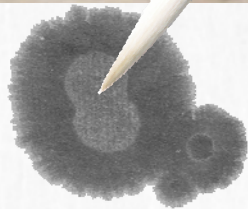




Experimental and kinetic modeling study of a premixed CH₄/O₂/Ar flame doped with components of diesel fuel: Indane



Zhenyu TIAN

LRGP, CNRS, Nancy Université, ENSIC

Roscoff, Mar. 3rd, 2010



Outline

Experimental and kinetic modeling study of a premixed CH₄/O₂/Ar flame doped with components of diesel fuel: Indane

1

Introduction

2

Experimental

3

Kinetic modeling

4

Results and discussion

5

Conclusion

1. Introduction

More efficient, but cleaner engines and fuels is of interest. A better understanding of combustion chemistry is a high priority challenge which must be taken up before any further developments of innovative combustion processes are undertaken.

Diesel fuel



Alkanes
Alkylcyclohexanes
Alkyldecalines
Alkylbenzenes
Polycyclic naphthoaromatic

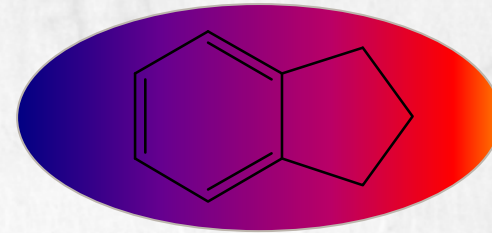
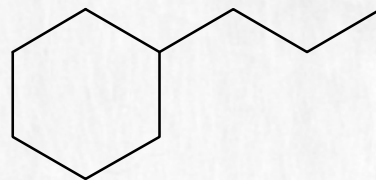
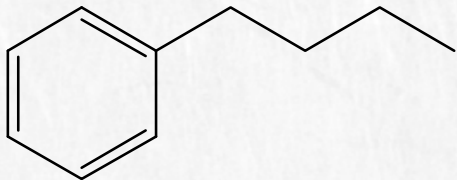


1. Introduction



Naphtheno-aromatics (6.9% wt).

Indane, the simplest naphtheno-aromatic, only one experimental study has been performed in a jet-stirred reactor at Orléans [1] and no models regarding its oxidation has been reported previously.



n-butylbenzene [2] and *n*-propyl-cyclohexane [3]

The purposes of the present work are to experimentally investigate the structure of a premixed laminar methane flame doped with indane and develop a new mechanism for the oxidation of indane.

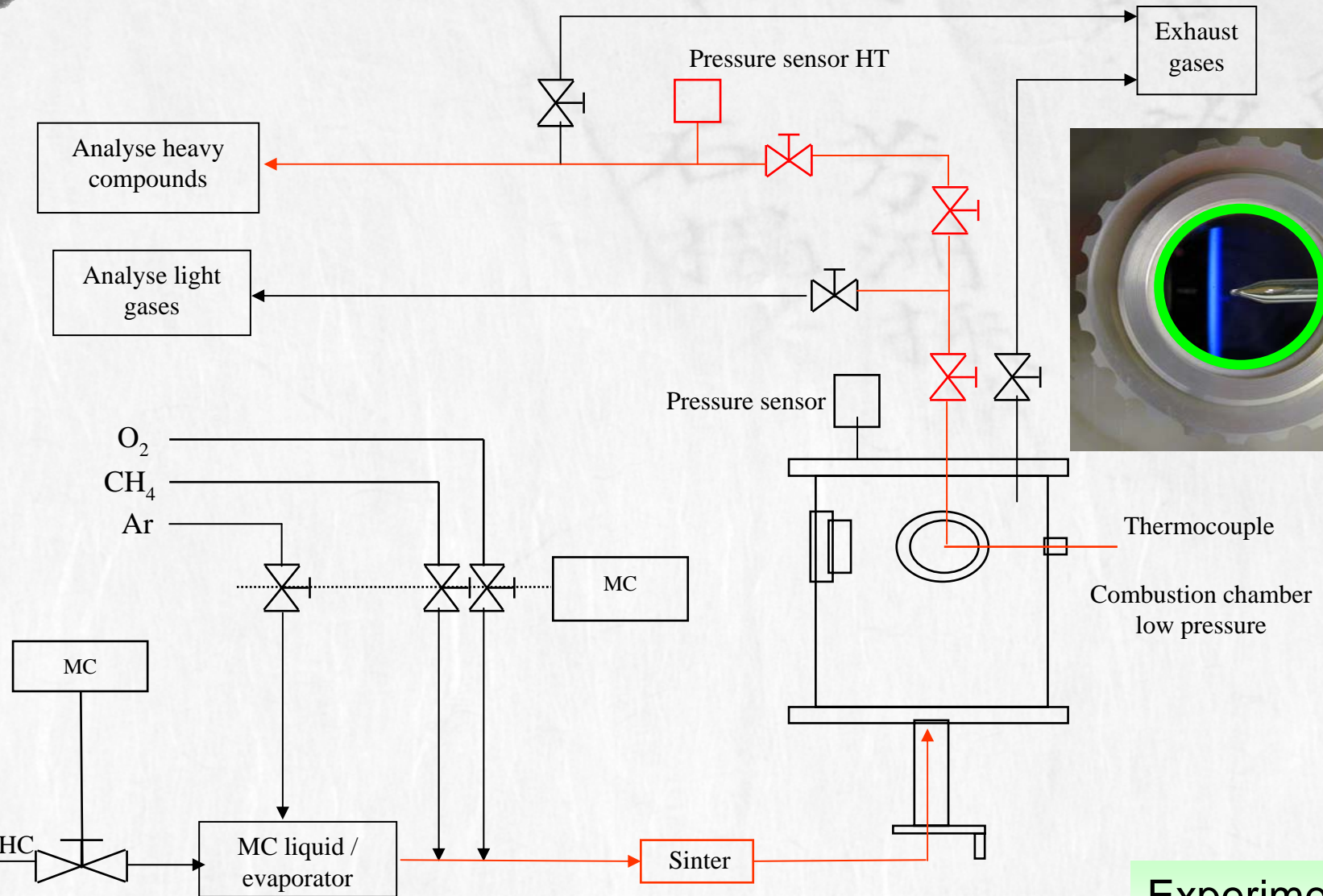
[1] Energy & Fuel 15 (2001) 372-376.

