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Autoignition, Knock, Detonation and the Octane Rating of Hydrogen

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Acknowledgements

- First, my thanks to KAUST and in particular Profs. Roberts, Im and Turner for inviting me.
  - I apologise for not being able to be with you in person today.

- I also acknowledge my colleagues and students at the University of Melbourne, particular Dr. Farzad Poursadegh who undertook the experiments and modelling that I present today, which has just been published:

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Autoignition, knock, detonation and the octane rating of hydrogen

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What is the octane number of hydrogen?

Introduction

- The literature on hydrogen's susceptibility to knock is contradictory and not traceable:
  - some consider hydrogen to be high-octane, whilst others consider it to be low-octane;
  - reported **Research Octane Numbers (RONs)** vary from **60 to over 130**; and
  - we were unable to find any primary references reporting these octane ratings.
- And:
  - hydrogen's high autoignition temperature and high flame speed suggest that it will have superior knock resistance; but
  - hydrogen's low low ignition energy could *potentially* initiate uncontrolled combustion.
- Also:
  - the apparent absence of published studies that demonstrate how the RON and MON of hydrogen was measured calls into question these reported values;
  - the reliance of the **Methane Number** test on the assumption that hydrogen is knock-prone is inconsistent with studies that consider hydrogen to be high octane.
- This study was therefore intended to clarify this situation using the standard octane rating engine.

Experimental methods

- Experiments were conducted on a standard Waukesha CFR F1/F2 engine with a variable CR.
- This engine was equipped with a gaseous fueling system that introduced hydrogen upstream of the standard carburetor.
- Two sets of octane rating tests were conducted:
  - **Standard tests** were based on the ASTM's RON test method;
  - **Modified tests** were also undertaken where hydrogen was rated at λ values that were more relevant to SI engine operation and with spark timings that matched the combustion phasing of iso-octane at its standard test condition.
- In-cylinder pressure measurement was acquired using a piezoelectric pressure transducer (Kistler 6125C).
- It is important to note that pre-ignition was **not** observed at any of the conditions examined in this work.

Table 1: Operating conditions studied

Engine speed	600 ± 6 rpm
Intake air temperature [a]	52 ± 1°C
Intake air pressure	barometric
Coolant temperature	100 ± 1.5°C
Compression ratio	varied

