DIELECTRIC BARRIER DISCHARGES IN HUMID AIR*

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AGENDA

- **Atmospheric Pressure Dielectric Barrier Discharges**
- **Model**
- **Base Case**
- **Effect of Flow Rate on ROS/RNS**
- **Effect of Humidity on ROS/RNS**
- **Conclusions**

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ATMOSPHERIC PLASMAS

- **Plasma-Medicine**
  - **Reactive oxygen species (ROS) and reactive nitrogen species (RNS) are produced in plasma discharges**
  - **ROS/RNS signal cells, optimal dose is difficult to determine [1]**
  - **Sanitize sensitive wounds without tissue damage [2]**
  - **Reduce the size of cancerous tumors. [3]**
  - **Greater certainty in the fundamental processes required before it could be used on humans − modelling is essential**
- **Environmental Remediation**
  - **Air and surface sterilization, control of air pollutants, CO_2 sequestration have shown promising results. [4]**
  - **Air discharges used on pilot scale for the removal of NO_x and SO_2 from incinerator exhaust. [5]**
  - **Many challenges with scaling up, modeling is valuable.**

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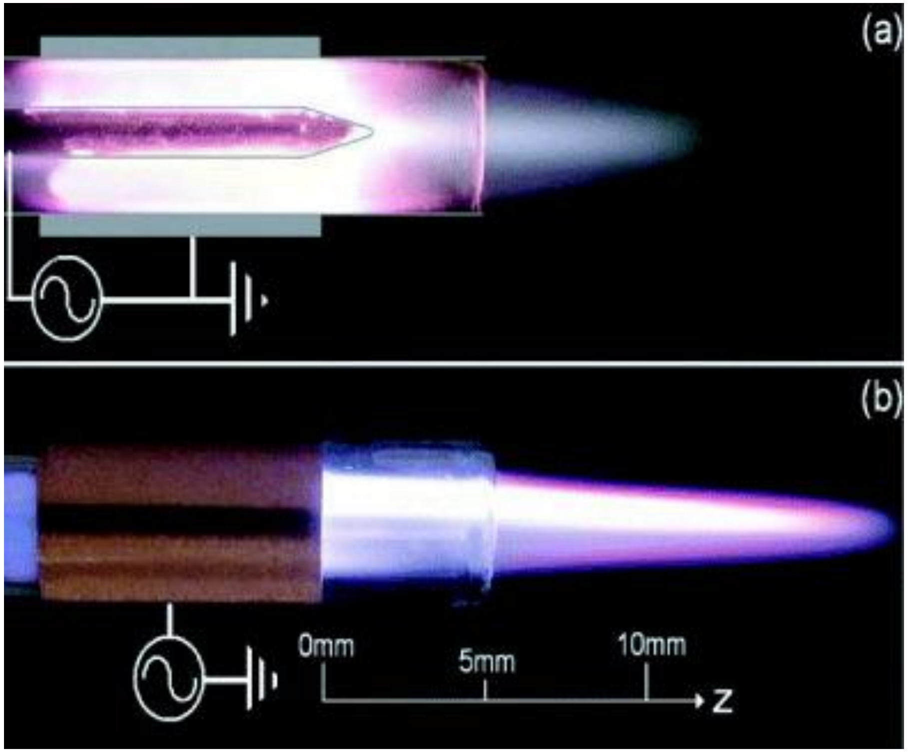
ATMOSPHERIC PLASMAS

- **Examples of atmospheric pressure plasmas devices**
- **This type of DBD discharges below may be used to directly treat wounds or tumors**



- **MG Kong [et al]**

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MODEL: GLOBAL-KIN

- **Global model (0-D) - assumes all densities are uniform throughout plasma volume.**
- **Electron temperature:**

$$\frac{\partial\left(\frac{3}{2}n_e k_b T_e\right)}{\partial t} = \vec{j}\cdot\vec{E} + n_e\sum_i \Delta\varepsilon_i k_i N_i - \sum_l \frac{3}{2} n_e \nu_{mi}\left(\frac{2m_e}{M_i}\right) k_b (T_e - T_i)$$