[2] Combust. Flame 156 (2009) 954-974.

[3] Combust. Flame 157 (2009) 75-90.

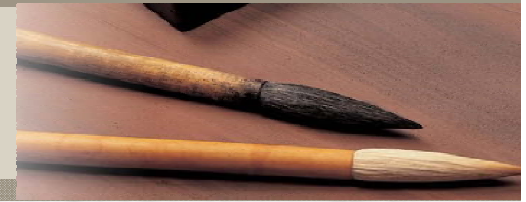


2. Experimental



Experimental

3. Kinetic modeling



Flame data

Chemkin 2.0 Premix Codes

257 species in 1658 reactions (one year)

Jet-stirred reactor data

950 - 1350 K
atmospheric pressure
N₂ as bath gas
indane of 800 ppm
 $\Phi = 1$ and 0.5



4. Results and discussion

4.1 Identification of flame species

($P = 6.7$ kPa, $\Phi = 0.67$, $\text{CH}_4/\text{indane}/\text{O}_2/\text{Ar} = 0.071/0.009/0.368/0.552$)

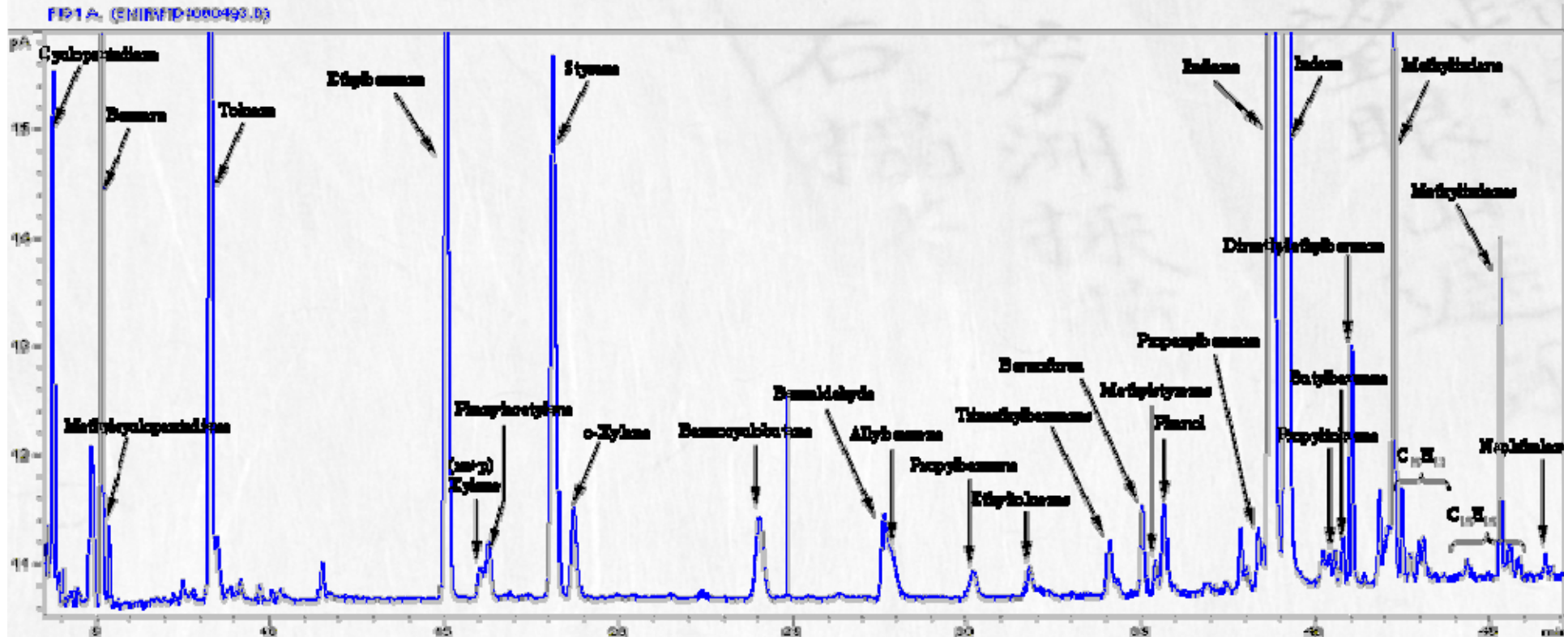


