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EXPERIMENTAL AND NUMERICAL STUDY OF LAMINAR FLAME SPEED OF AMMONIA/ETHANOL AT HIGH PRESSURE AND TEMPERATURE

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Introduction

- Ammonia = promising energy and hydrogen carrier.
- To optimize the global efficiency of energy systems : to retrieve its energy content through optimized combustion processes.
- To enhance the ignition and combustion development → blend ammonia with another 'neutral' carbon fuel as bio-alcohols

Objectives:

- To provide laminar flame speed data for NH₃-C- Bio-ethanol blend
- simultaneously different levels of temperature and pressures
- as usual in an internal combustion engine, up to 10 bar and 600K.

Experimental set-up

- Flame chemiluminescence visualization to obtain the radius evolution with a CMOS camera (PHANTOM V1611) with adapted frame rate :
 - 5 000 fps for ammonia only
 - up to 15 000 fps for ethanol only due to the laminar flame speed difference.

- Initial pressure P₀ = 1 and 2 bar , initial temperature = 423.15 K,
 - enabling to process data up to 650 K and 10 bar (for P₀=2bar).

- Stoichiometric equivalence ratio with the following equation of combustion :

$$X_{NH_3} NH_3 + (1 - X_{NH_3}) C_2H_5OH + \frac{3(1-0.75X_{NH_3})}{0.21} (0.21O_2 + 0.79N_2) = Products \quad (1)$$

With:
$$X_{NH_3} = \frac{n_{NH_3}}{n_{C_2H_5OH} + n_{NH_3}}$$

- Measurement of the laminar flame speed S_u** by using both pressure and flame radius growth relying on the hypothesis of **an isentropic compression of the unburned gases** following the ignition and resulting in a **simultaneous increase of both pressure and temperature for the unburned gases within the vessel**.

Determination of S_u
$$S_u = \frac{dR_f}{dt} - \frac{(R_0^3 - R_f^3) dP}{3\gamma_u R_f^2 P dt}$$

- Where R_f and R₀ are the radius of the flame and the spherical chamber respectively, P, the pressure, and γ_u, the heat capacity ratio of the unburnt gases at the corresponding radius R_f.

- Two kinetics mechanisms tested : CEU [1] and one merged from PCRL [2] and Shrestha [3] and with the PREMIX module from the ANSYS CHEMKIN-PRO package.
- The numerical simulations set with a 10 cm grid, curvature and gradient criteria of 0.1 and 0.05 respectively, multicomponent transport, and Soret effect.

Table 1: Mechanisms tested with their range of validation

Mechs	Fuels	Φ	P	T	Ref
CEU	NH ₃ /H ₂ -CH ₄ -CH ₃ OH-C ₂ H ₅ OH	0.7-1.6	1 atm	298-448K	[1]
PCRL	C ₂ H ₅ OH	0.6-1.4	1-10 atm	300-600K	[2]
Shrestha	NH ₃	0.8-1.4	1-10bar	298-473K	[3]