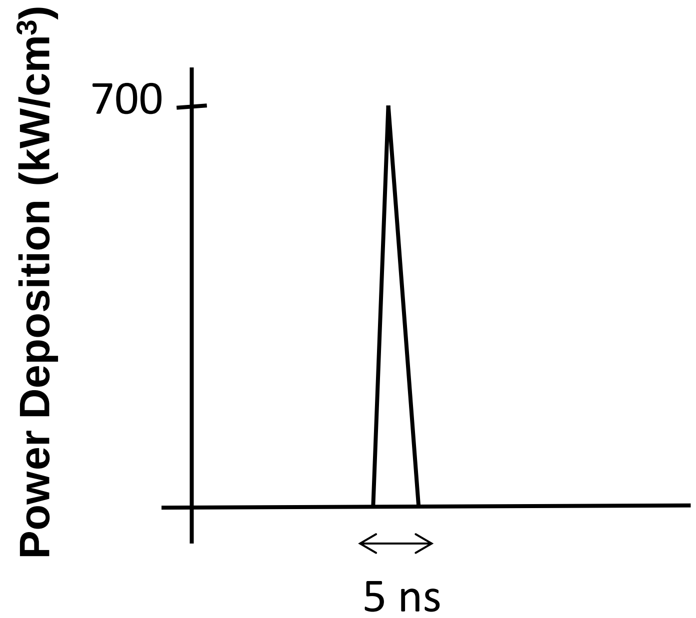
- **Species densities:**

$$\frac{dn_i}{dt} = \sum_j \left\{ \left(a_{ij}^{(L)} - a_{ij}^{(R)}\right) k_j \prod_l n_l^{a_{lj}^{(R)}} \right\}$$

$a_{ij}^{(L)}$ and $a_{ij}^{(R)}$ LHS and RHS stoichiometric coefficients

GAS FLOW & APPLIED POWER

- **Power deposition approximates a DBD**
  - **5 ns pulse**
  - **1 kHz pulse repetition freq.**
- **Flow gas (humid air):**
  - **$N_2/O_2/H_2O$ = 78/21/1**
  - **CO_2 3.5 x 10^{-2} %**
  - **CH_4 4 x 10^{-4} %**
- **Air flow direction, and electrode configuration need not be specified for the global model.**
- **Flow produces a "residence time" for gas in plasma.**



- **Single pulse power deposition**

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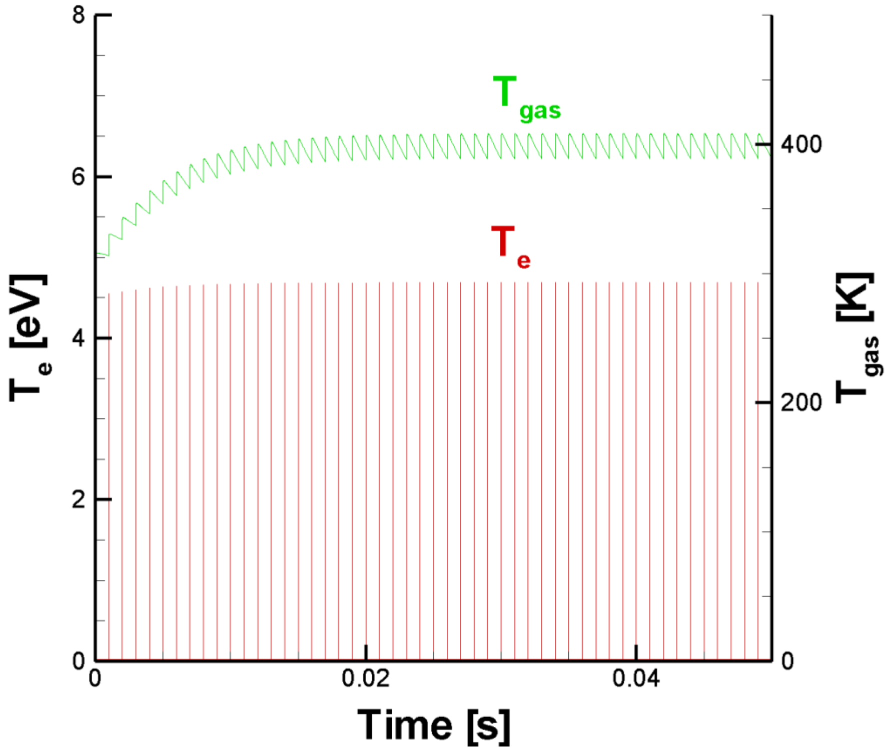
BASE CASE CONDITIONS