Figure 1 Typical chromatogram of heavy compounds obtained at a distance of 2.70 mm from the burner at 1800 K (oven temperature program: 313 K during 30 min, then a rise of 5 K/min until 453 K).

Feature article with cover page
in *Combustion and Flame*

Results and Discussion



4. Results and discussion

4.2 Temperature profile

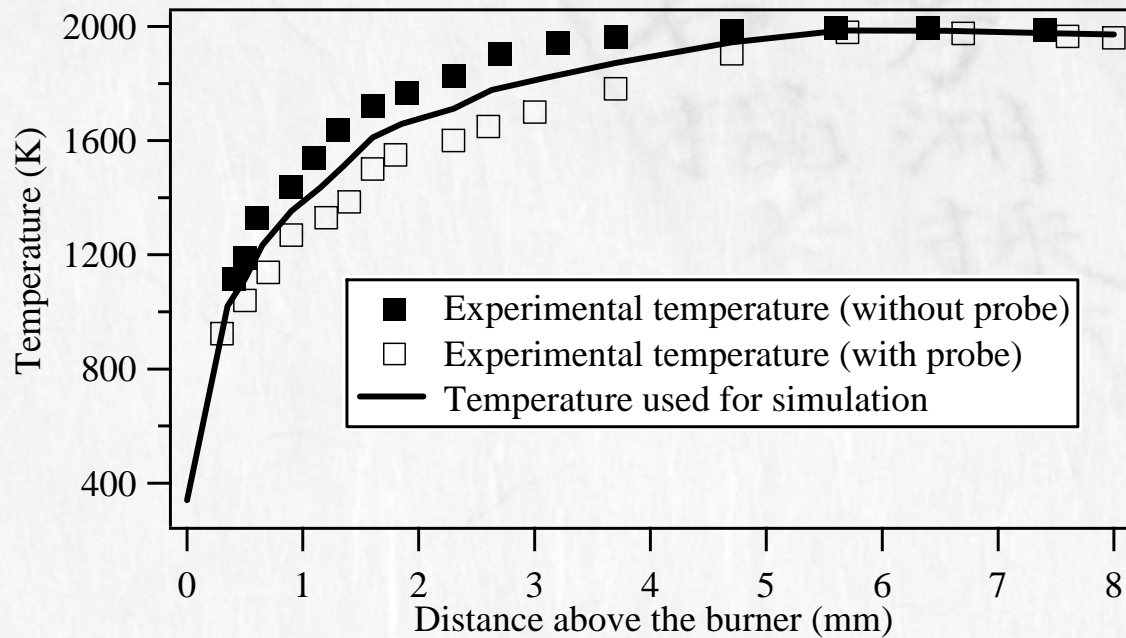


Figure 2 Experimental temperature profiles performed without and with the sampling probe and profile used for simulation.

4. Results and discussion

4.3 Kinetic modeling results

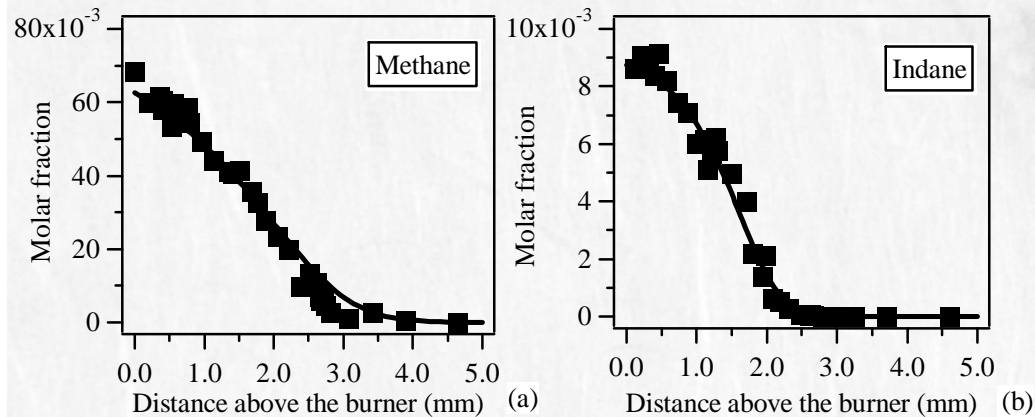


Figure 3 Experimental (points) and predicted (lines) mole fraction profiles of hydrocarbon reactants.

