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



Ronan PELÉ¹, DAYMA Guillaume², MOUNAIM-ROUSSELLE Christine¹,

BREQUIGNY Pierre¹, Fabien HALTER²

¹Laboratoire PRISME, Univ. Orléans, INSA CVL, EA4229, Orléans 45072, France

² Univ. Orléans, CNRS-ICARE, Orléans, France

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]

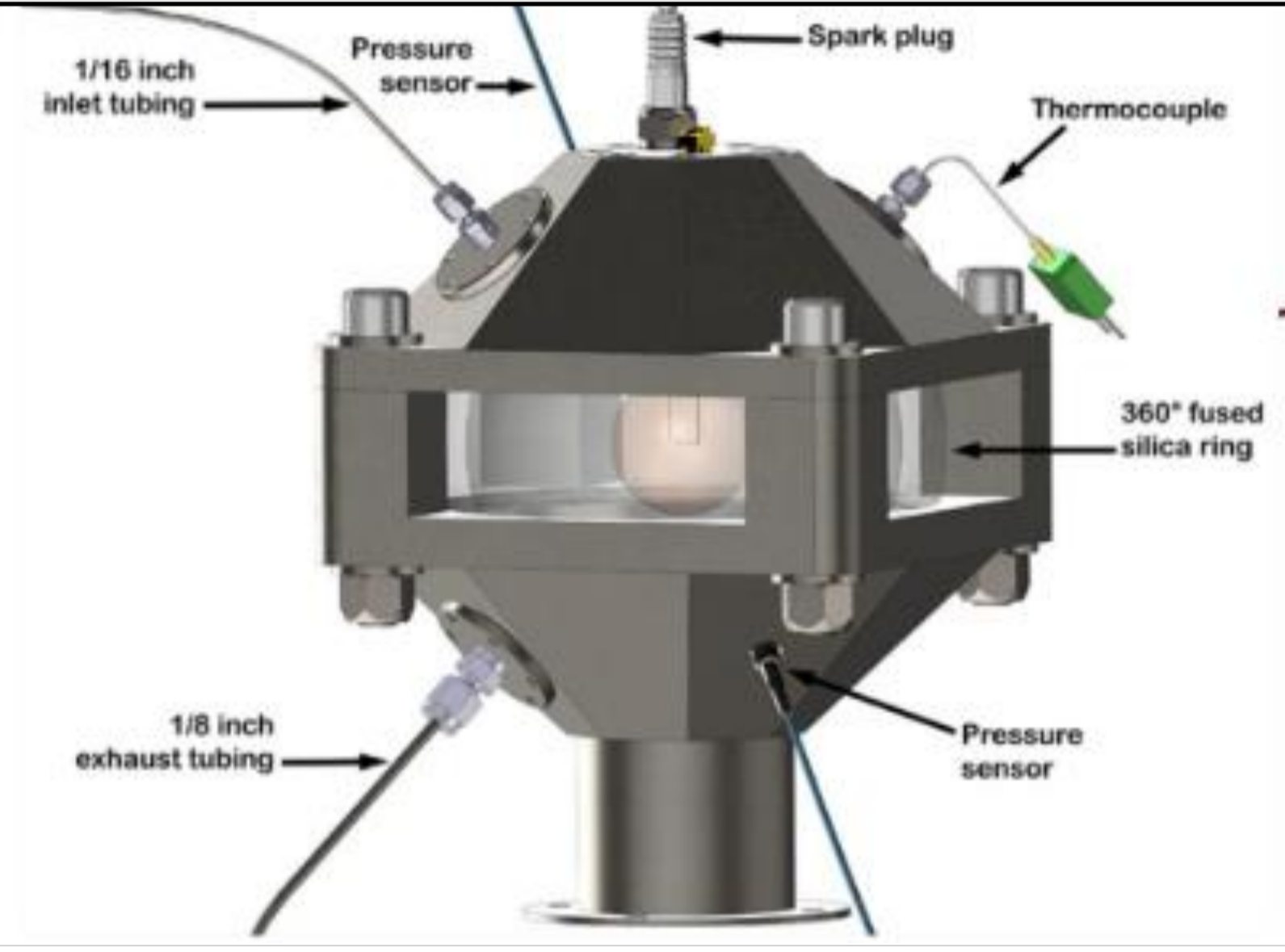


Figure 1: Experimental set-up of the isochoric methodology used [4]