- **500 sccm humid air**
- **25% relative humidity**
- **1 kHz pulse repetition rate**
- **Initial and inlet gas are the same composition – all species flow out.**
- **$T_e \approx 4.5$ eV during pulse**
- **T_{gas} increases during pulses due to joule heating – decreases between pulses due to conduction, flow.**



- **T_e, T_{gas} at 1 kHz.**

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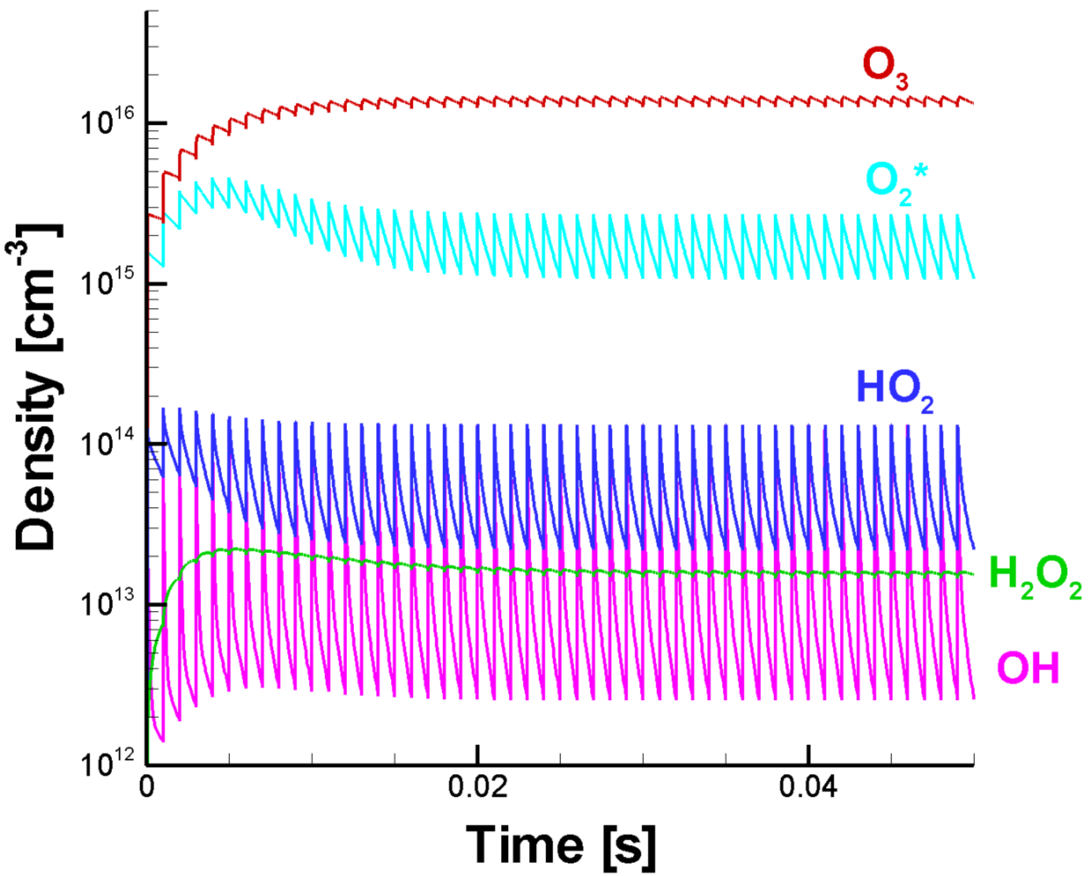
REACTIVE OXYGEN SPECIES (ROS)



