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Electronic State-to-State Modeling of a Recombining Nitrogen/Argon Plasma

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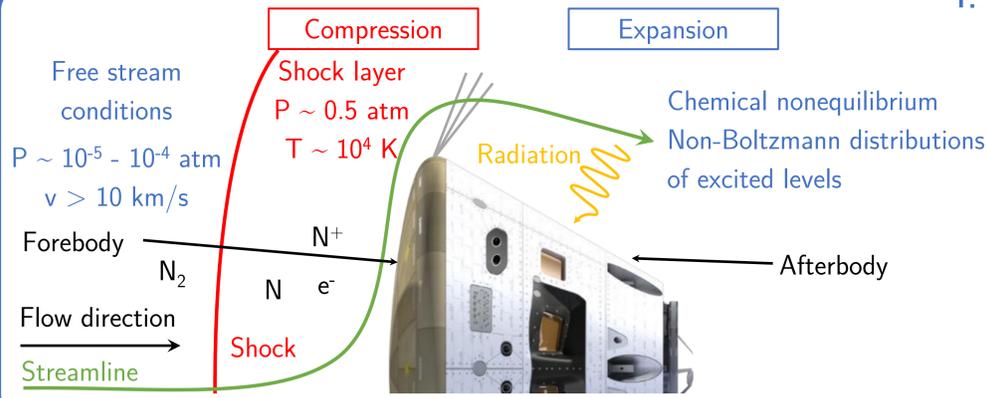
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I. Context



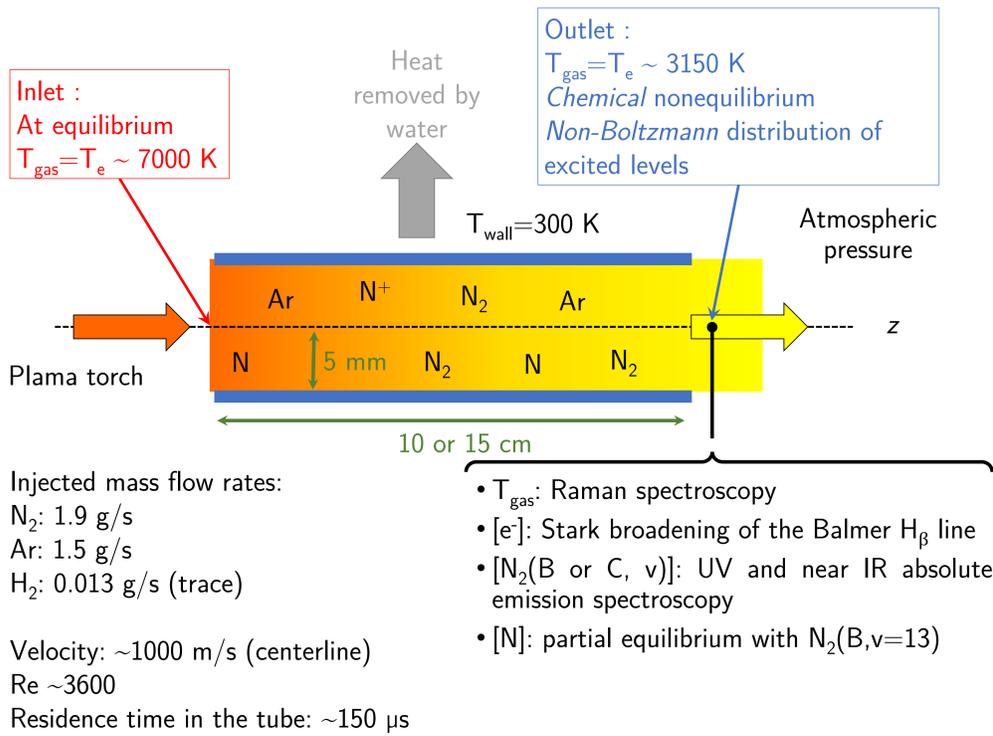
Radiative heat flux on afterbody heatshield is poorly known, which leads to **oversizing of heatshield** (up to 50% of total heatshield mass [1]).

Radiative heat flux is controlled by **atomic recombination**.

Our goal is to **model atomic recombination** of N with a Collisional Radiative (CR) model **validated versus experiments** in a recombination tube. A **vibronic-specific** and an **electronic-specific CR models** are presented and compared.

II. Experiment

Recombination tube experiment [4,5] designed to study N-atom recombination:



Injected mass flow rates:

N₂: 1.9 g/s
Ar: 1.5 g/s
H₂: 0.013 g/s (trace)

Velocity: ~1000 m/s (centerline)
Re ~3600

Residence time in the tube: ~150 μs

- T_{gas}: Raman spectroscopy
- [e⁻]: Stark broadening of the Balmer H_β line
- [N₂(B or C, v)]: UV and near IR absolute emission spectroscopy
- [N]: partial equilibrium with N₂(B, v=13)

III. State-to-State (StS) Models

Comparison between a vibronic-specific StS CR model [6] and the reduced electronic-specific StS CR model assuming Boltzmann distributions of the vibrational levels.