Results

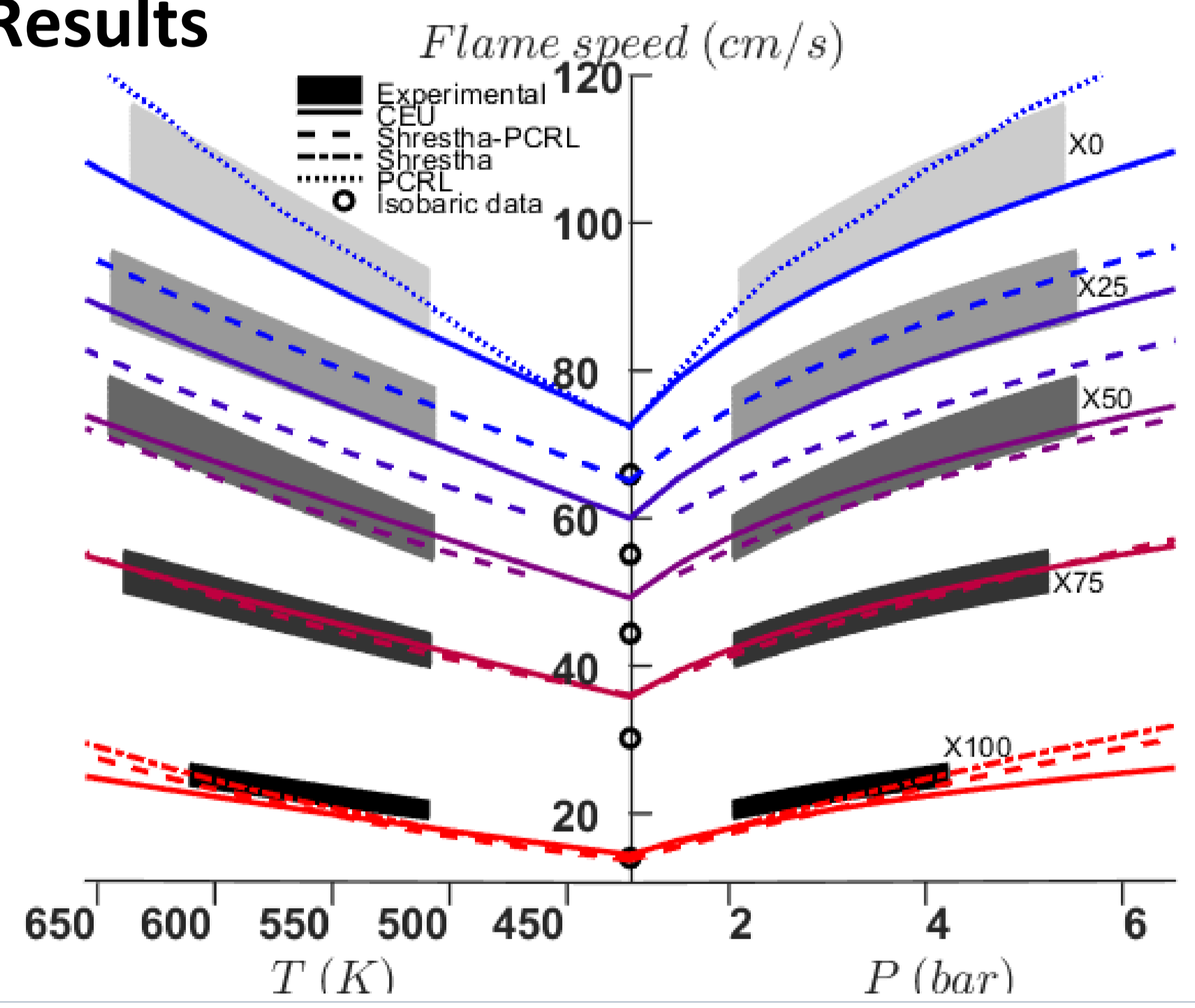


Figure 2. Comparison of predicted laminar flame speed with 2 kinetic mechanisms with experimental values for ammonia/ethanol blends; experimental values: Thickened line colored with a grey scale ; mixing rules: The different linestyles correspond to the laminar flame speed simulated with several mechanisms (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.