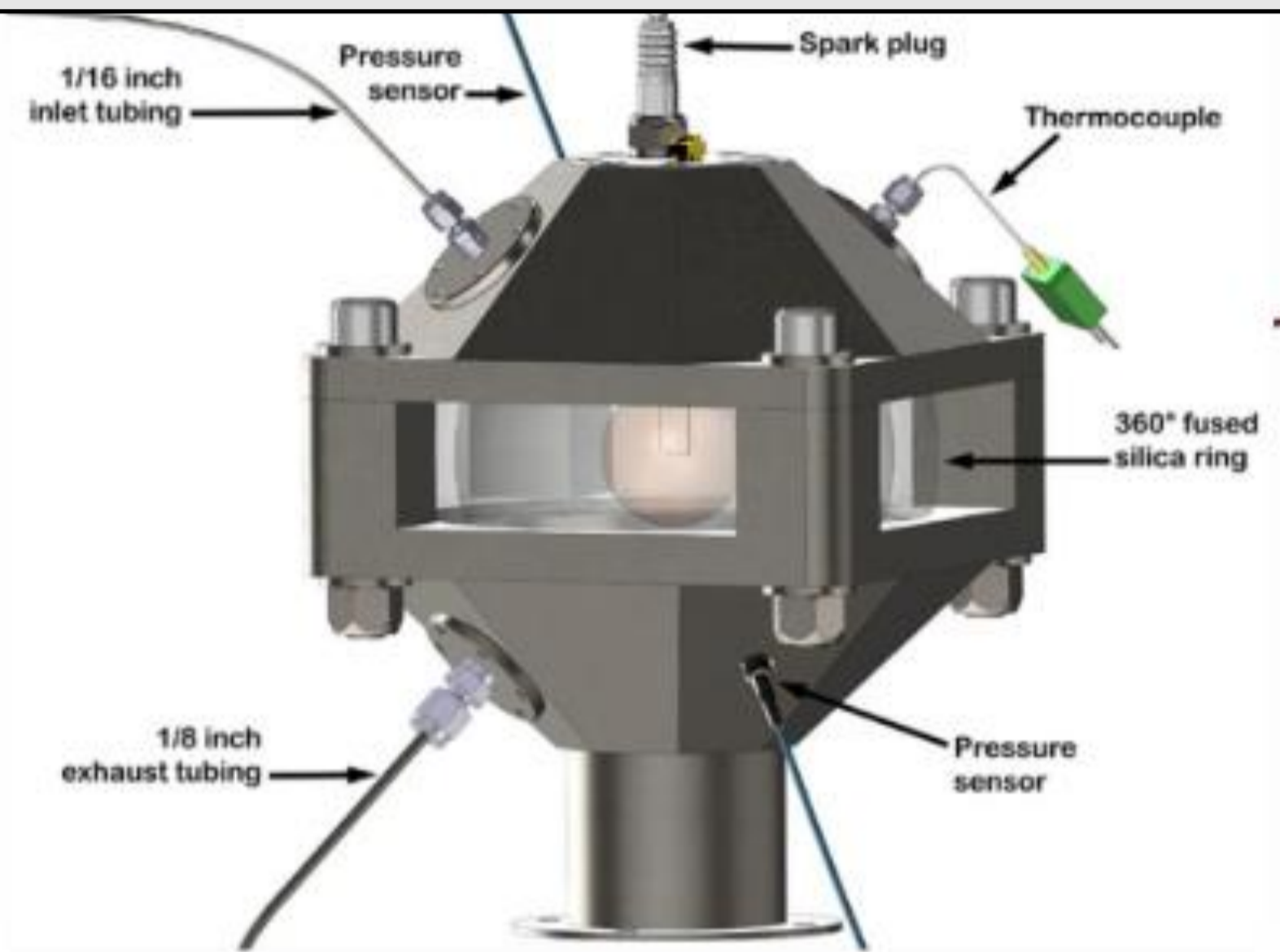


Figure 1: Experimental set-up of the isochoric methodology used [4]