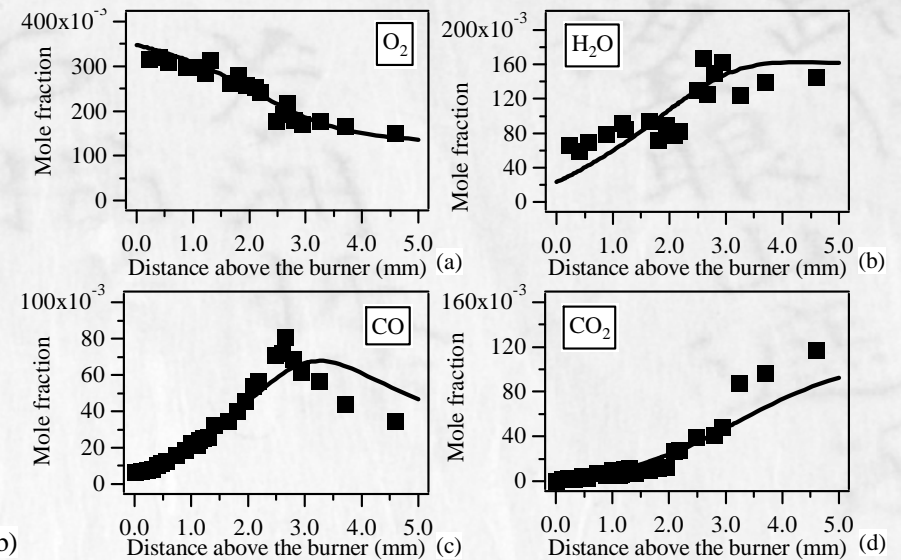


Figure 4 Mole fraction profiles of O_2 , H_2O , CO and CO_2



4. Results and discussion

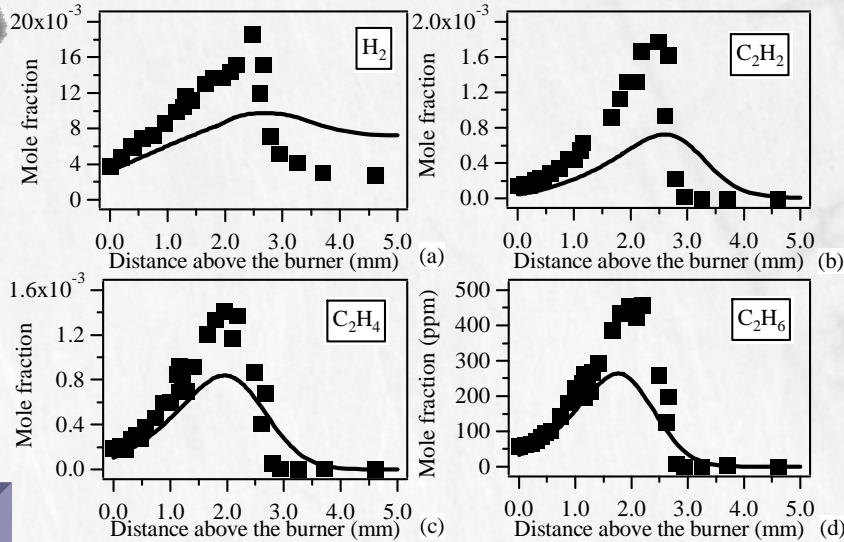


Figure 5 Mole fraction profiles of H₂ and C₂ species.

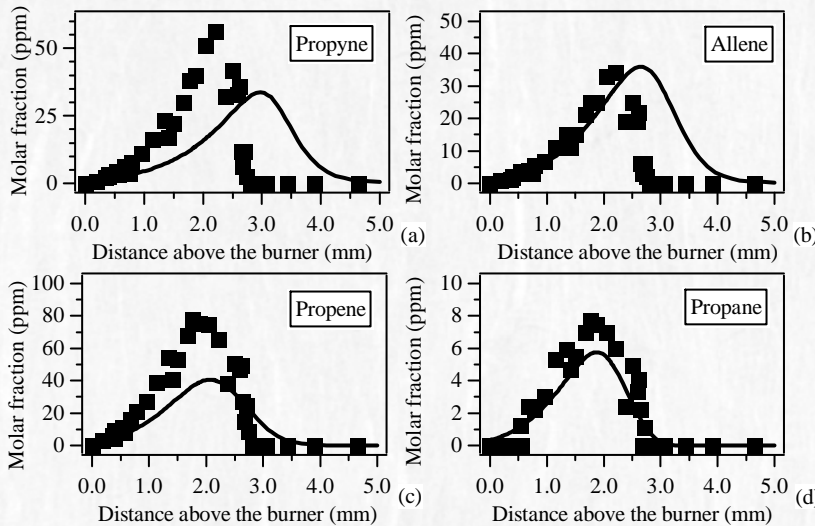


Figure 6 Mole fraction profiles of C₃ species.