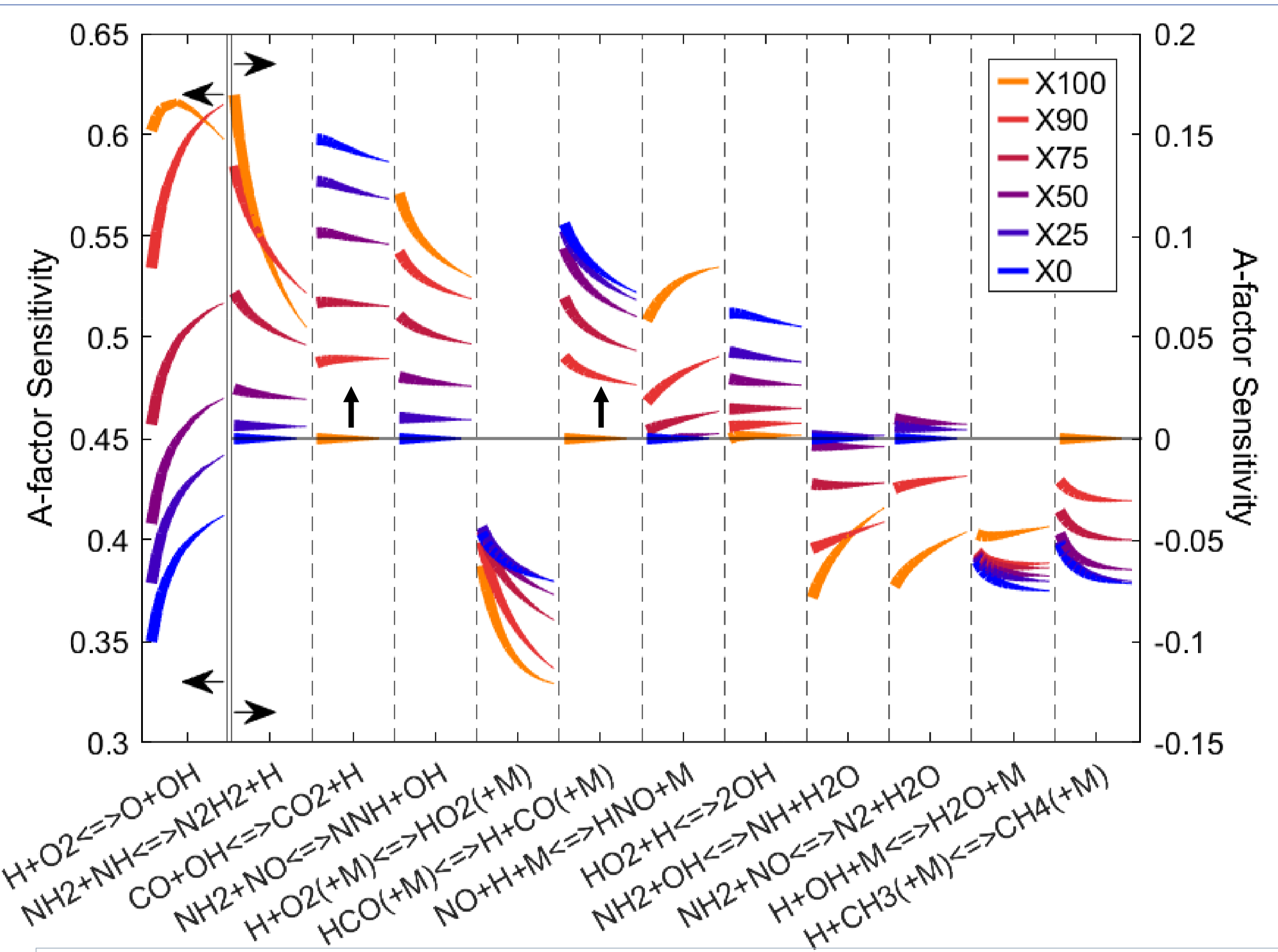


Figure 3. Sensitivity analysis on the flame speed with the CEU mechanism. The thickness of the line corresponds to the evolution of the pressure between 1 bar (thick) to 8 bar (narrow) and the color corresponds to NH₃ content (X).

- 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 :

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

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

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