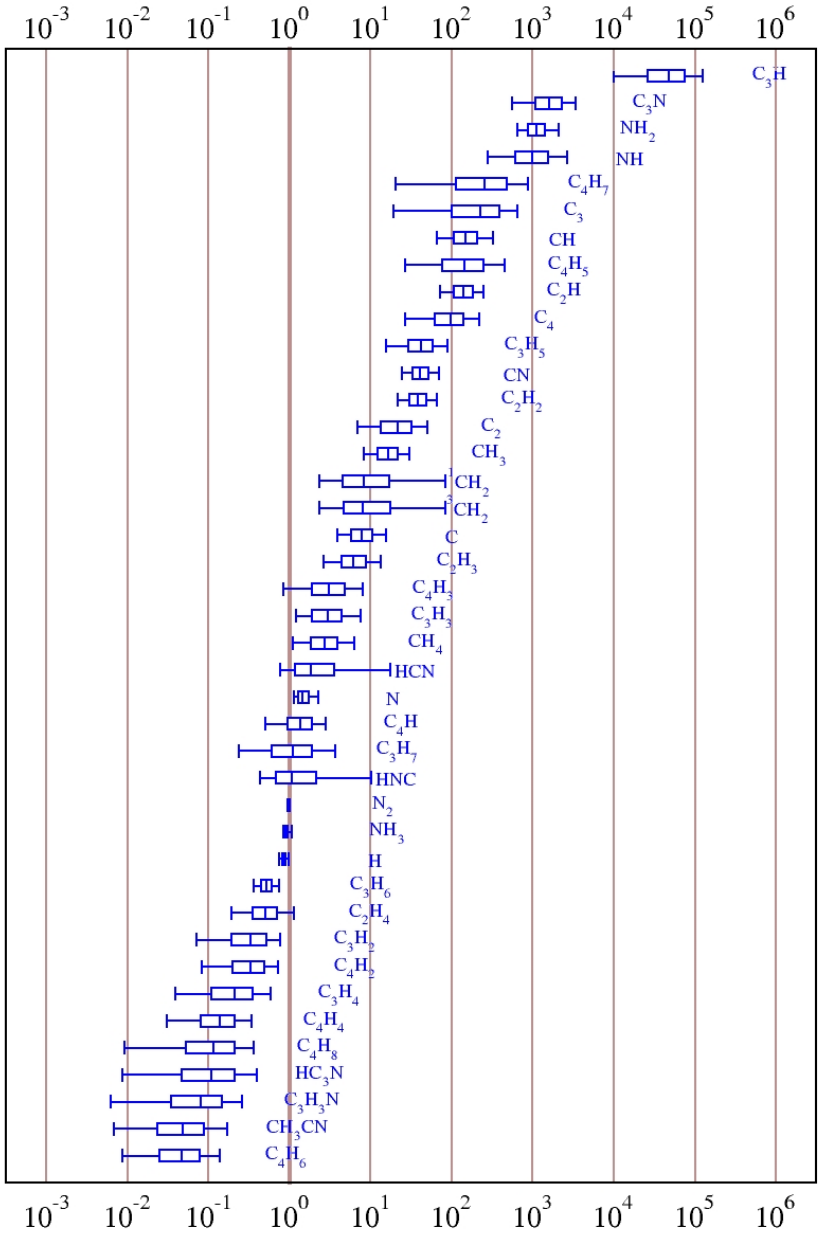

Figure 1: Ratio v_M^{Full}/v_M^{H-loss} of neutrals production rates between the proposed "Full" and standard "H-loss" models of dissociative recombination in Titan's ionosphere.