Ignition delay times of diluted mixtures of ammonia/methane at elevated pressures

C. Filipe Ramos[1], Bo Shu[2], Ravi Fernandes[2] and Mário Costa[1,*]

[1] Instituto Superior Técnico, Lisboa, Portugal
[2] Physikalisch-Technische Bundesanstalt, Germany

*mcosta@tecnico.ulisboa.pt

Ammonia Energy Conference 2019

Motivation

Searching for alternative fuels with zero CO_2 emissions after combustion and high fuel efficiency is today an important research topic.

NH_3 is attracting attention because has good energy density, does not produce any soot or CO_2 during its chemical conversion in a combustion process and can be produced with renewable energy sources…

… thus NH_3 looks like a promising alternative fuel and a green energy storage carrier.

Combustion properties of ammonia, however, are still not fully understood, particularly at high pressures.

Objectives

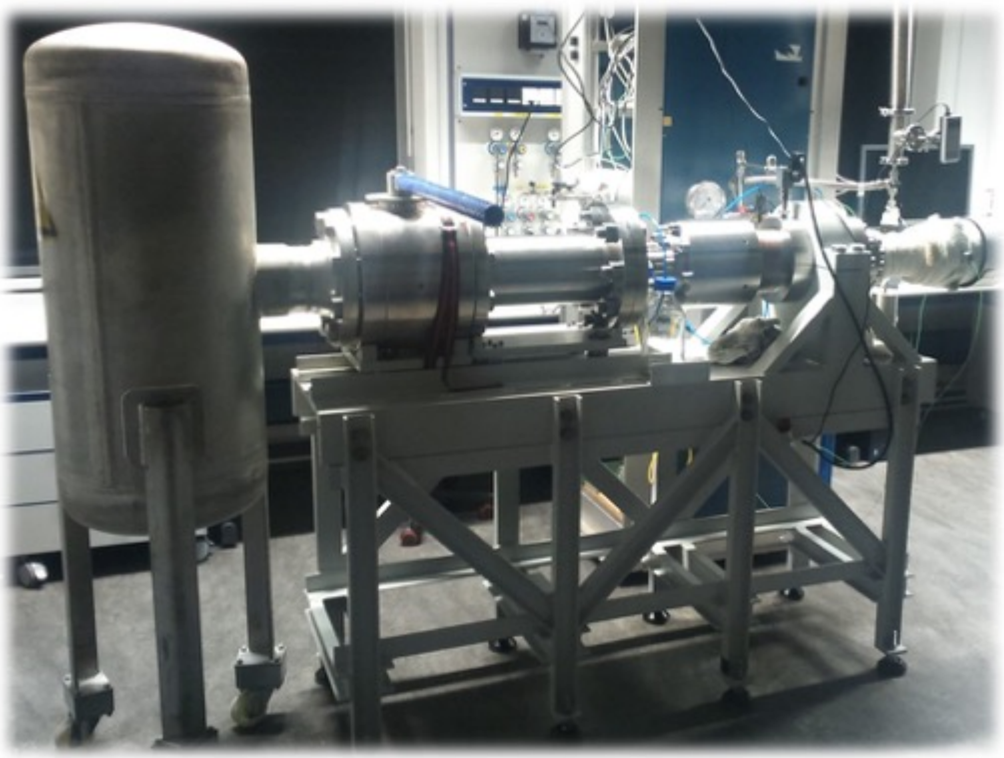
To study the ignition characteristics of diluted $NH_3/CH_4/O_2$ mixtures at elevated pressures;

To measure ignition delay times (IDT) in a rapid compression machine at pressures of 20 and 40 bar, temperatures between 920 and 1100 K, and equivalence ratios ranging from 0.5 to 2;