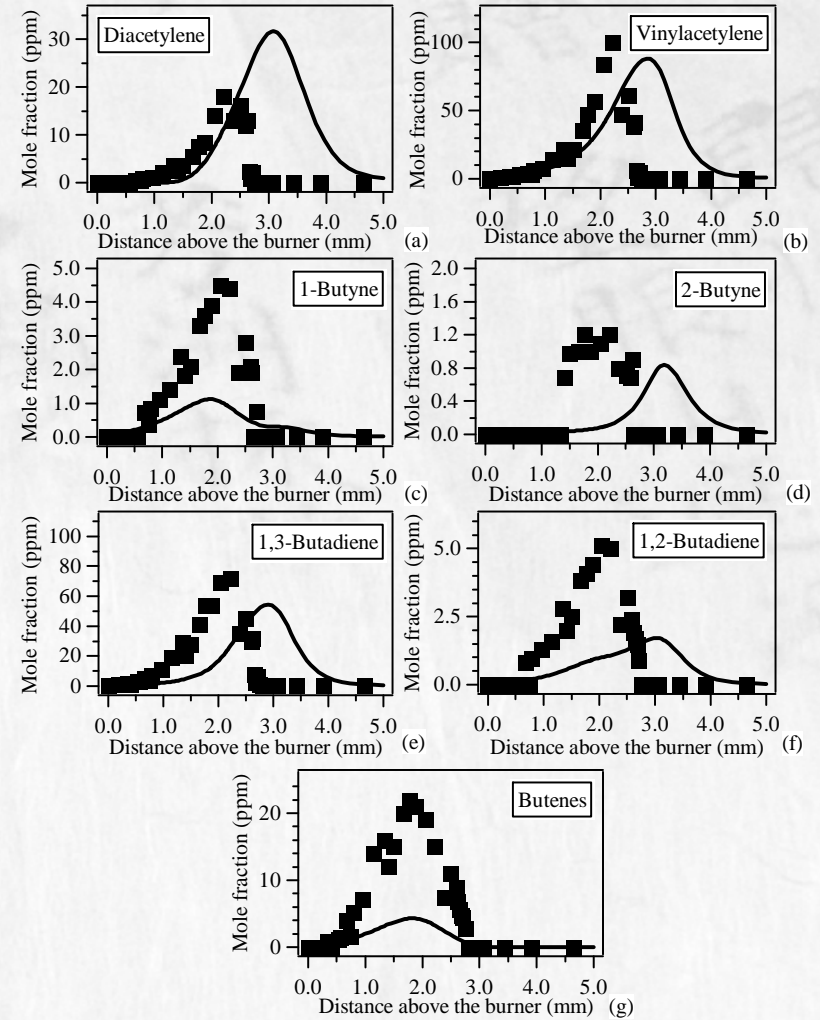


Figure 7 Mole fraction profiles of C₄ species.

Results and Discussion

4. Results and discussion

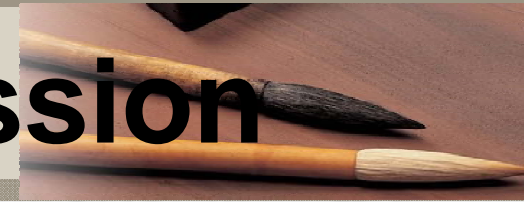
34.	$C_9H_9O \rightleftharpoons C_6H_6 + B_2CO + R_{10}C_2H_3V$	0.347
84.	$indene + R_2OH \rightleftharpoons R_{10}C_2H_3V + B_2CO + C_6H_6$	0.252
106.	$C_9H_7O \rightleftharpoons C_6H_6 + B_2CO + R_9C_2H$	0.155
204.	$C_6H_5 + R_1H (+M) \rightleftharpoons C_6H_6 (+M)$	0.048
206.	$C_6H_6 + R_1H \rightleftharpoons C_6H_7$	-0.134
207.	$C_6H_6 + B_1O \rightleftharpoons C_6H_5O + R_1H$	-0.378
208.	$C_6H_6 + R_2OH \rightleftharpoons C_6H_5OH + R_1H$	0.011
210.	$C_6H_6 + R_{10}C_2H_3V \rightleftharpoons styrene + R_1H$	0.036
211.	$C_6H_6 + R_1H \rightleftharpoons C_6H_5 + H_2$	-0.019
213.	$C_6H_6 + R_2OH \rightleftharpoons C_6H_5 + H_2O$	-0.460
357.	$toluene + R_1H \rightleftharpoons C_6H_6 + R_4CH_3$	0.064
416.	$C_6H_5CHO + R_1H \rightleftharpoons C_6H_6 + R_5CHO$	0.035
501.	$etC_6H_5 + R_1H \rightleftharpoons C_6H_6 + R_{11}C_2H_5$	0.037

Figure 8 Mole fraction profiles of C5-C6 non-aromatic species.

Figure 9 Mole fraction profiles of C6-C8 mono-aromatic species.