[a] compensated for variations in barometric pressure

Numerical methods

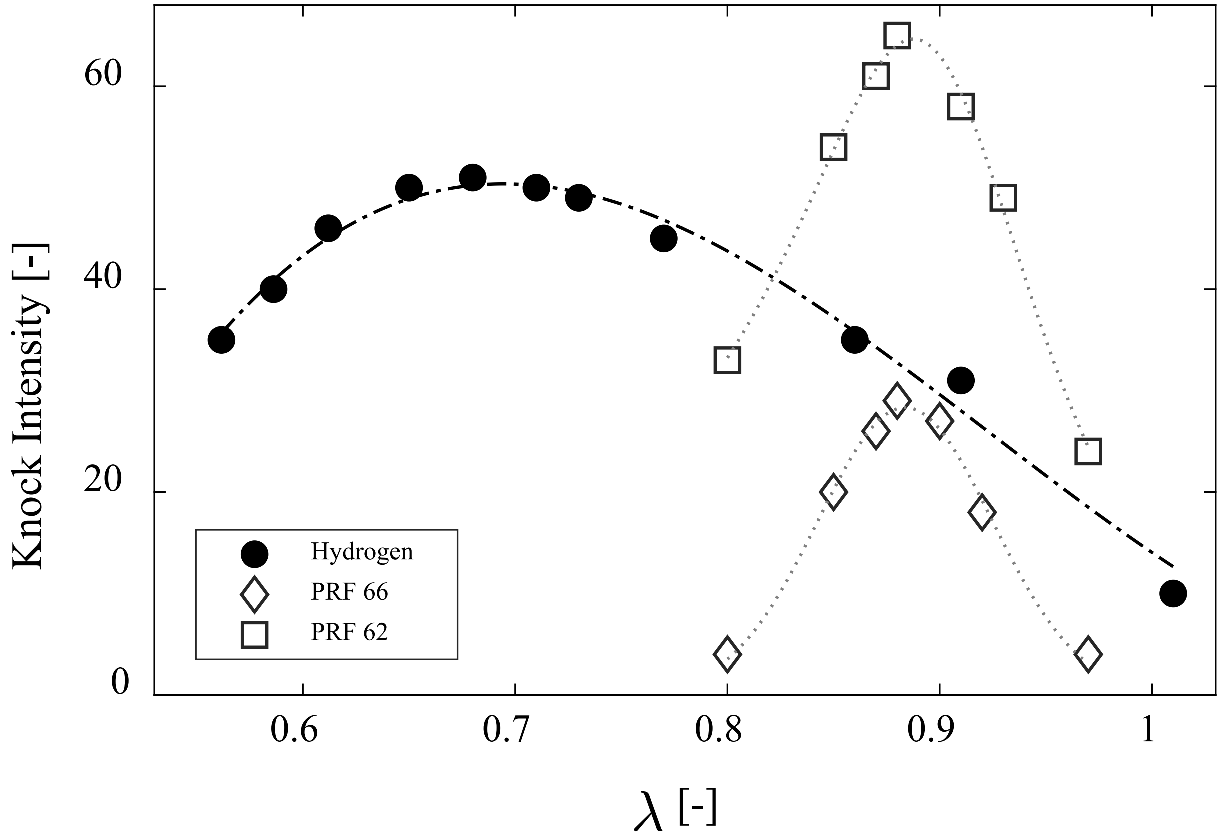
Two-zone combustion modelling

- A two-zone model of the closed part of the CFR engine cycle was implemented in GT-Suite's 'Reverse Run' mode.
- This obtained the fuel's mass fraction burned (MFB) profile and the in-cylinder heat transfer.
- This requires the volumetric efficiency, residual gas fraction and wall temperatures as inputs, and these were estimated using a model of the full CFR engine and was based on our previous work.
- GT-Suite's 'SI Turbulent Flame Module' was then used to model turbulent flame propagation during combustion.

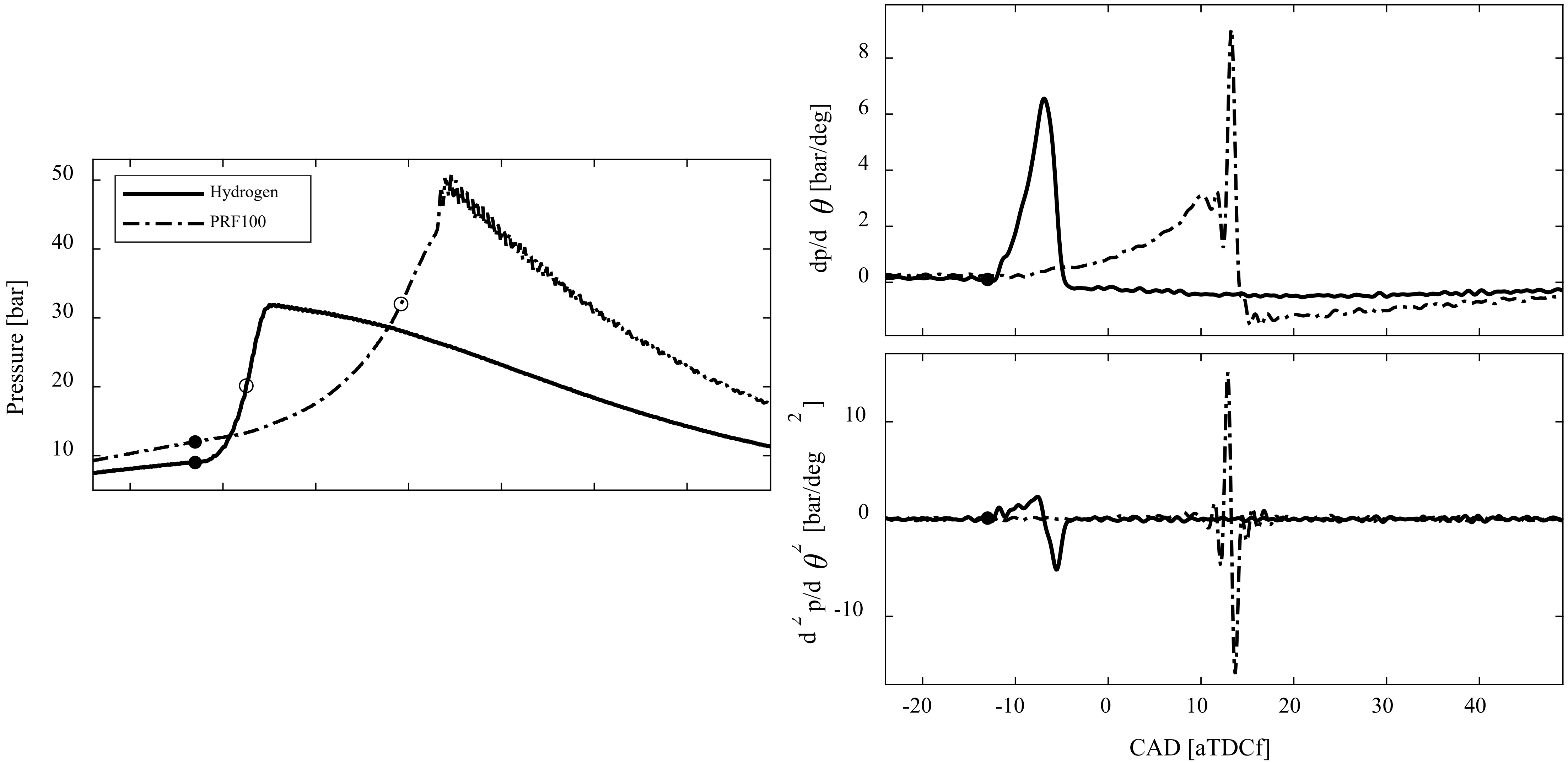
Kinetic modelling

- A closed, homogeneous and adiabatic reactor in Chemkin was used to study end-gas reactivity.
- The charge temperature and composition at intake valve closure (IVC) from GT-Suite and the *measured, non-autoigniting* in-cylinder pressure traces are imposed on this reactor.
- Autoignition was simulated using a kinetic model for synthesis gas which includes a nitric oxide sub-mechanism (Zhang et al, 2017, Combust Flame; 182:122–41).

