# Model and experiment comparison of RONS production with an atmospheric pressure plasma as a function of gas temperature

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**Abstract:** Here, a dielectric barrier discharge is investigated. The device is characterized to determine discharge current, dissipated power and plasma events. Deionized water is treated and aqueous nitrate is determined colorimetrically along with ozone density in the effluent. The relation between gas temperature and nitrate production is investigated. Experimental results agree with a 0D reaction network model, using the Zapdos application [1].

## 1. Introduction

Atmospheric pressure plasma production of nitrate has potential in various biological applications, such as agriculture. Water can absorb nitrate produced by these plasmas and then be applied to plants as fertilizer [2, 3]. For plasma production of nitrate ($NO_3$) to be industrially viable, it is important to characterize and optimize this process.

## 2. Methods

An atmospheric pressure dielectric barrier discharge device is used to produce aqueous $NO_3$. Dry air is flowed into the chamber, discharges, and flows out into a volume of deionized water. The effluent then diffuses the generated RONS into the liquid as it transports through. The plasma is characterized with a Pearson coil and voltage probe. The gas temperature of the plasma volume is determined by optical emission spectroscopy of the $N_2$(C-B, 0-0) rotational band, and is varied by adjusting the applied voltage and frequency. The reactive species $H_2O_2$, $NO_2$, $NO_3$, and $NH_4$ are tested for in the treated liquid via colorimetry, of these only $NO_3$ is detected. Optical absorption spectroscopy is used to measure $O_3$ in the plasma effluent as it exits the discharge chamber.

A 0D chemistry model of the plasma (using the Zapdos application in the MOOSE framework) is compared to these experimental results. The model attempts to mimic the resultant chemistry of the effluent as it exits the plasma chamber. It is informed by the physical and electrical characteristics of the experimental device. The primary variable of the model is gas temperature, and is the main point of comparison with the experimental results.

## 3. Results and Discussion

Figure 1 displays the comparison of the modeled and experimental results, with respect to gas temperature. The $O_3$ densities, which peak at $6.5 \times 10^{17}$ $cm^{-3}$ and $1.3 \times 10^{17}$ $cm^{-3}$, display similar trends. Nitrate, despite sharing a similar normalized trend, the modeled density is over an order of magnitude lower than would be expected experimentally, $9.7 \times 10^{15}$ $cm^{-3}$, for all the aqueous $NO_3$ to have originated in the gas phase.

## 4. Conclusions

Both species measured demonstrate strong trends with gas temperature over the measured range. Further investigation of liquid chemistry demonstrates the importance of various other RONS, such as $N_2O_5$, in the generation of $NO_3$ in the treated liquid. Counterintuitively, prioritizing $NO_3$ production in the gas may not be desirable, if trying to obtain higher concentrations.

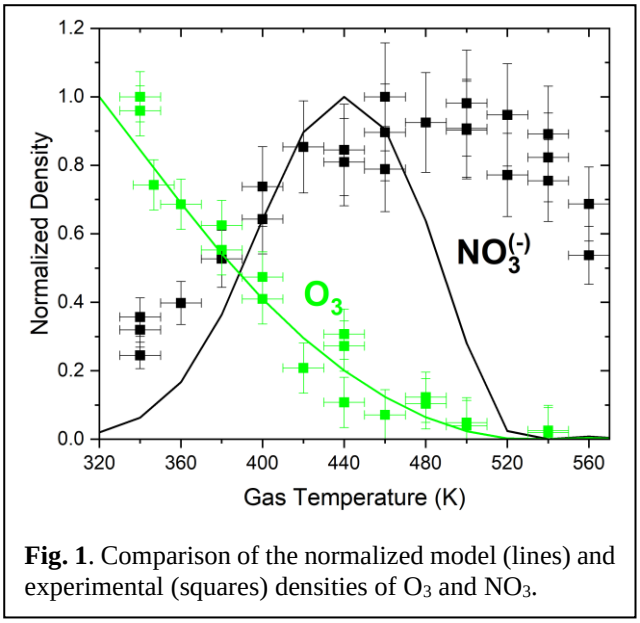


**Fig. 1**. Comparison of the normalized model (lines) and experimental (squares) densities of $O_3$ and $NO_3$.

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## References

[1] Alexander D. Lindsay et al., Journal of Physics D: Applied Physics 49.23 (2016), p. 235204.
[2] Ranieri, Pietro, et al. *Plasma Processes and Polymers* 18.1 (2021): 2000162
[3] C Robinson et al., Current Opinion in Green and Sustainable Chemistry (2024), p. 100978.