C5~C6

4. Results and discussion



C9
~
C10

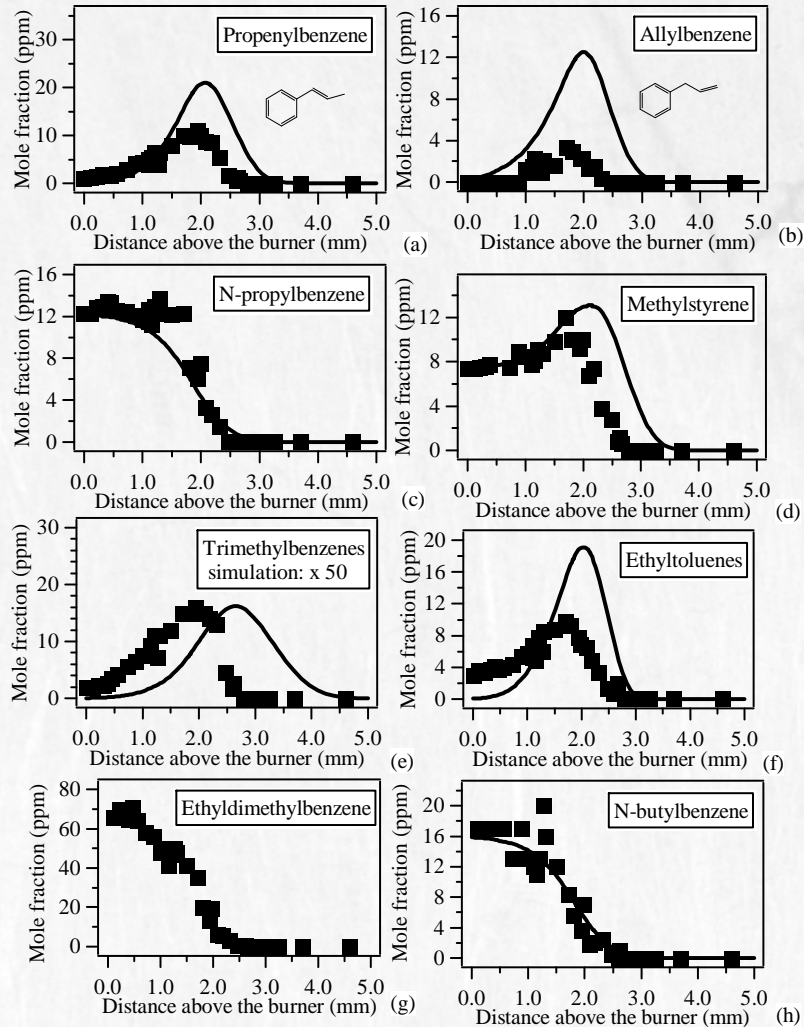


Figure 10 Mole fraction profiles of C9-C10 mono-aromatic species.

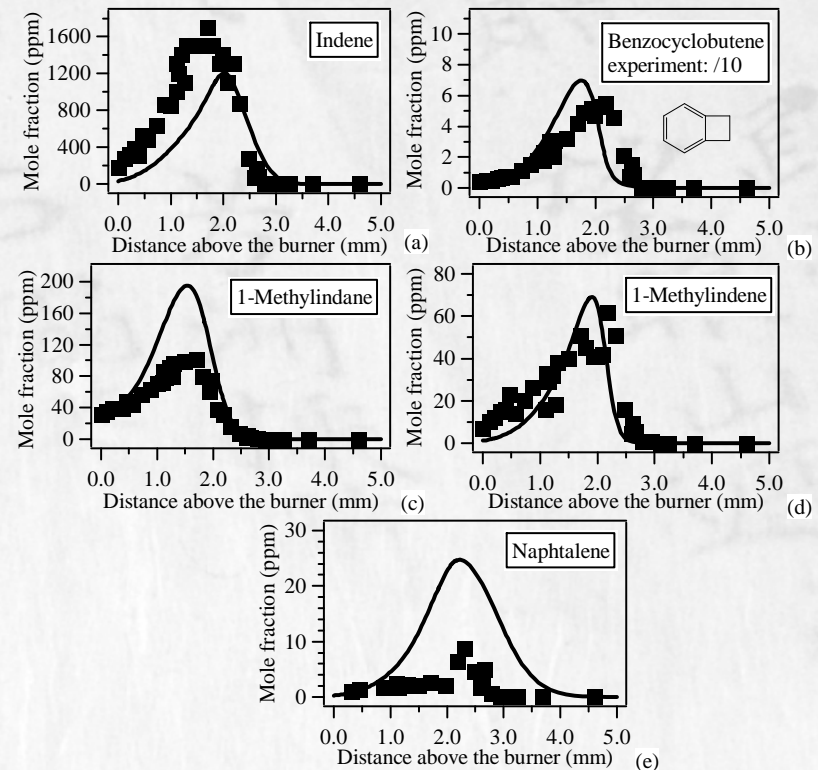


Figure 11 Mole fraction profiles of bicyclic aromatic species.