Rating at standard RON conditions

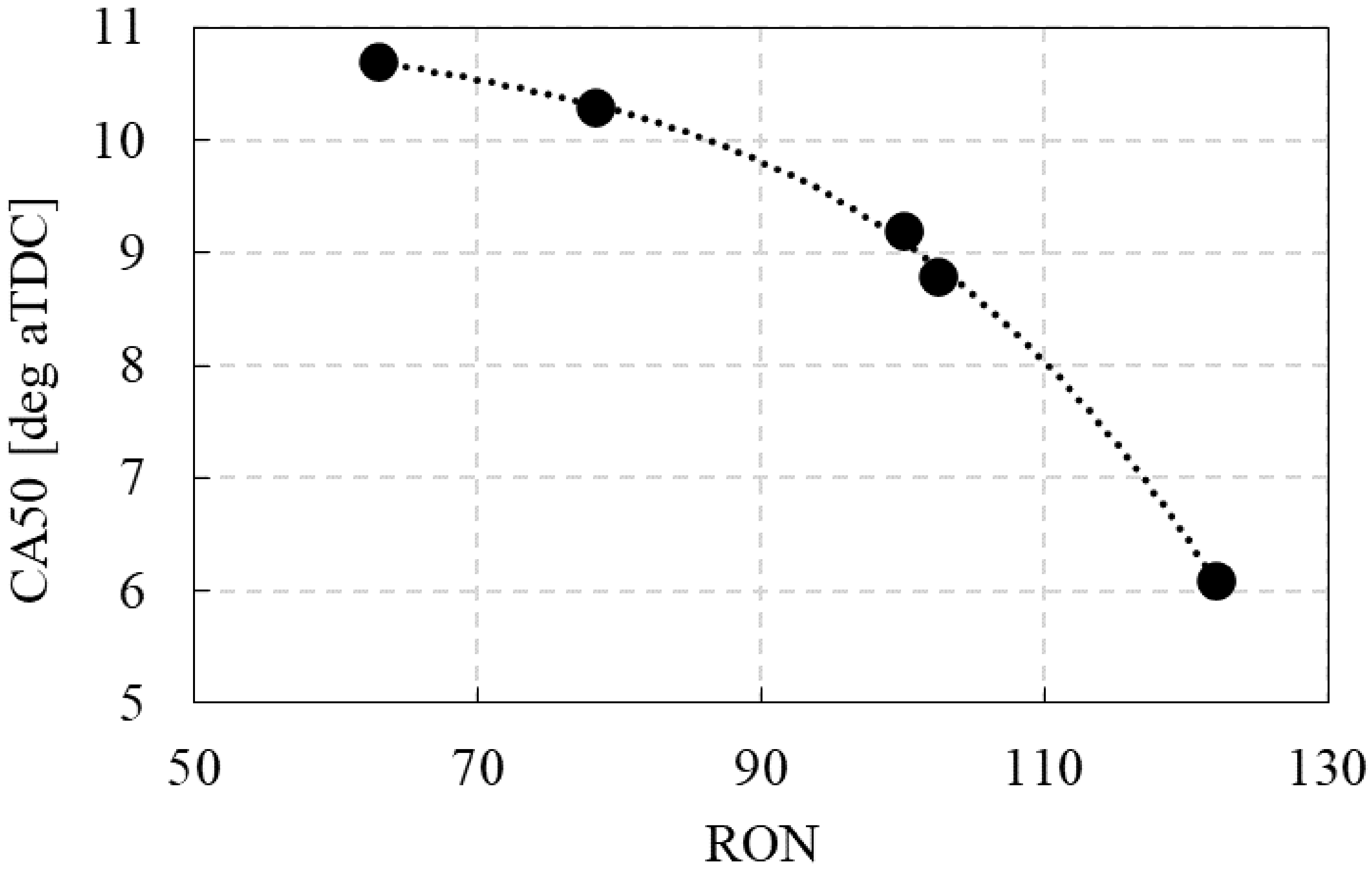


Rating at standard RON conditions



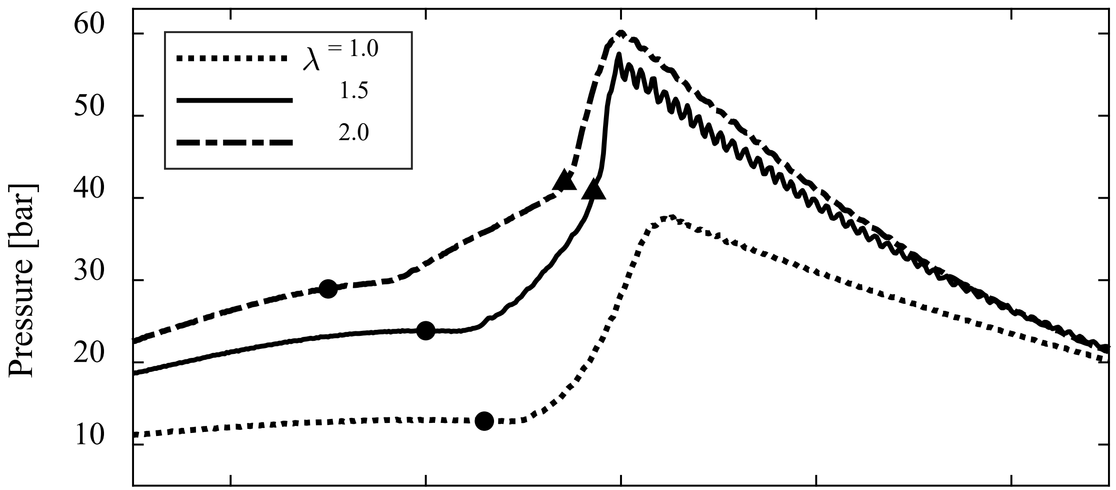
What spark timing for modified RON tests?