Species	Vib.-specific	Elec.-specific
N	142 levels (ungrouped)	142 levels (ungrouped)
Ar	3 level	1 level
N ₂	X, v ≤ 48 ; A, v ≤ 30 B, v ≤ 33 ; C, v ≤ 28 W, v ≤ 39 ; B', v ≤ 57 A', v ≤ 6 ; a, v ≤ 50 a', v ≤ 58 ; b, v ≤ 48	10 electronic levels
N ⁺	1 level	1 level
Ar ⁺	1 level	1 level
N ₂ ⁺	X, v ≤ 63 ; A, v ≤ 65 B, v ≤ 37	3 electronic levels
Electrons	-	-

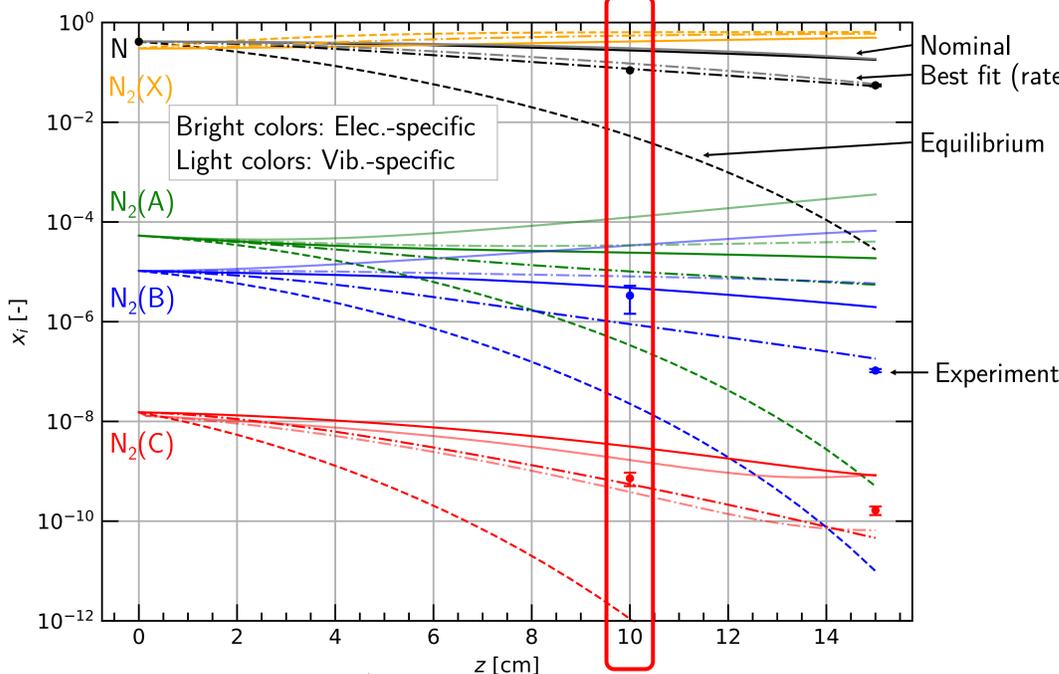
Processes included:

- Excitation
- Dissociation
- Ionization
- Predissociation
- Dissociative Recombination
- Charge exchange
- Quenching, Energy Transfer and Pooling
- Radiation

699 species vs 161 species
241,841 reactions vs 12,143 reactions

IV. Results

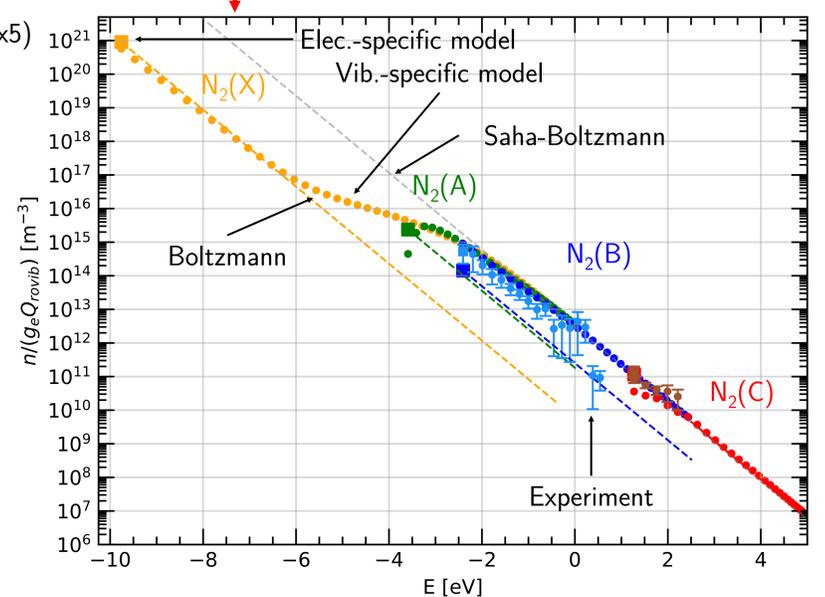
Computed Mole Fractions



Differences between measurements and models results (best fit simulation) at 10 and 15 cm:

	N	N ₂ (B)	N ₂ (C)
Elec.-specific	<1% ; ~6%	Factor 20 ; ~71%	~24% ; Factor 3.5
Vib.-specific	~36% ; ~16%	Factor 2.5 ; Factor 56	~50% ; Factor 2.4

Boltzmann Plot at z = 10 cm
(Best fit simulation)



V. Conclusions

We reduced a vibronic-specific StS CR model into an electronic-specific StS CR model assuming Boltzmann distributions of the vibrational levels and compared them with absolute population measurements in a N₂/Argon recombining plasma. The reaction rate coefficients should be multiplied by 5 to correctly predict N recombination.

Both models predict N and N₂(C) populations within a factor 4. There are larger discrepancies for N₂(B), due to the partial equilibrium between N₂(B, v) and N₂(A, v ≥ 8) that are not captured by electronic-specific StS CR models.

Future work will include concatenation of the electronic-specific model with NO electronic-specific model [7] and comparison with measurements in an Air/Argon mixture.

References

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 [6] Mariotto P., 2022, *Ph.D. thesis*, Université Paris-Saclay
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