Results

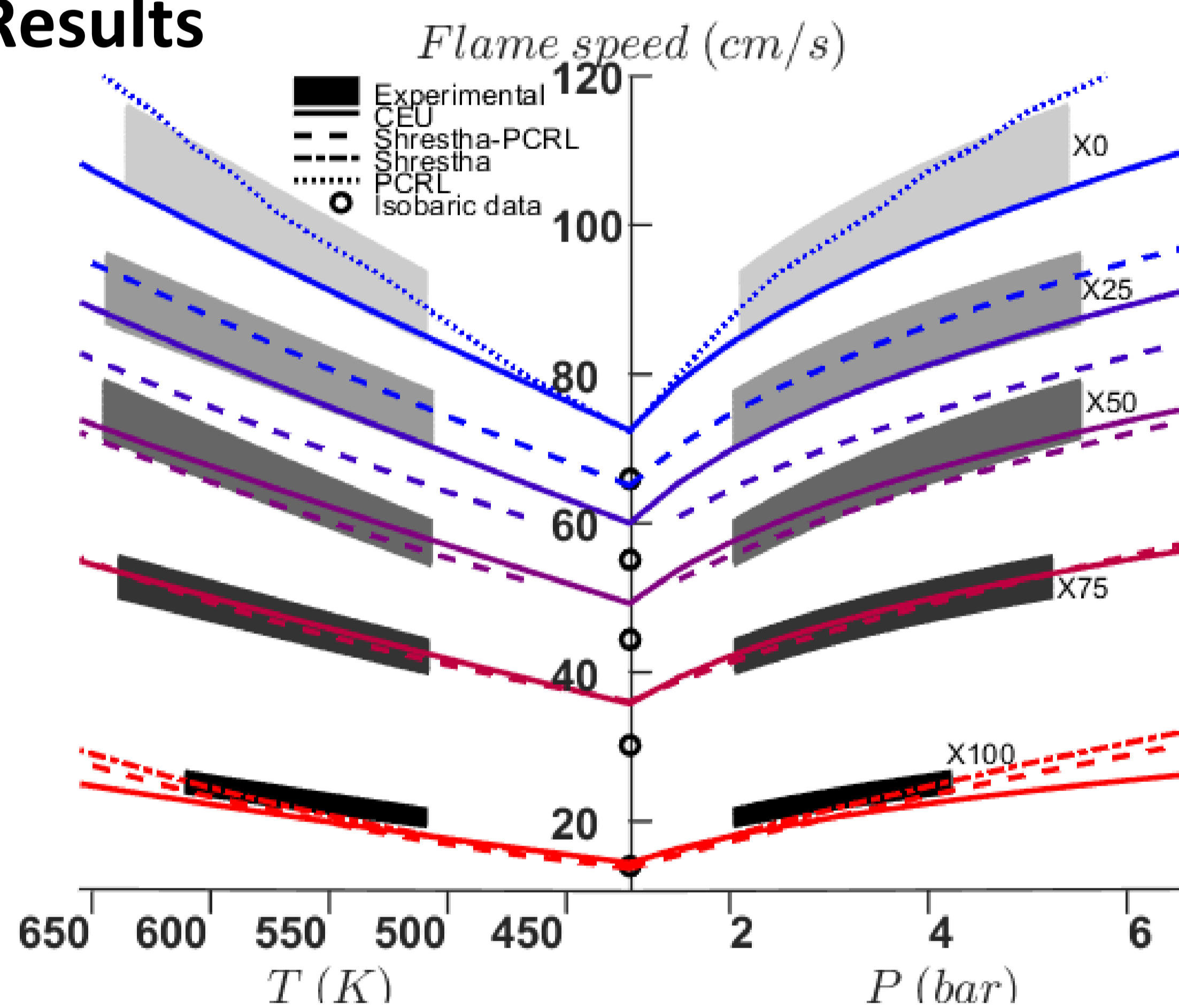


Figure 2. Comparison of predicted laminar flame speed with 2 kinetic mechanisms with experimental values for ammonia/ethanol blends; experimental values: Thickened line colored with a grey scale ; mixing rules: The different linestyles correspond to the laminar flame speed simulated with several mechanisms (blue for ethanol and red for ammonia) for P₀=1 and T₀=423.15 K .

- Simultaneous \nearrow of both P&T in the vessel due to the isentropic compression → laminar flame speed increase.
- Effect of ethanol addition on laminar flame speed not linear:
 - the addition of a small amount of ethanol to ammonia = important reactivity increase**
 - carbon chemistry plays a major role even for low ethanol content.
- CEU mechanism** agrees well with the laminar flame speed **at high temperature and pressure** for the initial pressure P₀ = 1bar but can not reproduce the isobaric points.
- Shrestha-PCRL mechanism** agrees well the laminar flame at high pressure and temperature **for low ratio of ethanol but fails with a high content of ethanol (X0 and X25)**. Oxidation kinetic well optimized for pure ammonia but not for pure ethanol.

Conclusion

- New laminar flame speed data for ammonia/ethanol blends using the isochoric methodology at representative engine condition of pressure and temperature with comparison to kinetic mechanisms.
- The laminar flame speed for the different blends = non linear dependence of ammonia content in the blend :
 - the laminar flame speed increases notably with the addition of a small amount of ethanol suggesting by HCO(+M) ↔ H+CO(+M) and CO+OH ↔ CO₂+H.
- The two mechanism tested reproduce globally the experimental laminar flame speed for the low content of ethanol but for high ethanol ratio X0 and X25 only CEU mechanism

[1] Z. Wang, X. Han, Y. He, R. Zhu, Y. Zhu, Z. Zhou, K. Cen, Combust. Flame 229 (2021) 111392.

[2] S. Roy, O. Askari, Energy & Fuels 34 (2020) 3691–3708.

[3] K.P. Shrestha, C. Lhuillier, A.A. Barbosa, P. Brequigny, F. Contino, C. Mounaim-Rousselle, L. Seidel, F. Mauss, Proc. Combust. Inst. 38 (2020) 2163–2174.

[4] F. Halter, Z. Chen, G. Dayma, C. Bariki, Y. Wang, P. Dagaut, C. Chauveau, Combust. Flame 212 (2020) 165–176.