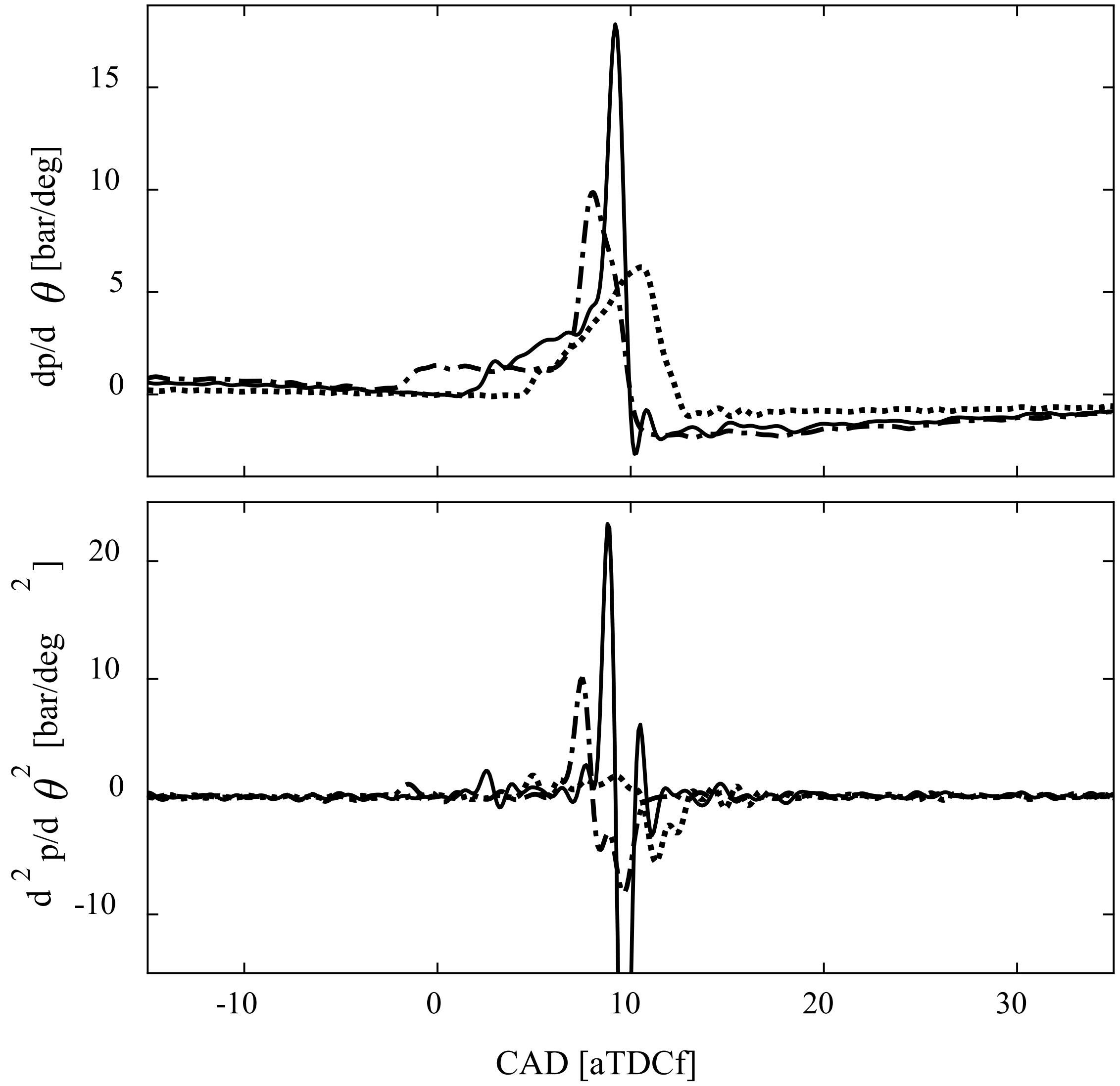
Use CA50 as a guide and choose PRF100



- We then retard spark for the hydrogen tests such that CA50 is close to that of PRF100 at its standard test condition.

