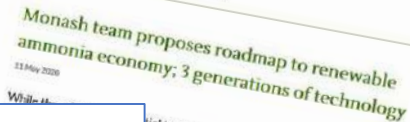




KAUST Research Conference

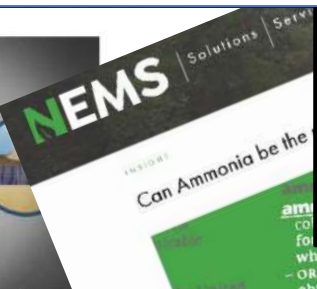
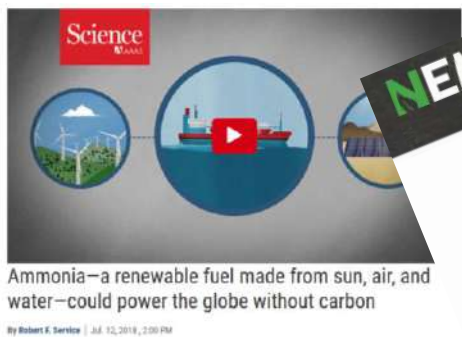
Near Zero-Carbon Combustion Technology

21-23, June, 2021



Ammonia as a fuel For Internal Combustion Engine

Prof Christine Mounaim-Rousselle
University of Orléans



Oxford University Looks To Power Aircraft With Ammonia

by Graham Snelgrove · August 11, 2020 · 41 shares · 3 minute read



PETROCHEMICALS

Is ammonia the fuel of the future?

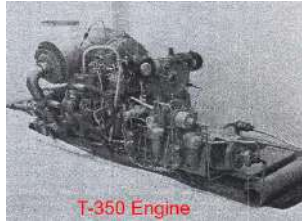
Industry sees the agricultural chemical as a convenient and sustainable means to transport hydrogen and save carbon dioxide emissions

ALEX TULLO, CAEN STAFF

Thanks to some co-workers
P. Bréquigny, R. Rabello, A. Mercier, U Orléans,
C. Lhuillier (UORL/UCL), F. Contino, UC Louvain



AMMONIA AS FUEL FOR TRANSPORTATION : A 'BRIEF' HISTORY



T-350 Engine



1940
Belgium
NH₃/Coal gas =
'syngas'
10 000 miles

1960-1966
US Army
Rocket record



2007-2012 :
Michigan University
50%NH₃/Gasoline
3 800 km

2012-2015 :
KIER, Korea
Dual Fuel
NH₃/Gasoline
10L/100km
until 70% NH₃



Marangoni Toyota GT-86
Eco-Explorer, 2013



Hydrofuel Project-2020



C-Free Run project,
Hydrogen Engine Center
(Iowa), 2018-2021

SOME RECENT EXAMPLES : SPARK IGNITION ENGINE



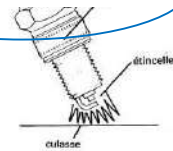
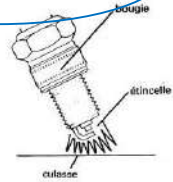
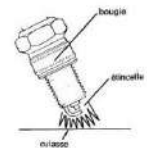
CFR
Gas PFI
Gaseous direct injection

Twin Lombardini (2 cyl./0,25 l)
Gas PFI
LPG injector

GM engine (4 cyl/0.6 l)
Gas PFI
Direct gas Inj
EMULSION

Heavy duty
6 cyl./1.8l
Premixed PFI – CR 10,5

4 cyl./0.9l
Gaseous PFI – CR 9



Texas university

Gasoline+ethanol
(max30%)+NH₃
(17%)

(Haputhanthri et al.
ASME 2017)

Pisa University

NH₃+H₂
Range Extender

Frigo et al. IJHE
2012

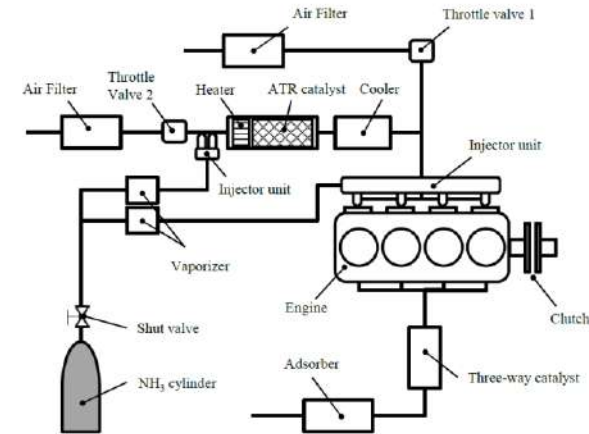
KIMM

Natural Gas + NH₃
(50%)
(Oh et al. FUEL
2021)

Toyota
NH₃ + H₂ Thermal
Reformer
cold start + SCR
catalyst
(Koike et al. IJHE
2021)

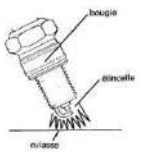
Iowa university,
DTU, ...