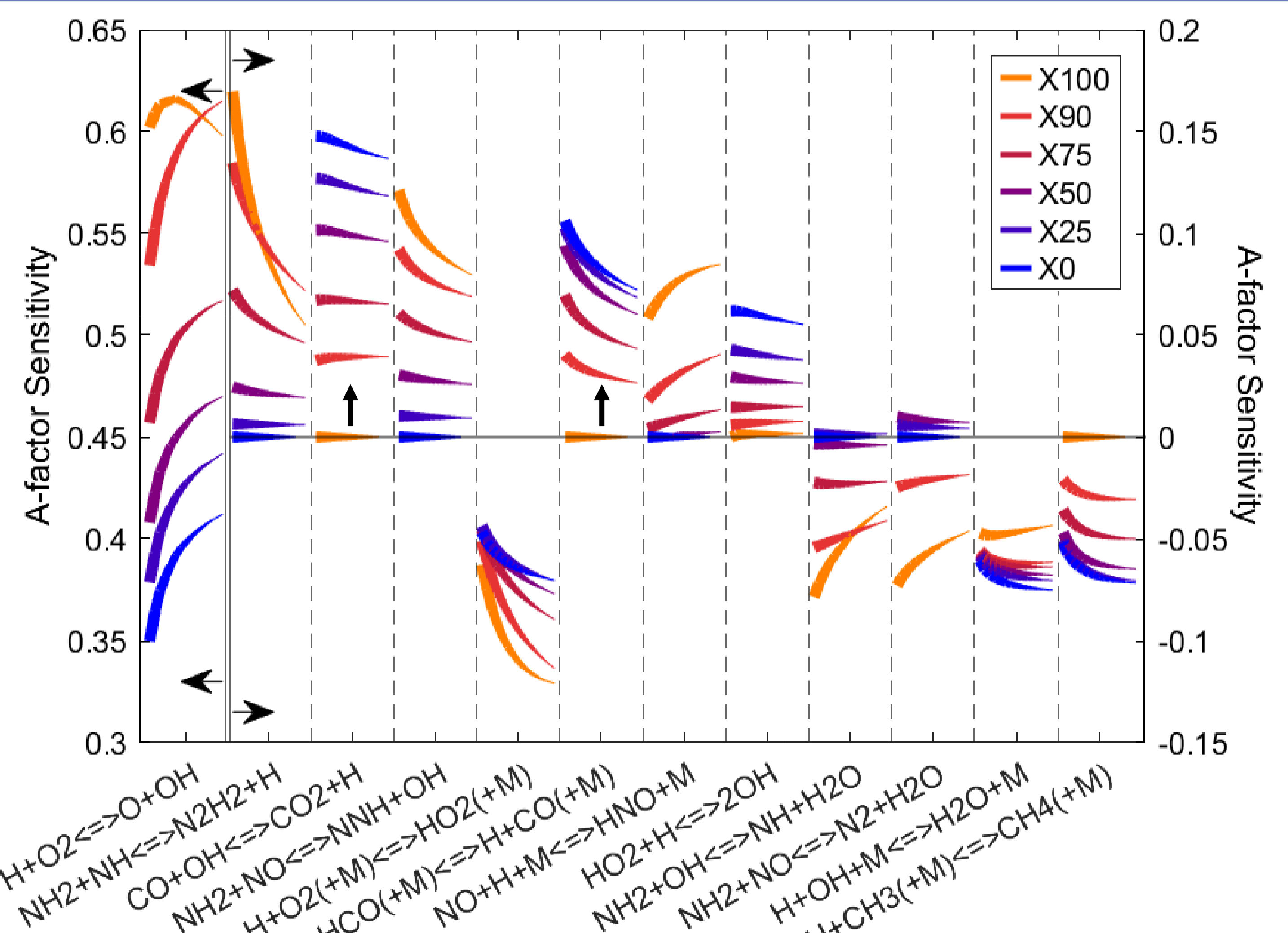


Figure 3. Sensitivity analysis on the flame speed with the CEU mechanism. The thickness of the line corresponds to the evolution of the pressure between 1 bar (thick) to 8 bar (narrow) and the color corresponds to NH₃ content (X).

- Sensitivity coefficients calculated for each blend and each couple (P,T).
- Thickest part of the trace (the left one) = initial condition (1 bar, 423.15K).
- Decrease of the thickness = (P,T) evolution up to 8 bar.
- Mechanism of the decomposition of HCO with the reaction and oxidation of CO :

$$HCO(+M) \leftrightarrow H+CO(+M) \quad CO+OH \leftrightarrow CO_2+H$$
- One of the key to understanding the behavior of the laminar flame speed as a function of the ethanol content.**