Rating at modified RON conditions





Rating at modified RON conditions

Standard RON

	$\lambda_{H_2,eq}{}^{b}$	ON	CCR
Hydrogen*	1.00	62-64	5.6
Gasoline [34]	1.24	90–100	6.6-7.6
Ethanol [34]	1.28	108	9.2
Toluene [35]	1.21	117	10.8
Propane [18]	1.23	109	9.4
Methane [37]	1.24	>120	>11.5

* Measured in this work.

[a] ON is beyond the measurement range of ASTM 2699.

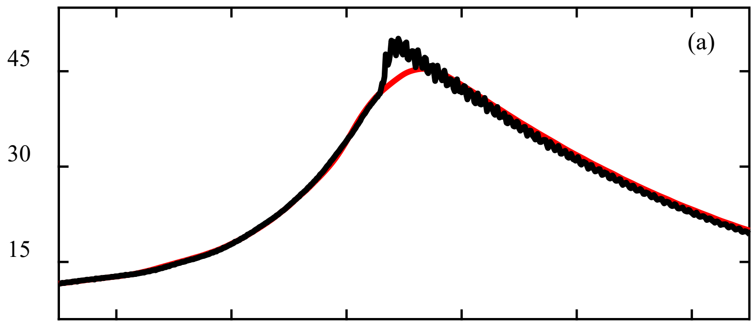
[b] λ of H_2/air with the same chemical energy as a given stoichiometric hydrocarbon/air mixture.

Modified RON

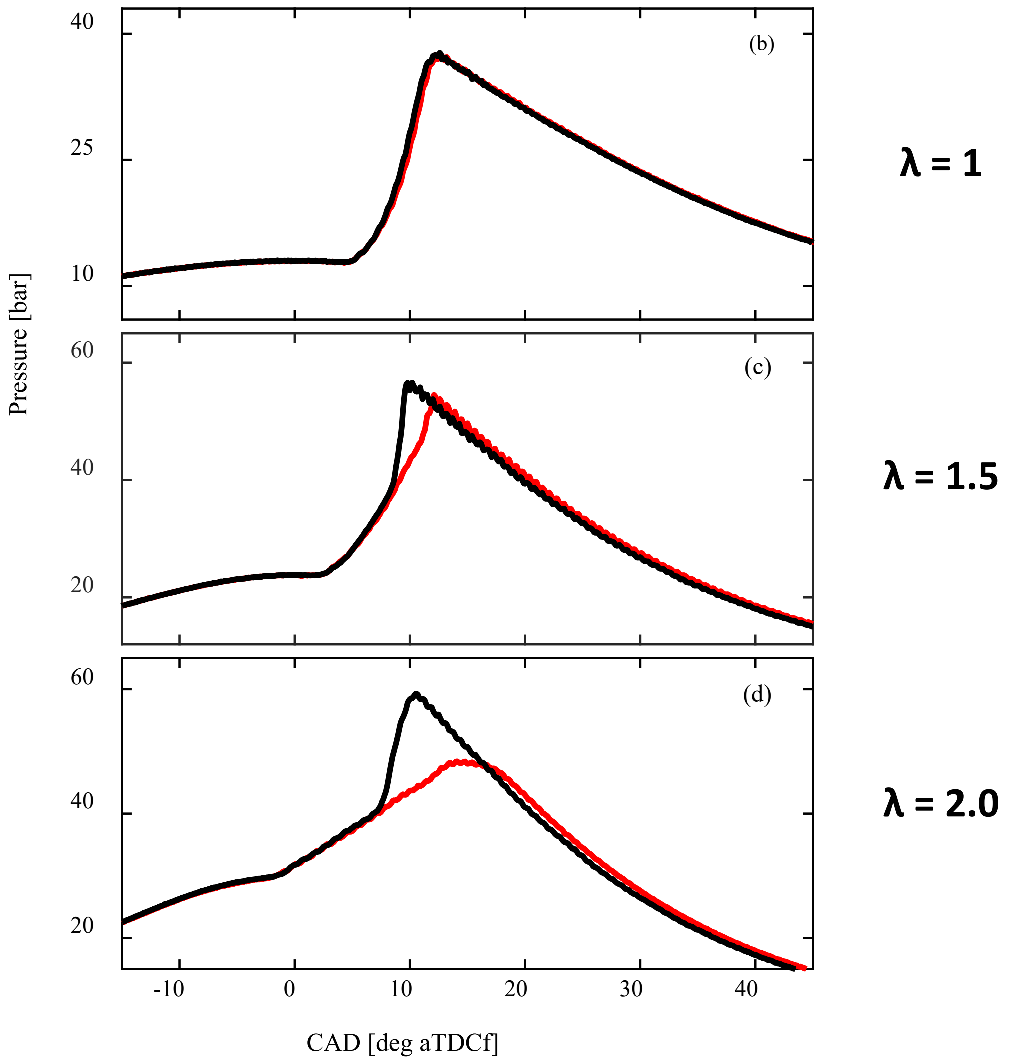
	λ	θ_{ign} [°aTDC]	ON	CCR
	1	3	93.7	6.9
Hydrogen*	1.5	0	117	10.8
	2 [a]	-4	>120	>11.5