NH₃+Gasoline
2012-2013



SOME RESEARCH EXAMPLES : COMPRESSION IGNITION ENGINE

Yanmar Engine (0.3 l)
Liquid premixture GDI (200 b)



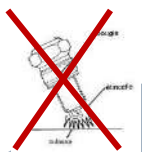
Iowa Energy Center
DUAL FUEL
Premixed DME(min 40%) /NH3
Ryu et al. 2014

3 cyl.CI engine
CR 17.5 (0.54l)



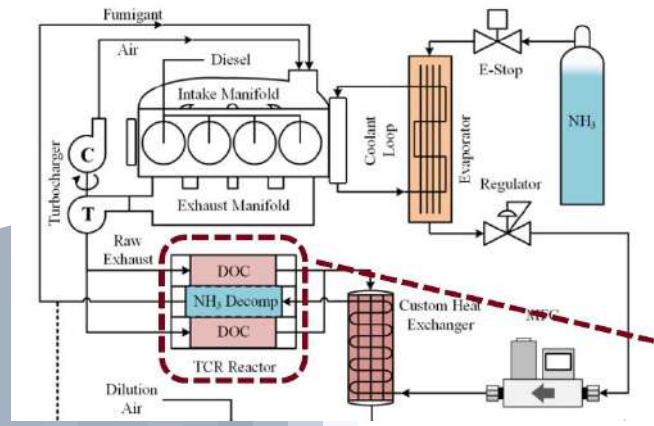
KIER
Diesel (Min 62%)/NH3
DUAL FUEL
Woo, NH3 conference, 2014

Single cylinder research
HCCI engine (0.5l)
Gas fully premixed



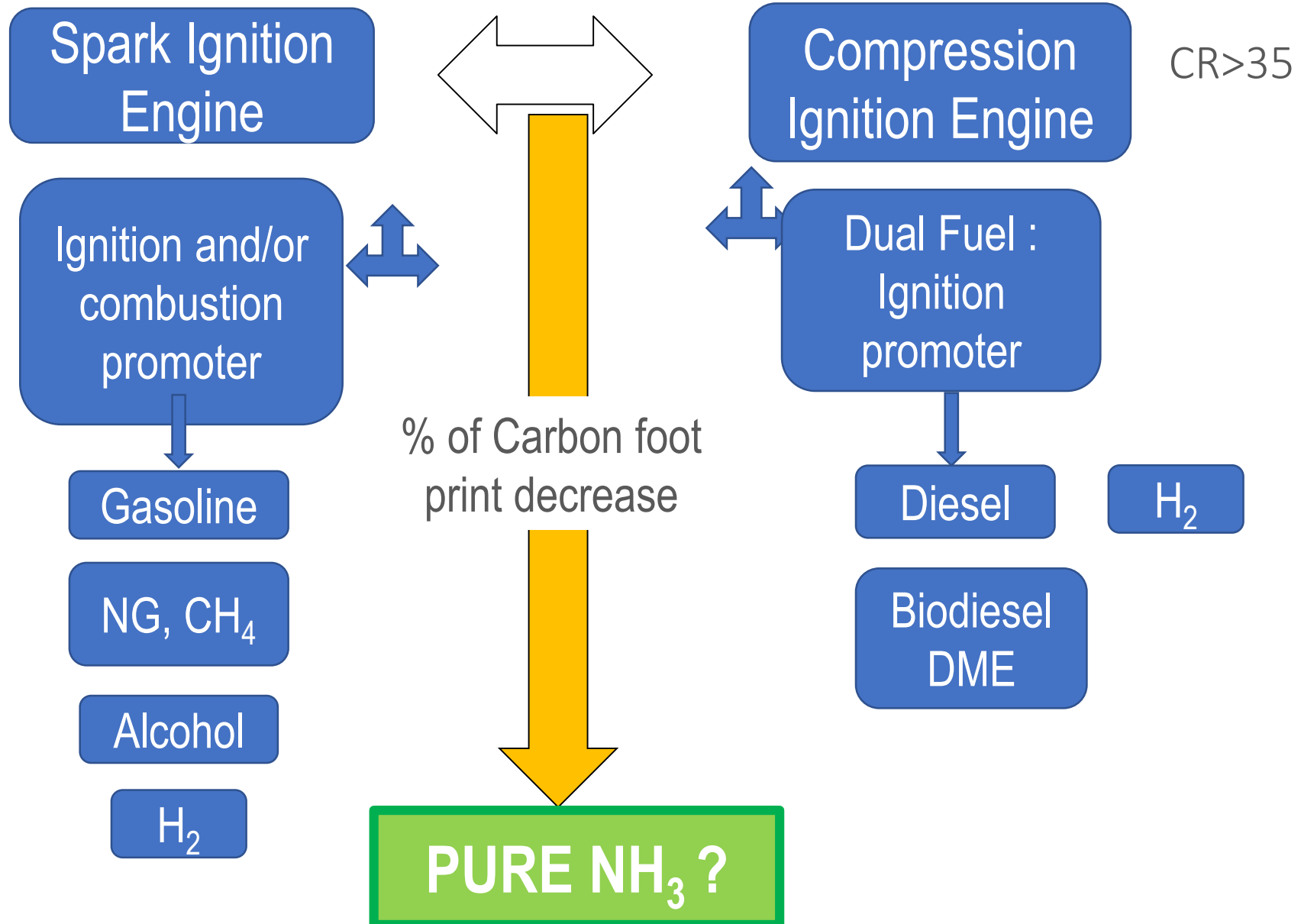
Louvain-VRIJE –
Université
d'Orléans
HCCI
NH3+H2
Pochet et al.,
PROCI 2018