- **Electron impact dissociation / attachment of O_2, H_2O during pulse produces O, OH, H, O_2^-**
- **Reactions between pulses:**

$$O + O_2 + M \rightarrow O_3 + M$$

$$H + O_2 + M \rightarrow HO_2 + M$$

$$OH + OH + O_2 \rightarrow H_2O_2 + O_2$$

- **Gas flow (residence time, τ = 9.6 ms) depletes products.**

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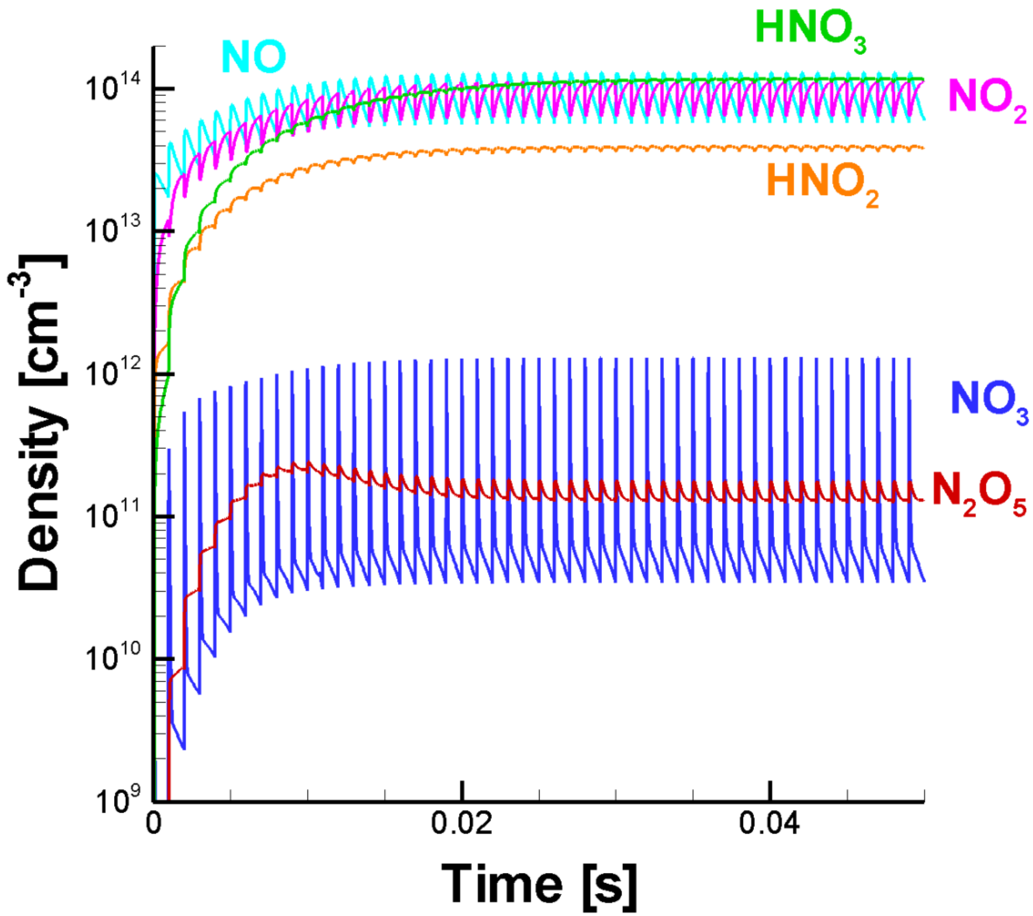
REACTIVE NITROGEN SPECIES (RNS)