Impact of TEL addition to the fresh charge

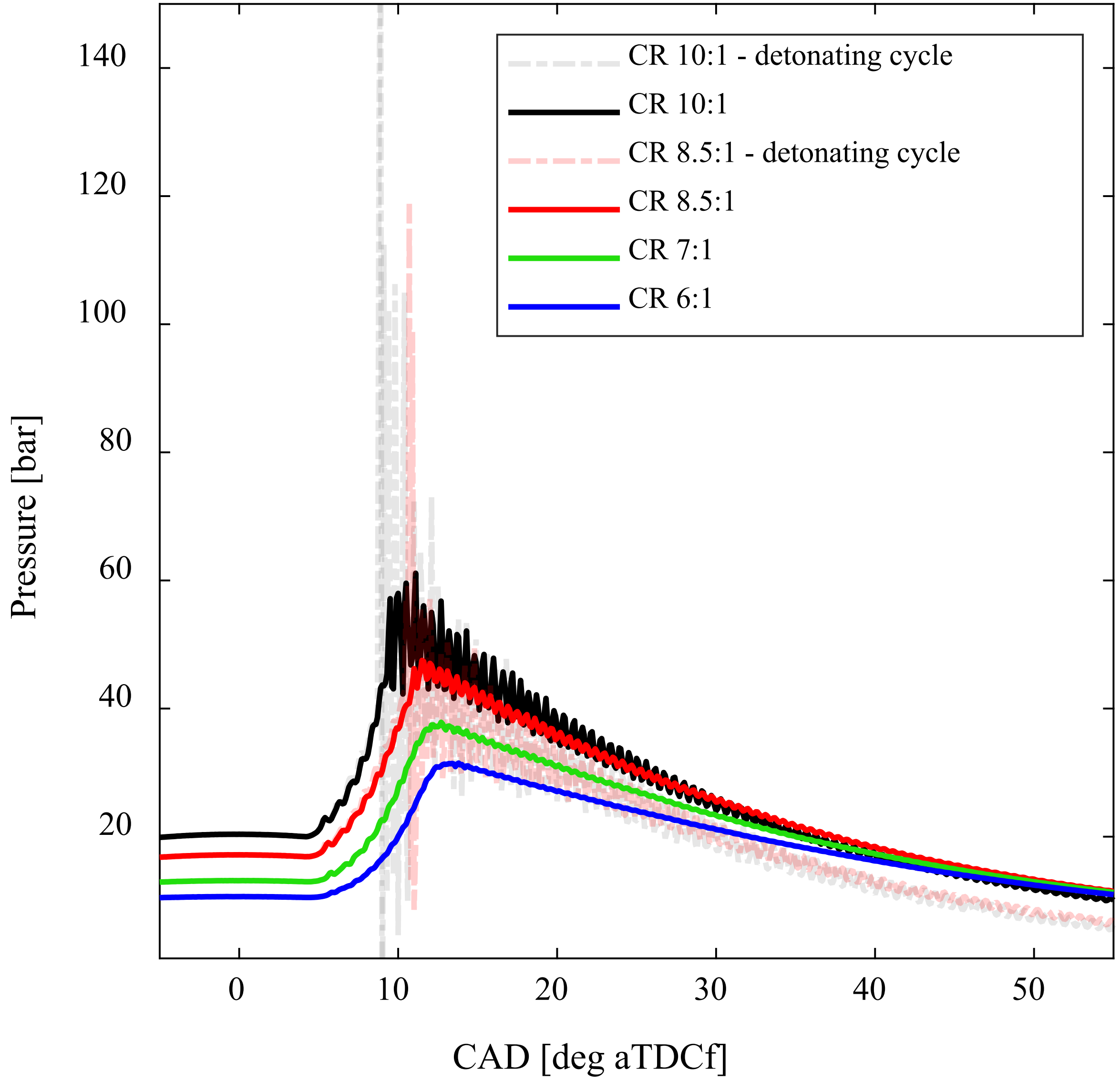
Iso-octane at its SKI standard RON condition