John Deere,
4 cyl. (1.125l)
CR 17



T.E. Murphy Engine
Research Lab
(Minneapolis) Diesel
(45% in Energy)/NH3
Thermal Chemical
Recuperation
- seed with H₂
Northrop et al.
NH3 event 2021

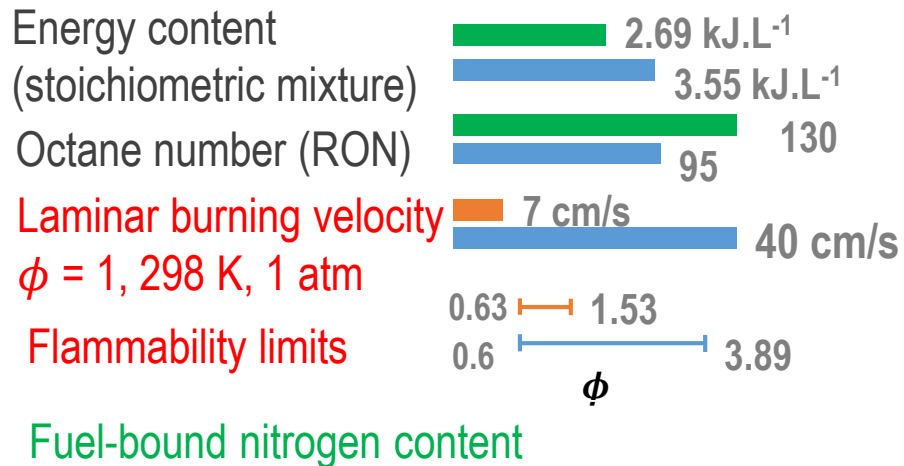
NH₃ AS FUEL FOR POWERTRAIN



RELEVANCE OF SPARK-IGNITION (SI) ENGINE FOR NH₃

Properties of ammonia VS gasoline

Carbon-free



- No CO₂, CO nor PM emissions
- Good energy density
- Potential for high compression ratios (CR)
- Combustion promoter (H₂...) to boost performance and ensure stability ??
- NO_x and NH₃ mitigation strategy required for pollutants

MAIN RESULTS FROM PREVIOUS SI ENGINE STUDIES

For zero-carbon footprint : how ignite ammonia-air mixture,

How obtain complete combustion without any use of conventional fuels ?

Combustion and Performances in SI engines				
Minimum H ₂ for combustion stability	Efficiency		Output energy	
Between 5-10% in vol	Higher for ER>=1		Less than gasoline at low and partial load	
Amount needed decreases with load increase (full load: 0%)	Higher than gasoline		Increase with CR or boosted pressure	
slight effect of engine speed	Decrease with H ₂ increase			
Pollutant Emissions before any aftertreatment device				
	ER decrease (lean)	ER increase (rich)	H ₂ increase	Load
NO _x (ppm)	++ maximum > gasoline	--	+	slight increase but no universal trend
Unburnt NH ₃	--	++	-- H ₂ at exhaust	no universal trend