- **Terminal RNS include nitrogen oxides (N_xO_y) and acids (HNO_x)**

$$N + OH \rightarrow NO + H$$

$$O + NO + N_2 \rightarrow NO_2 + N$$

$$O + NO_2 + M \rightarrow NO_3 + M$$

$$NO + OH + M \rightarrow HNO_2 + M$$

$$OH + NO_2 + N_2 \rightarrow HNO_3 + N_2$$

- **RNS stabilize after about 0.02 s (20 pulses), which is about 2.1τ**

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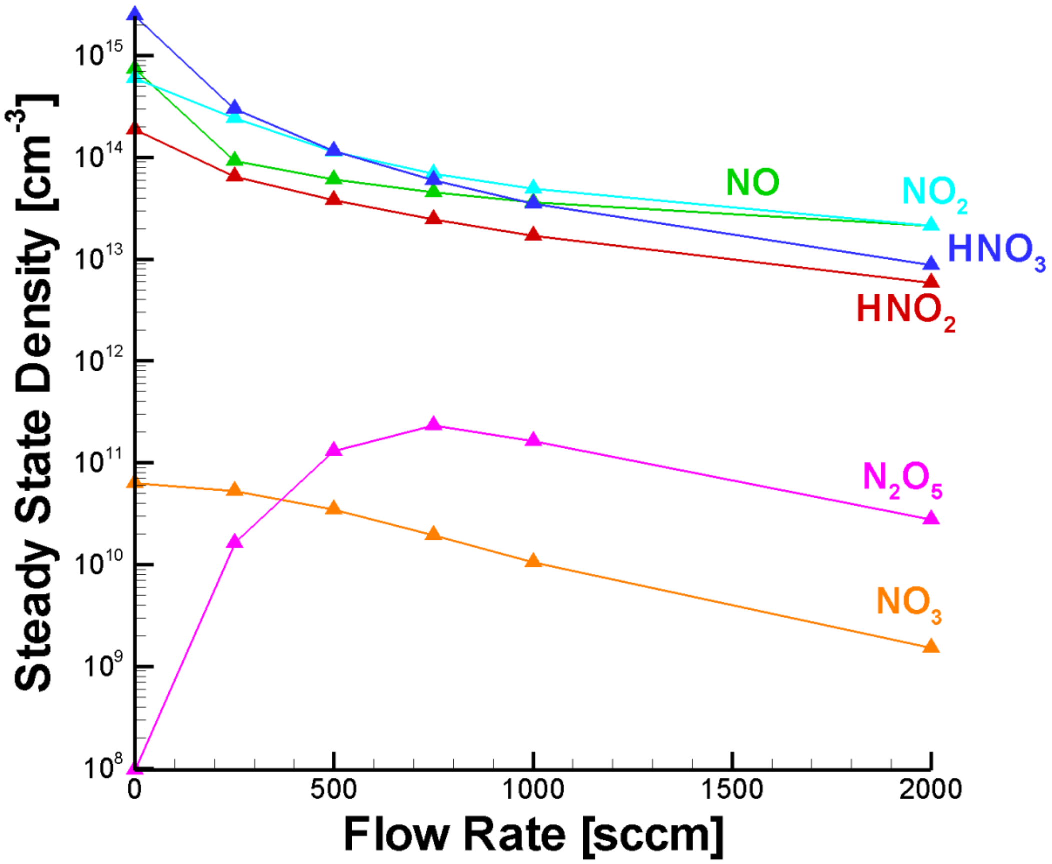
EFFECT OF FLOW RATE - RNS



- Residence time τ decreases with increasing flow rate.
- RNS increase with smaller flow rate as longer τ enables more formation reactions.
- N_2O_5 is an exception:

$$NO_2 + NO_3 + M \rightarrow N_2O_5 + M$$

$$NO_2^- + N_2O_5 \rightarrow NO_3^- + NO_2 + NO_2$$

- N_2O_5 is consumed by a NO_2^- at low flow, limited by NO_3 at high flow.