bicyclic



4. Results and discussion

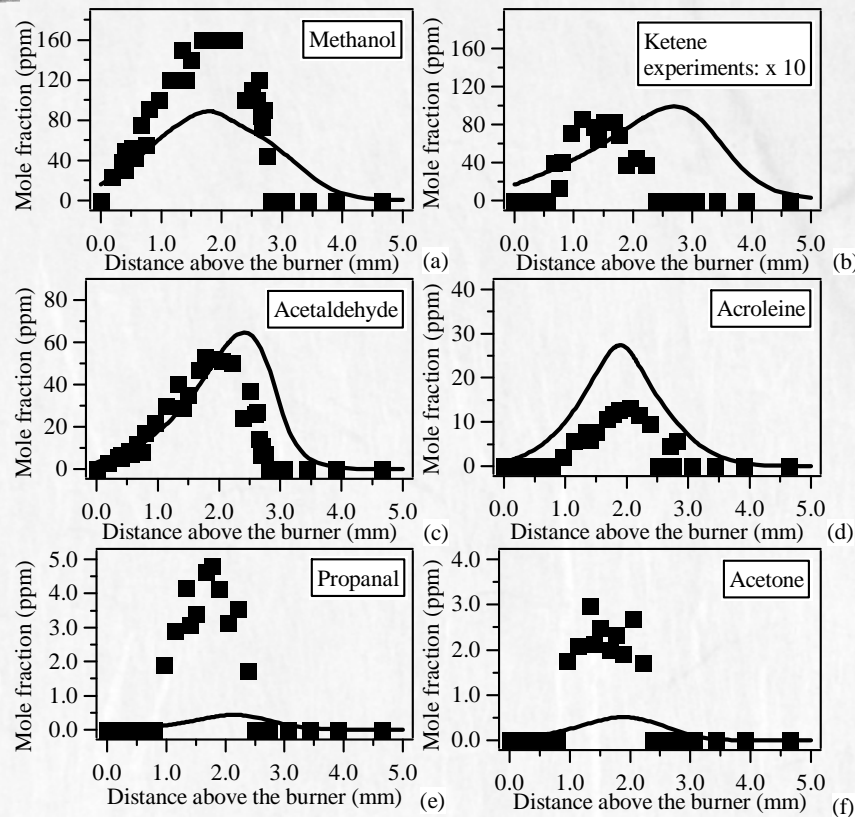


Figure 12 Mole fraction profiles of C1-C3 oxygenated species.

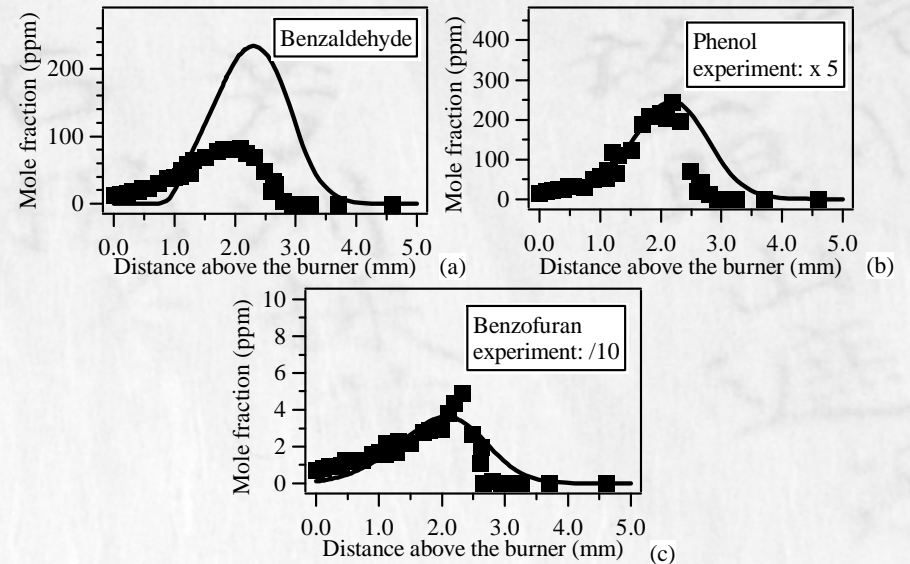


Figure 13 Mole fraction profiles of oxygenated aromatic species.

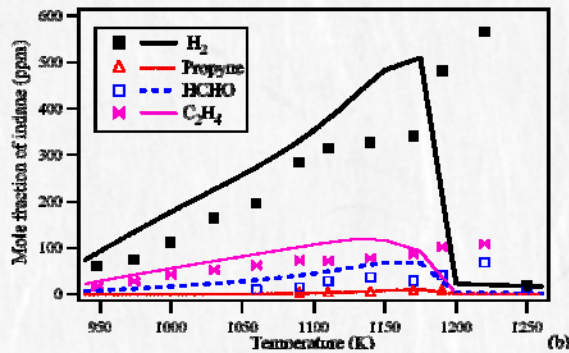
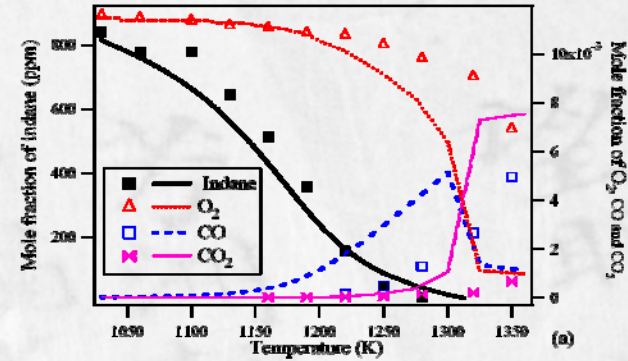
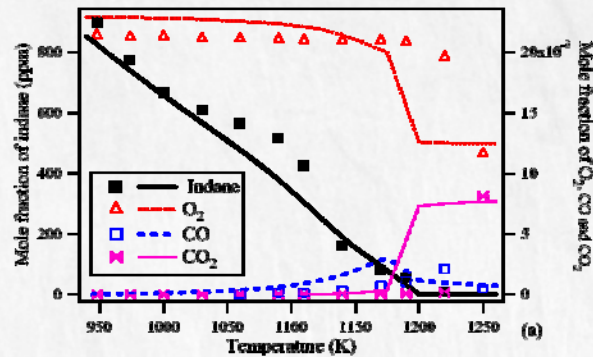
Oxygenated species