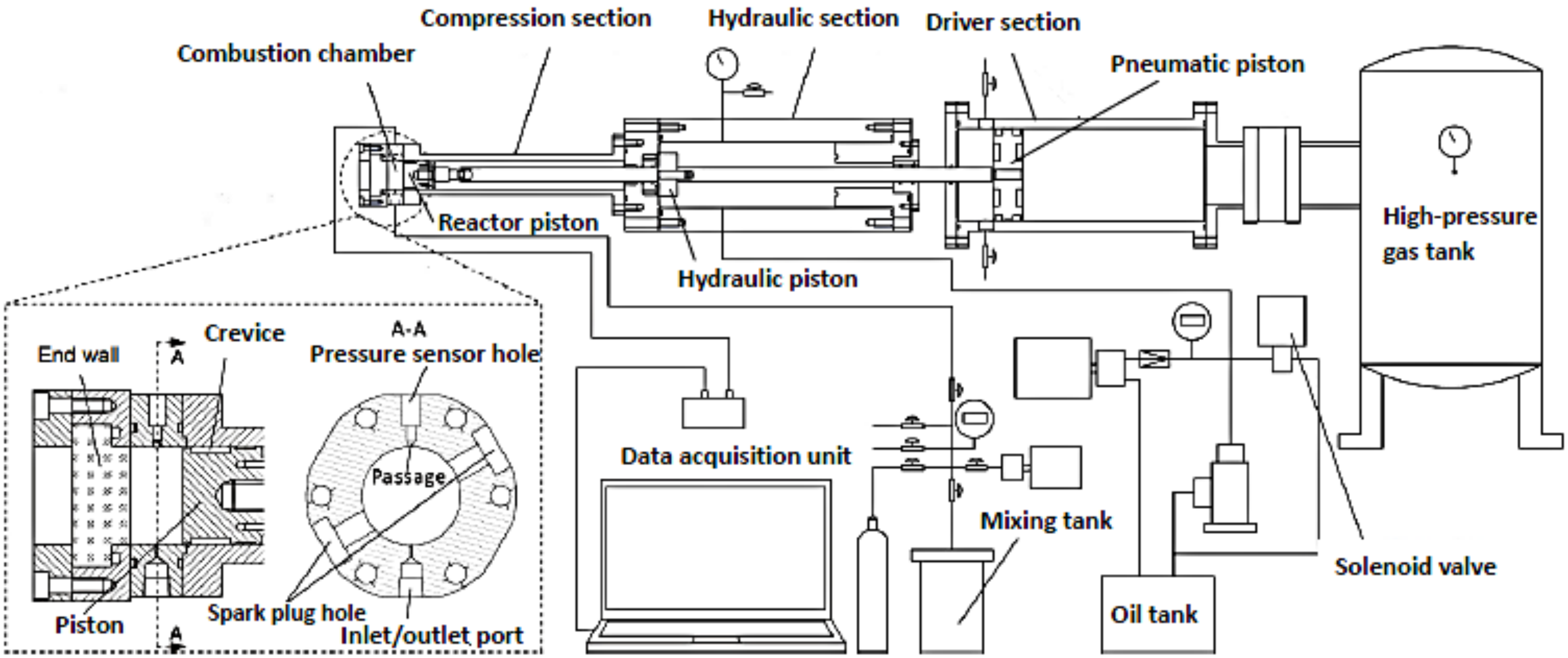
To evaluate the performance of literature chemical kinetic mechanisms in predicting the present data.

Experimental

The auto-ignition experiments were performed in a rapid compression machine (RCM) at Physikalich-Technische Bundesanstalt (PTB), Germany.



Experimental



RCM consists of a single piston design, pneumatically driven and hydraulically braked.

Combustion chamber includes 6 ports for pressure sensors, gas inlet and exhaust gas outlet.