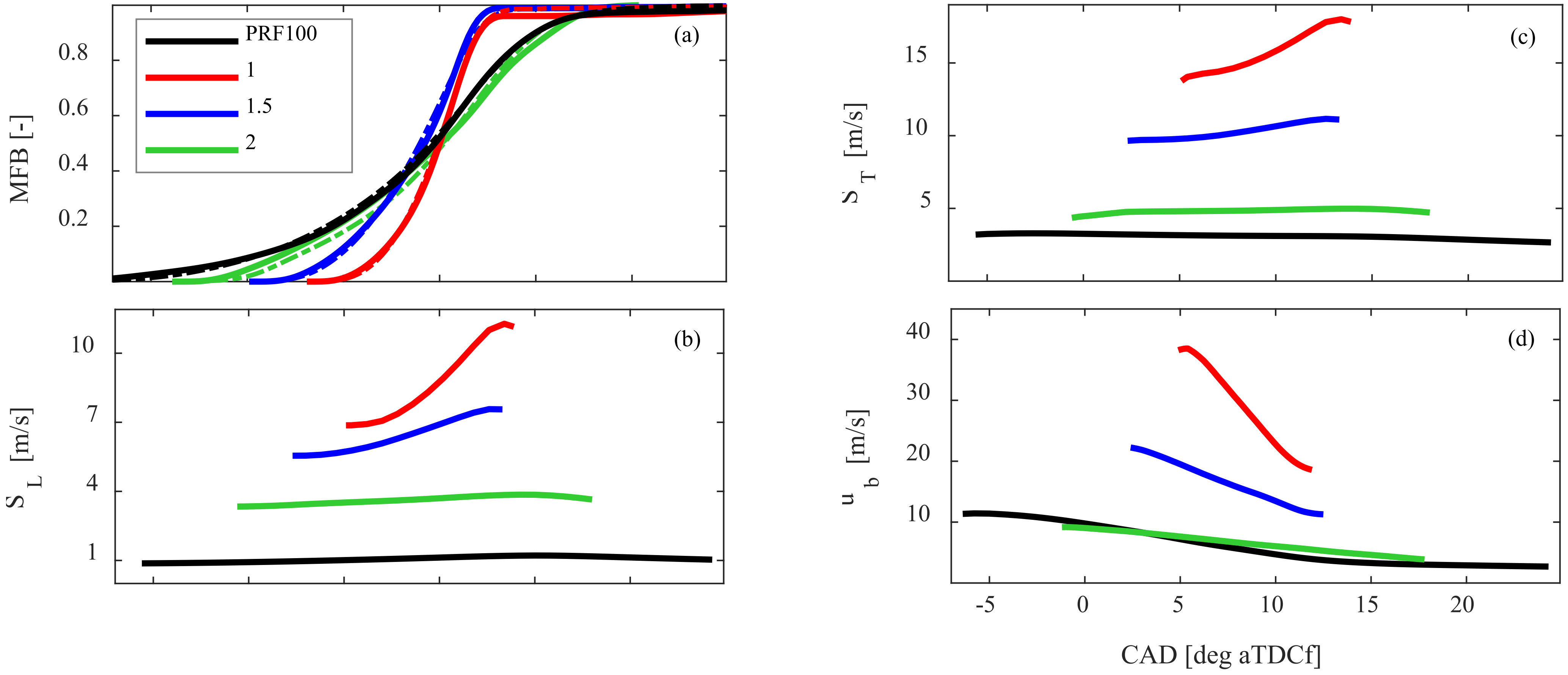
Hydrogen at its SKI modified RON conditions