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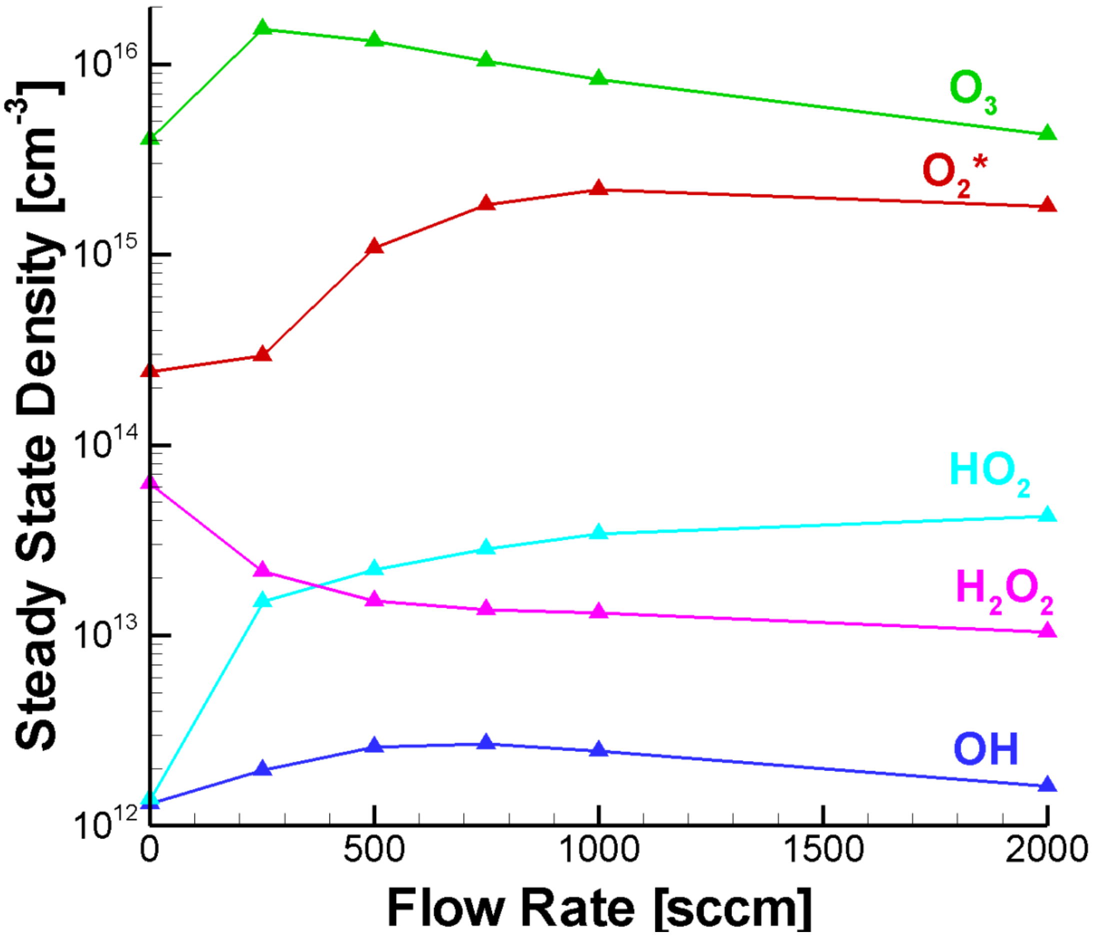
EFFECT OF FLOW RATE – ROS



- In absence of hydro-carbons, ROS are fairly stable and accumulate in discharge.
- ROS do react with RNS:

$$HO_2 + NO + M \rightarrow HNO_3 + M$$
$$HO_2 + NO_2 \rightarrow HNO_2 + O_2$$
$$NO + O_3 \rightarrow NO_2 + O_2$$

- Shorter residence times produce less RNS and so less depletion of ROS.
- Control of ROS/RNS by varying flow rate