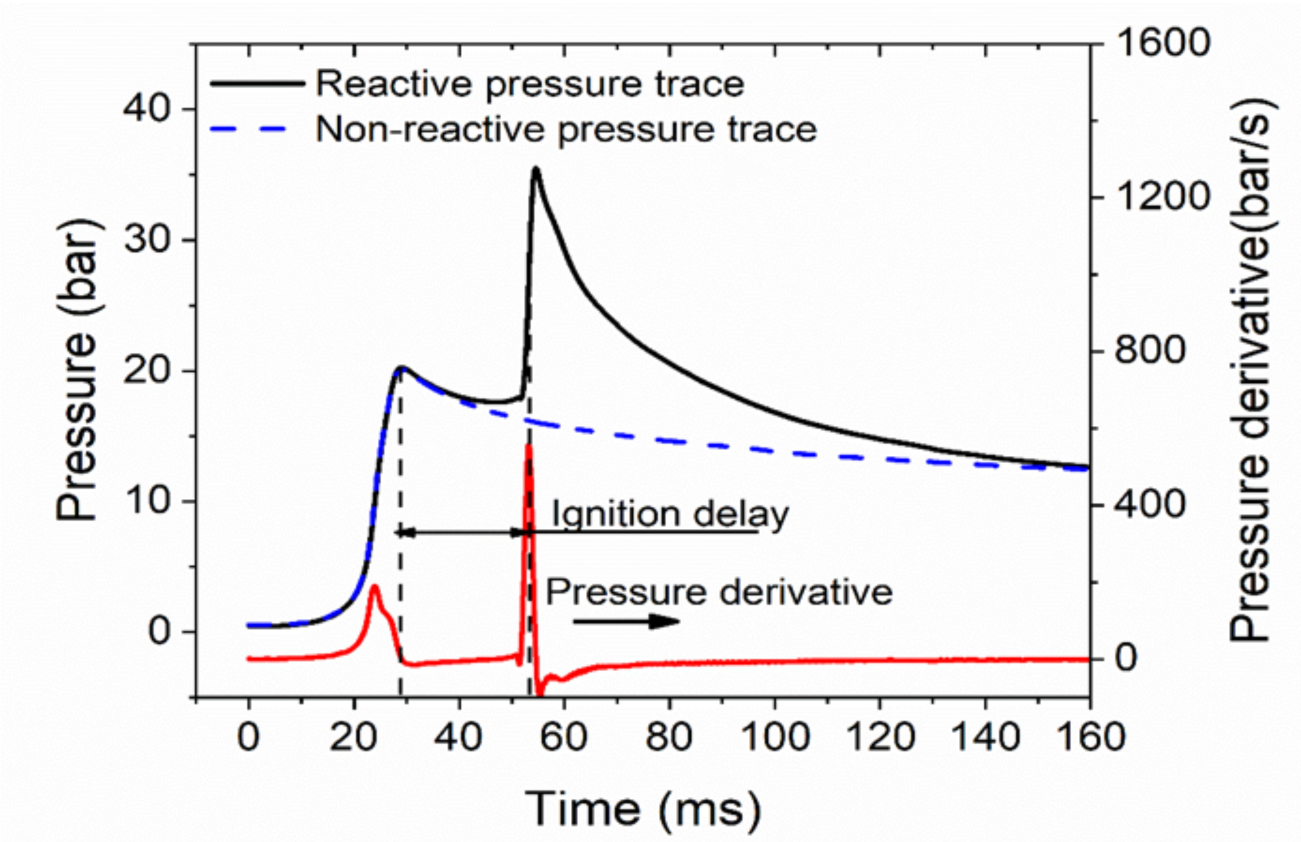
Maximum working pressure is 200 bar.

Compression ratio used in this work was fixed at 20.93.

Experimental

IDTs were measured through the pressure time histories.

Typical pressure trace measurement for a NH_3/CH_4 fuel mixture



IDT = time difference between EOC (first maximum of pressure history) and ignition onset (point of maximum derivative after compression of gases)

Mixtures studied

No.	NH_3 in fuel	CH_4 in fuel	Equivalence ratio (ϕ)	Temperature range (K)	
				20 bar	40bar
1	80%	20%	0.5	1000-1090	920-990
2	80%	20%	1	1020-1100	940-990
3	80%	20%	2	1000-1070	940-1020
4	90%	10%	0.5	1020-1090	950-1010
5	90%	10%	1	1030-1100	980-1020
6	90%	10%	2	1050-1090	960-1030

Mixtures prepared in stainless steel tanks at room temperature, with only Ar or Ar/N_2 as diluent gases. For all cases, dilution applied was 70%.