Further examination of stoichiometric conditions

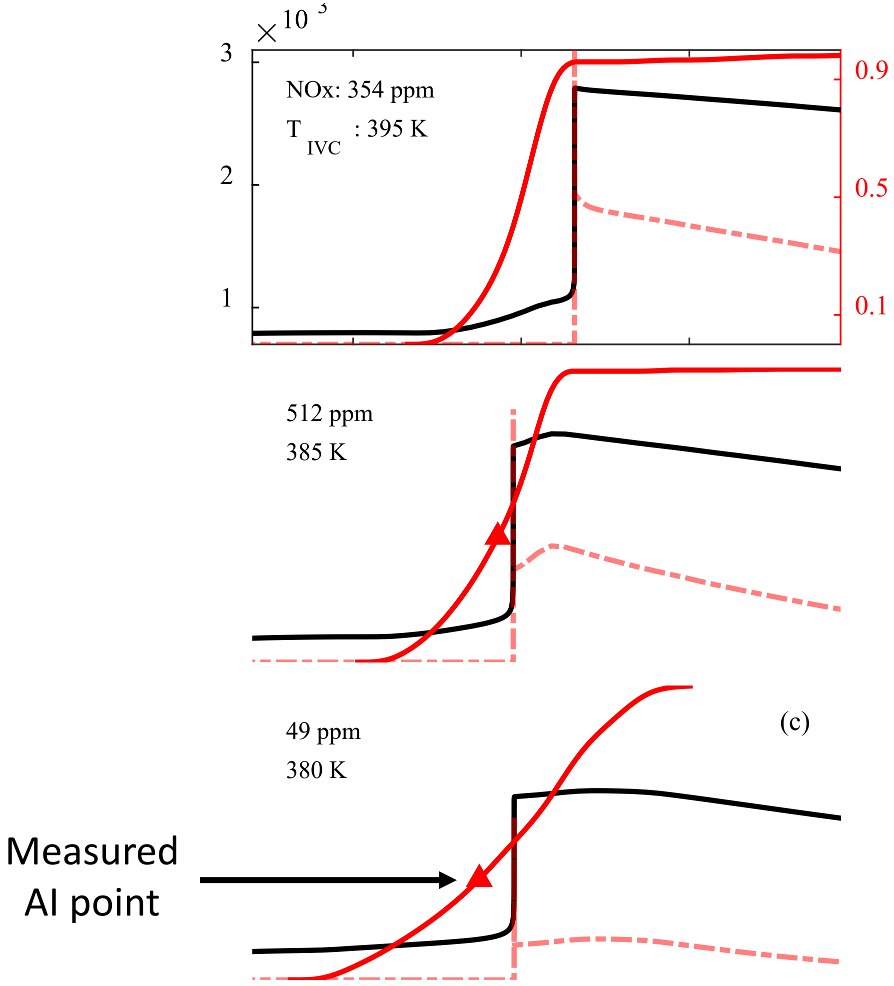


Two zone combustion modelling



One zone kinetic modelling

Reference cases

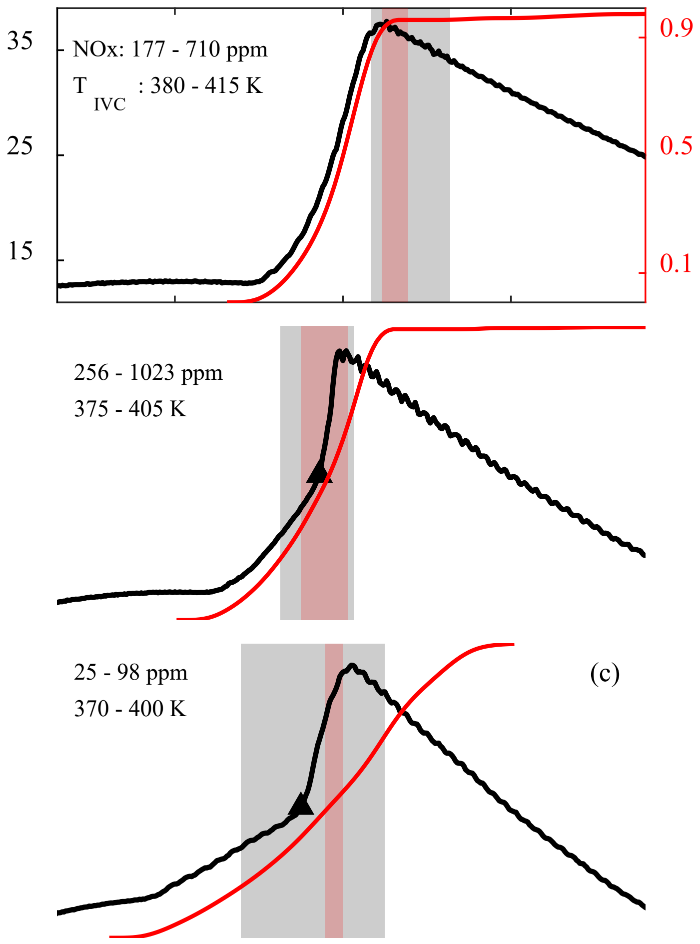


λ = 1

λ = 1.5

λ = 2.0

Sweeping NO (red) and T_{IVC} (grey)



Summary and Conclusions

- Application of the standard RON method showed that hydrogen had a **RON of 62–64.** However, this standard method:
  - required very rich operation on hydrogen at its ‘standard knock intensity’ (SKI) cf. PRFs of similar RON; and
  - the resulting hydrogen combustion featured 50% mass fraction burned (MFB50) *occurring before top dead center.*
- *Modified RON tests* were therefore undertaken for λ = 1, 1.5 and 2, with
  - the spark timing retarded such that the location of hydrogen’s MFB50 matched that of iso-octane at its RON standard condition; and
  - all other operating parameters were maintained as per the standard RON method.
- This modified RON testing is more representative of practical engines and indicated that:
  - hydrogen at λ = 1, 1.5 and 2 had a **modified RON of 93.7, 117 and >120** respectively; with
  - these λ values spanning those that match the energy delivered by common SI engine fuels.
- But these modified RON tests also demonstrated different abnormal combustion regimes between λ = 1 to 2.

Summary and Conclusions, continued

- Between **λ = 1.5 and 2** and SKI conditions, consistent with prior studies of conventional knock in this standard engine:
  - pressure traces featured deflagration and then autoignition followed by a rapid pressure rise;
  - the addition of small amounts of dilute TEL suppressed this rapid pressure rise without modifying the earlier burn.
- At **λ = 1** and SKI conditions:
  - a rapid pressure rise *wasn't observed* and the addition of TEL *had negligible effect*, **suggesting no autoignition!;**
  - **detonation** started to occur as CR was increased above that at SKI, first appearing at around CR = 8.5:1.
- Numerical modelling at SKI conditions demonstrated consistent trends to the experiments:
  - **λ = 1** featured S_t ~ 15−20 m/s and autoignition timings that were very near the end of combustion;
  - λ = 1.5 and 2 featured S_t more similar to typical fuels, and these enabled autoignition timings close to those seen in the experiments.
- Together, these results show that hydrogen:
  - *can* be more knock-resistant than standard gasolines *when used appropriately* (watch out if you don't?);
  - requires the careful application and interpretation of standard test methods; and
  - requires the careful use of diagnostic tools to avoid mistakenly classifying normal and abnormal combustion.

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