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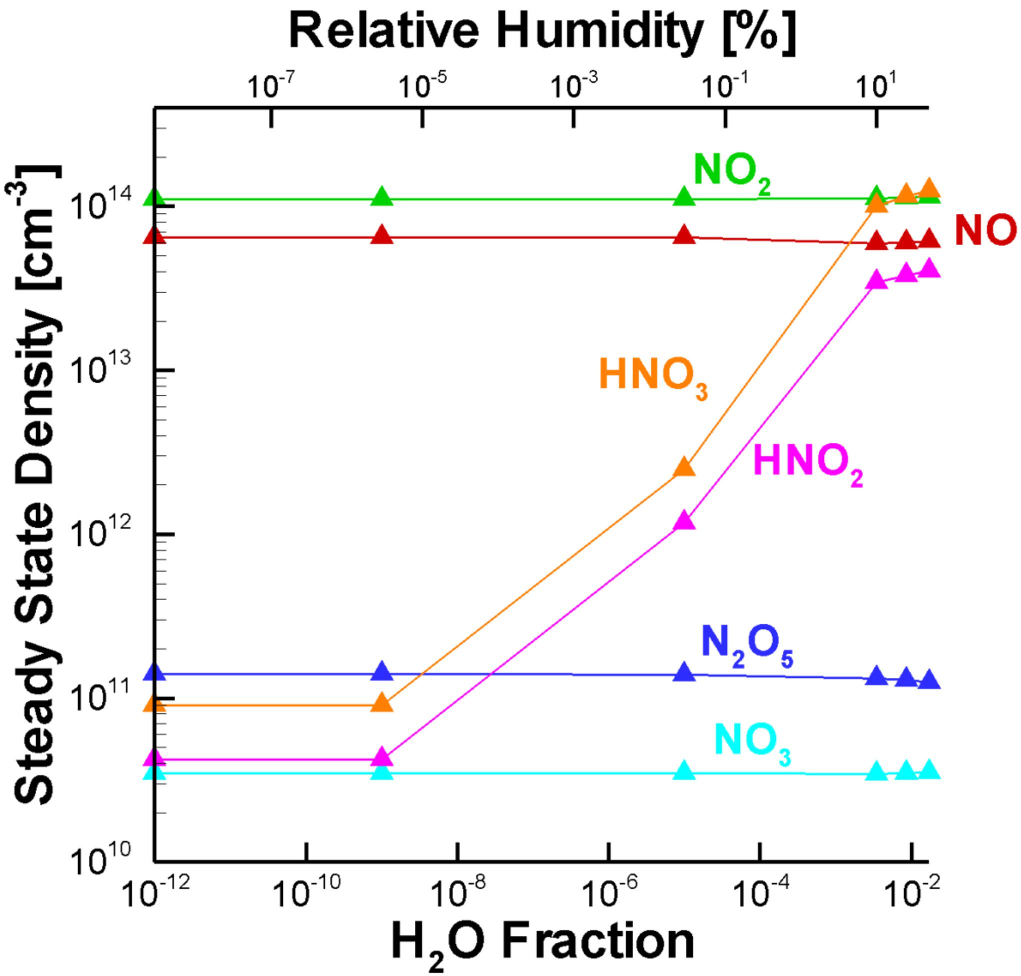
HUMIDITY – RNS PRODUCTION



- **Production of HNO_2 and HNO_3 increase with increasing humidity.**

$$NO + OH + M \rightarrow HNO_2 + M$$

$$OH + NO_2 + N_2 \rightarrow HNO_3 + N_2$$

- **Humidity above 10% does not effect RNS generation**
- **Water impurities below 1 ppb do not effect RNS generation**

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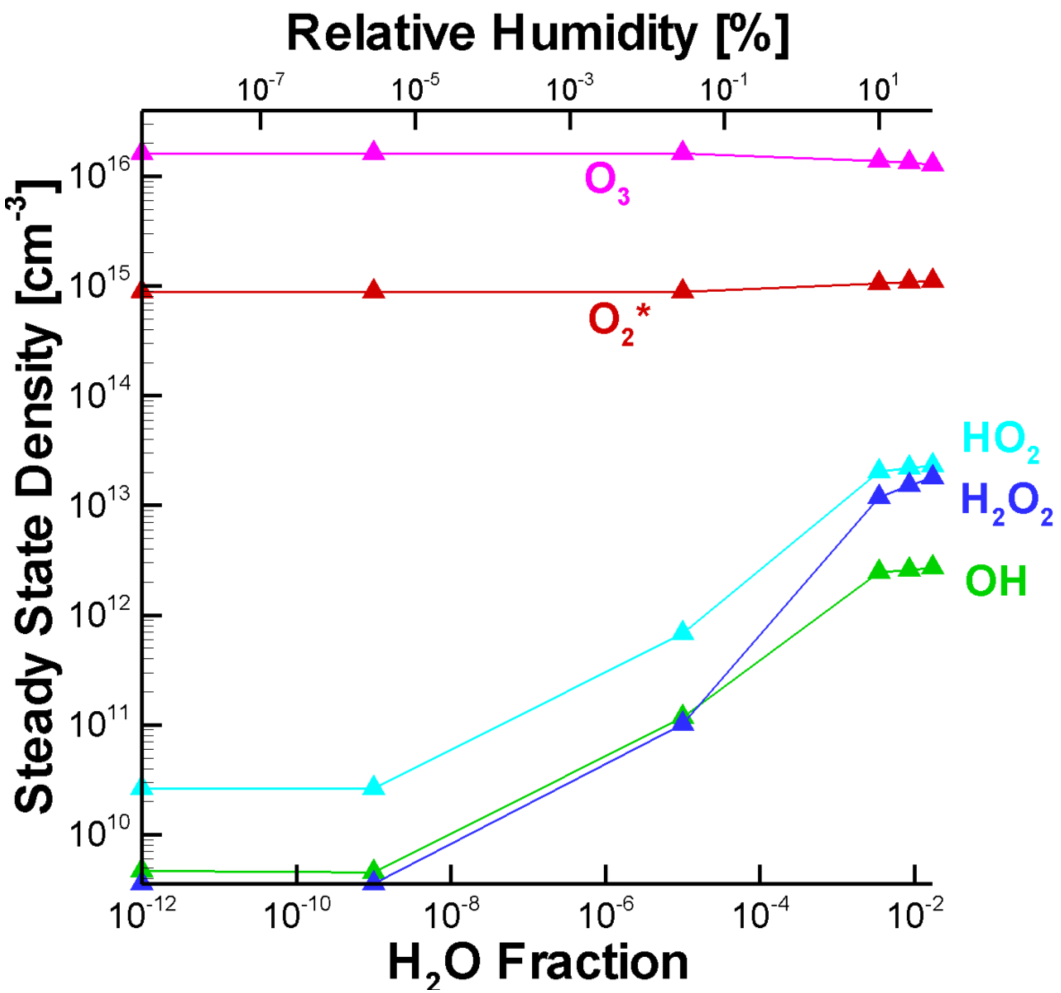
HUMIDITY – ROS PRODUCTION