Data for pure NH_3 and mixtures of NH_3/H_2 at high pressure were obtained in previous work.

Kinetic models

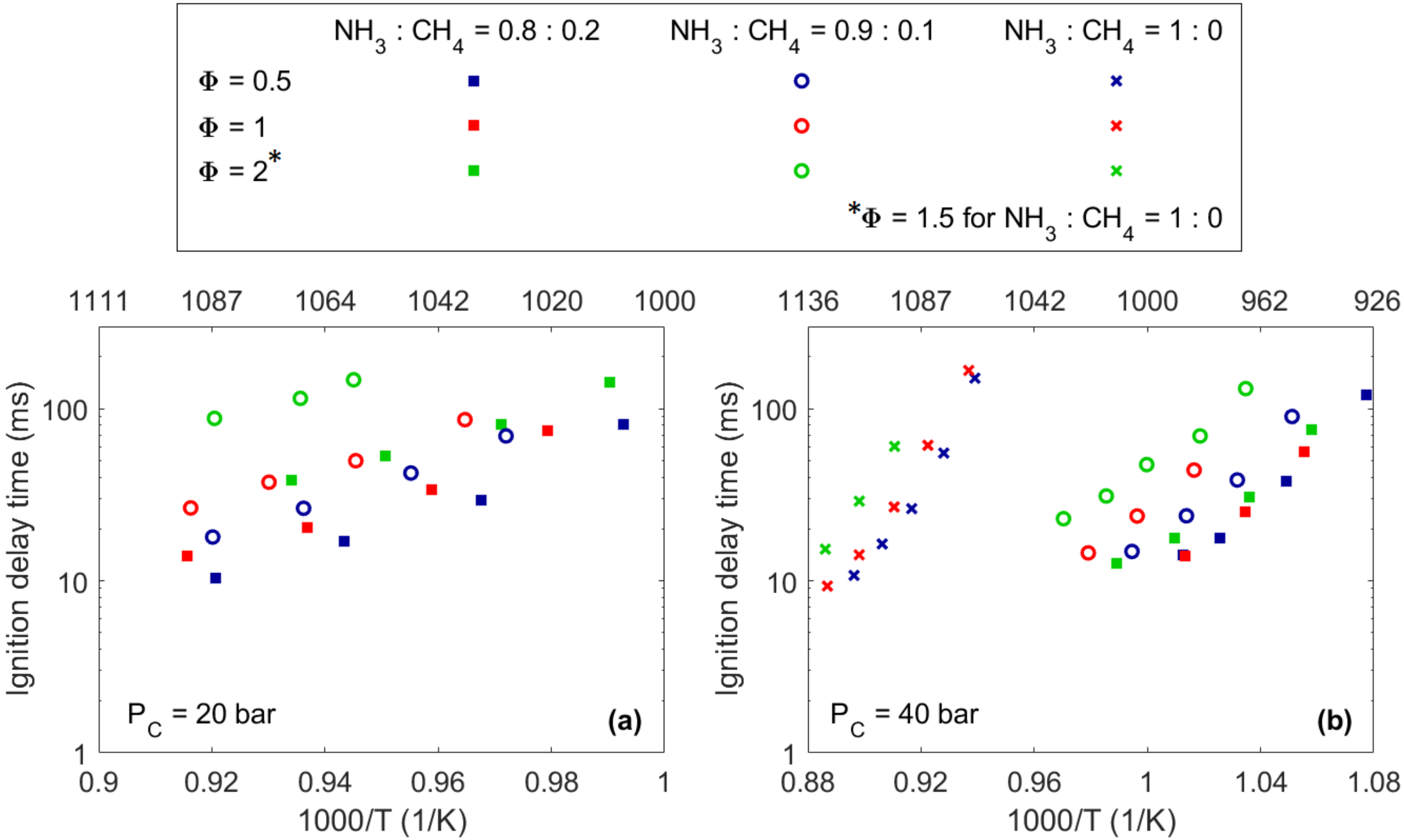
No.	Author	Species nr	Reaction nr	Year	Comments
1	Dagaut et al.	25	135	2008	
2	Mendiara et al.	31	191	2009	
3	Konnov	31	242	2009	
4	Klippenstein et al.	31	202	2011	no Carbon
5	Song et al.	32	204	2015	improvement of No. 4 – no C
6	Mathieu et al.	30	159	2015	improvement of No. 1
7	Otomo et al.	33	222	2017	improvement of No. 5 – no C
8	Nakamura et al.	32	224	2017	combination of No. 3 and 6
9	Glarborg et al.	33	211	2018	improvement of No. 4