Results and Discussion

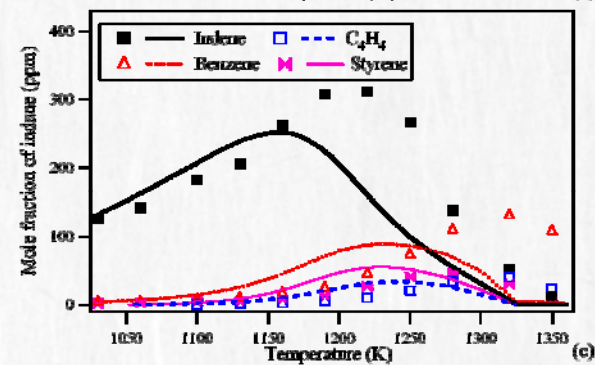
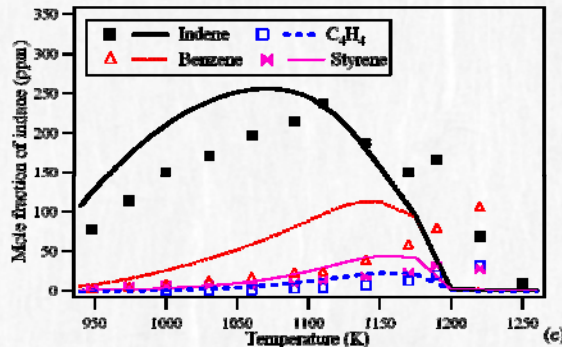
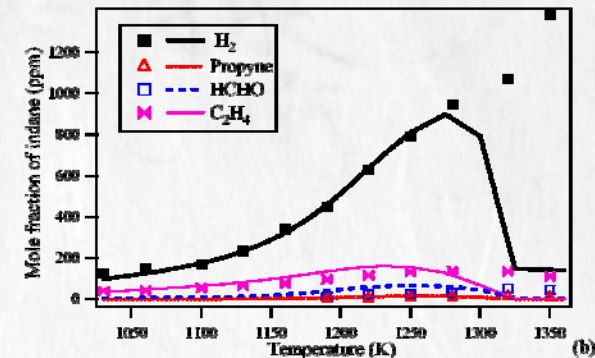


4. Results and discussion

4.4 Validation to jet-stirred reactor data



$\Phi = 1.0$



Results

$\Phi = 0.5$



5. Conclusion



1

This work presents new experimental results for a lean premixed laminar flame of methane seeded with indane.

2

A new mechanism is developed to reproduce the combustion of this diesel model compound.

3

Profiles of temperature are measured and mole fraction profiles are obtained for 48 identified stable species from C0 to C10, including 21 aromatic products and 9 oxygenated compounds other than the reactants.

4

The mechanism is validated to both flame and the jet-stirred reactor results.



Acknowledgement



Dr. Frederique Battin-Leclerc *

Dr. Emir Pousse

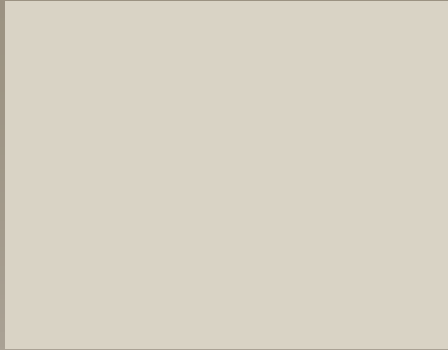
Dr. Pierre-Alexandre Glaude

Prof. Rene Fournet

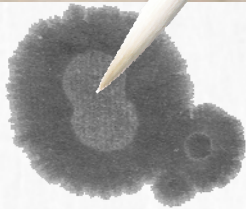
Region Lorraine, PSA Peugeot Citroën, TOTAL

Frederique.Battin-Leclerc@ensic.inpl-nancy.fr





Thank You!



The Great Wall

长城



Yellow Mountain

黄山





Waterfall

黄果树瀑布



West Lake
西湖