- H_2O_2, HO_2, and OH increase with humidity – origins are traced to electron impact dissociation of H_2O.
- Humidity above 10% does not affect ROS – likely due to finite energy deposition.
- Impurities less than 1 ppb not important

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CONCLUDING REMARKS

- **Increased flow rates (smaller residence times) decrease RNS densities, except for N_2O_5 .**
- **Increasing humidity increases production of HNO_2, HNO_3 H_2O_2, HO_2, and OH – electron impact dissociation of H_2O.**
- **Water impurities in dry air below 1 ppb, have a negligible effect on ROS and RNS.**
- **Increasing humidity above 10% has a negligible effect on ROS and RNS**
- ***Future Work:***
- **Expand reaction mechanism and validate by comparison to experiment**
- **Improve functionality of Global_Kin to include interaction with a liquid**
- **Analyze devices with a broad range of flow rates, from surface micro-discharges to DBDs and plasma jets.**

REFERENCES

[1] D. B. Graves, "The emerging role of reactive oxygen and nitrogen species in redox biology and some implications for plasma applications to medicine and biology," *J. Phys. D. Appl. Phys.*, vol. 45, no. 26, p. 263001, Jul. 2012.

[2] G. Fridman, G. Friedman, A. Gutsol, A. B. Shekhter, V. N. Vasilets, and A. Fridman, "Applied Plasma Medicine," *Plasma Process. Polym.*, vol. 5, no. 6, pp. 503–533, Aug. 2008.

[3] M. Vandamme, E. Robert, S. Dozias, J. Sobilo, S. Lerondel, A. Le Pape, and J.-M. Pouvesle, "Response of Human Glioma U87 Xenografted on Mice to Non Thermal Plasma Treatment," *Plasma Med.*, vol. 1, no. 1, pp. 27–43, 2011.

[4] S. Samukawa, M. Hori, S. Rauf, K. Tachibana, P. Bruggeman, G. Kroesen, J. C. Whitehead, A. B. Murphy, A. F. Gutsol, S. Starikovskaia, U. Kortshagen, J.-P. Boeuf, T. J. Sommerer, M. J. Kushner, U. Czarnetzki, and N. Mason, "The 2012 Plasma Roadmap," *J. Phys. D. Appl. Phys.*, vol. 45, no. 25, p. 253001, Jun. 2012.

[5] H.-H. Kim, "Nonthermal Plasma Processing for Air-Pollution Control: A Historical Review, Current Issues, and Future Prospects," *Plasma Process. Polym.*, vol. 1, no. 2, pp. 91–110, Sep. 2004.