Cantera was used.

Most models perform poorly; only Meldiara et al., Konnov and Glarborg et al. performed reasonable.

Experimental results

Experimental results of IDT of NH_3/CH_4 fuel mixtures and pure NH_3 at (a) 20 bar and (b) 40 bar.

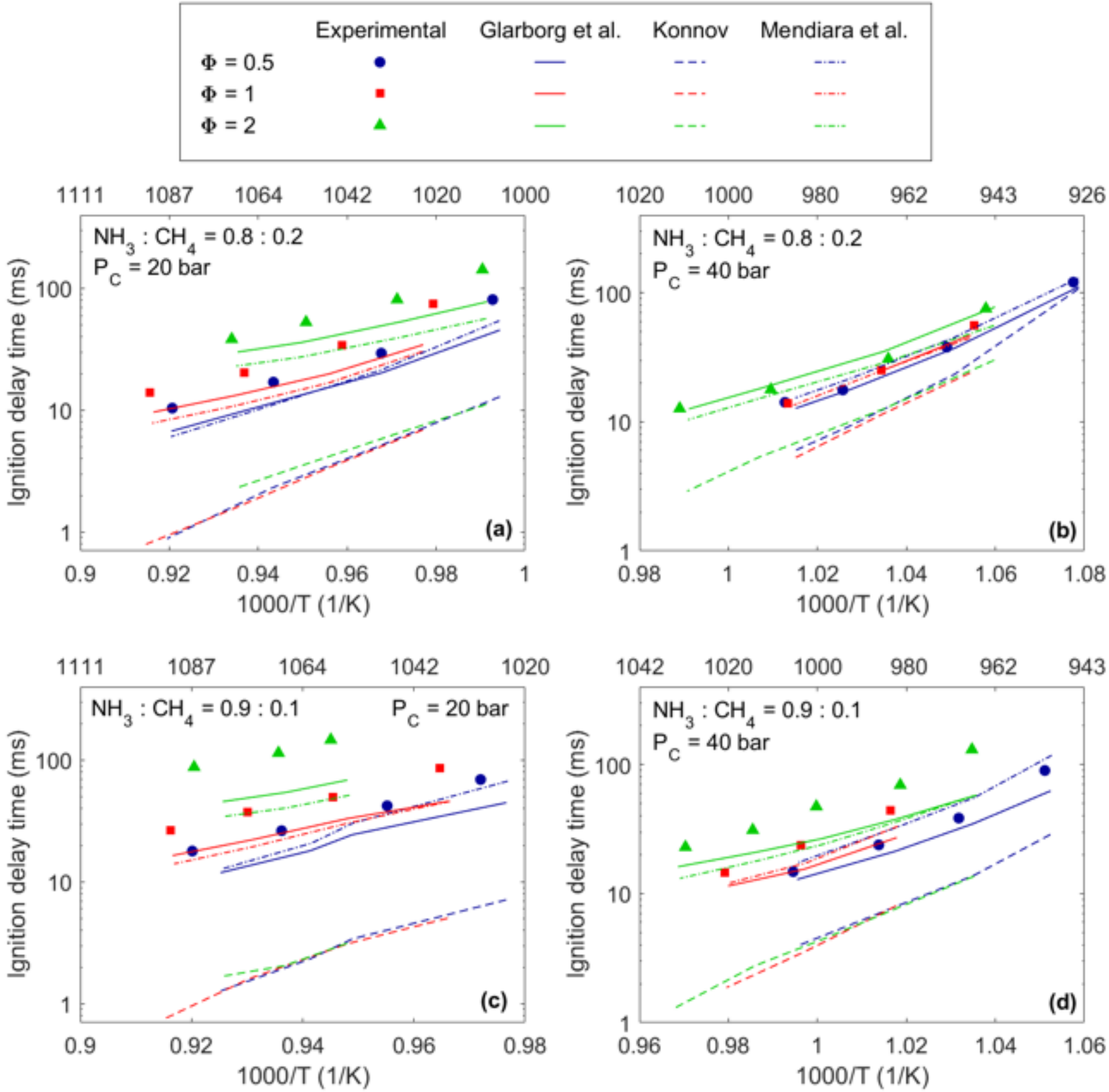


Increase in ϕ increases IDT

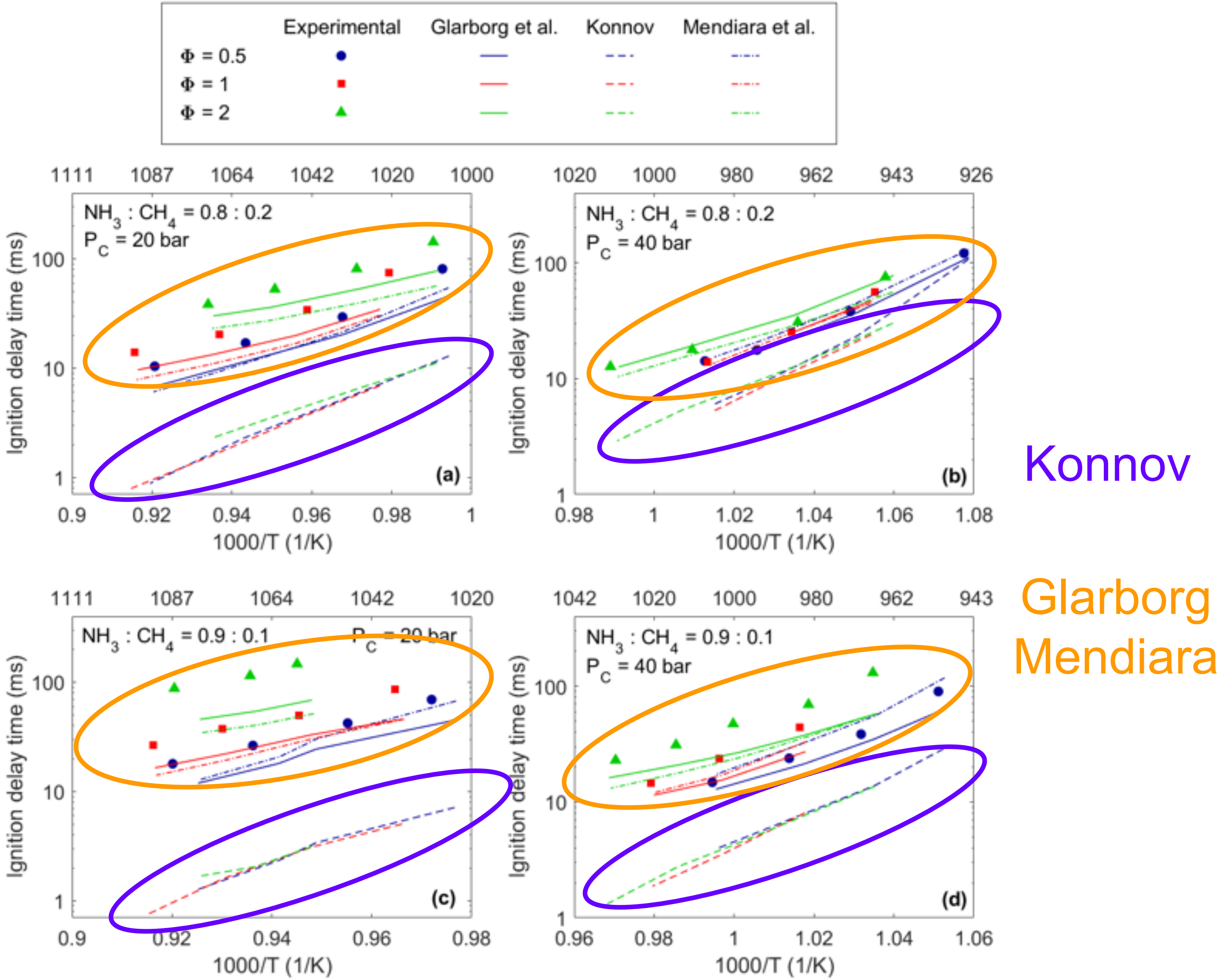
Increase in NH_3 in fuel mixture increases IDT

Increase in pressure decreases IDT

Comparison with numerical models



Measurements and numerical results of IDT of NH_3/CH_4 fuel mixtures, using the chemical kinetics mechanisms from Glarborg et al., Konnov, and Mendiara et al.



Measurements and numerical results of ignition delay times of NH_3/CH_4 fuel mixtures, using chemical kinetics mechanisms from Glarborg et al., Konnov, and Mendiara et al.

Conclusions

An increase in ϕ leads to longer IDT.

An increase in NH_3 in the fuel mixture leads to longer IDT.

Addition of CH_4 facilitates ignition at lower temperatures, thus increasing the reactivity of the mixture.

An increase in pressure leads to faster ignition. In addition, the separation between the IDTs of fuel mixtures with different NH_3/CH_4 ratios becomes clear as the pressure increases.

The three mechanisms studied under-predicted the measurements. The mechanisms by Glarborg et al. and Mendiara et al. were capable of matching more closely the experimental results than the mechanism of Konnov, which was off by ~1 order of magnitude.

Studies at high pressure are still scarce; more experimental data is needed in order to help the development and validation of chemical kinetics mechanisms.

Acknowledgments

This work was partially supported by Fundação para a Ciência e a Tecnologia (FCT), through IDMEC, under LAETA, project UID/EMS/50022/2019.

C.F. Ramos acknowledges the COST Action CM1404 "Chemistry of Smart Energy Carriers and Technologies (SMARTCATS)" for the financial support.

FCT

Fundação para a Ciência e a Tecnologia

COST

CM1404

SMARTCATs

References

- S.K. Vallabhuni, A.D. Lele, V. Patel, A. Lucassen, K. Moshammer, M. AlAbbad, A.Farooq, R.X. Fernandes, Autoignition studies of Liquefied Natural Gas (LNG) in a shock tube and a rapid compression machine, Fuel 232 (2018) 423–430.
- D.G. Goodwin, H.K. Moffat, R.L. Speth, Cantera: An Object-oriented Software Toolkit for Chemical Kinetics, Thermodynamics, and Transport Processes, 2017.
- P. Glarborg, J.A. Miller, B. Ruscic, S.J. Klippenstein, Modeling nitrogen chemistry in combustion, Prog. Energy Combust. Sci. 67 (2018) 31–68.
- A. A. Konnov, Implementation of the NCN pathway of prompt-NO formation in the detailed reaction mechanism, Combust. Flame 156 (2009) 2093–2105.
- T. Mendiara, P. Glarborg, Ammonia chemistry in oxy-fuel combustion of methane, Combust. Flame 156 (2009) 1937–1949.
- X. He, B. Shu, D. Nascimento, K. Moshammer, M. Costa, R.X. Fernandes, Auto-ignition kinetics of ammonia and ammonia/hydrogen mixtures at intermediate temperatures and high pressures, Combust. Flame 206 (2019) 189-200.