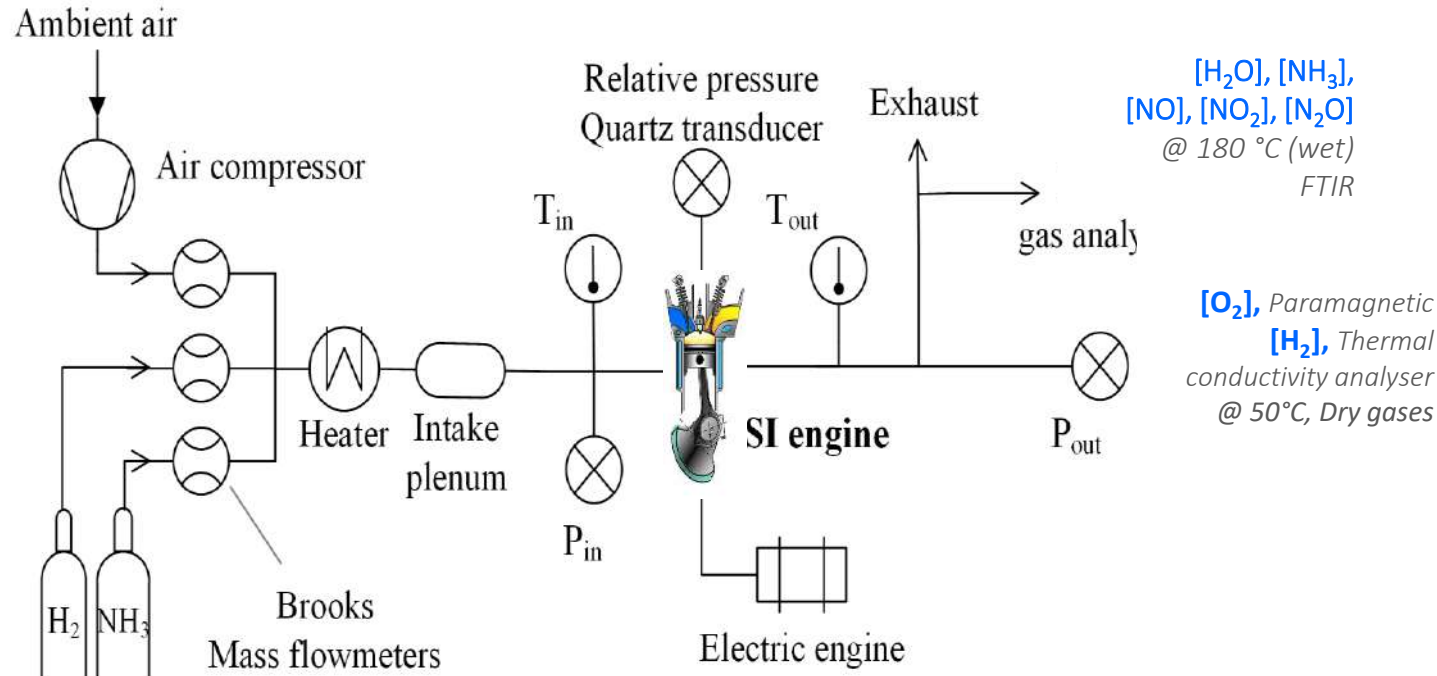
Frigo et al. : from 2000 to 4000 rpm (small engine)

Mounaïm-Rousselle C., Brequigny P. (2020) Ammonia as Fuel for Low-Carbon Spark-Ignition Engines of Tomorrow's Passenger Cars. *Front. Mech. Eng.* 6:70. doi: 10.3389/fmech.2020.00070

Some recent Highlights of combustion process in Single-cylinder engines

- 'CURRENT' ENGINE
 - no optimisation of piston/chamber design
 - no optimisation of ignition device
 - fully premixed NH_3/air (+minimum H_2)
 - to avoid injection process impact

SI SINGLE CYLINDER ENGINE



Piston geometry (GDI)



Engine Characteristics	
Engine Type	Current PSA EP6DT
Bore	77 mm
Stroke	85 mm
Connecting Rod Length	138.5 mm
Displacement Volume V _{cyl}	395.81 cm ³
Compression Ratio	10.5

MINIMUM OPERATING LIMITS WITH PURE AMMONIA

□ Engine speed effect - stable conditions ($s_{IMEP} \leq 5\%$)

		650 rpm			1000 rpm			1500 rpm			2000 rpm					
		%H ₂														
Φ	Pin (bar)	0%	5%	10%	0%	5%	10%	0%	5%	10%	0%	5%	10%			
0.9	<=0,65	■			■			X	■			X	■			
	0,8-0,85	■			X	X	X	■			X	X	X	■		
	1	■			X	X	X	X	X	X	■			X	X	

- impossible to ignite at low and high rpm without H₂
- difficult at low load
- possible 'sometimes' to ignite with NH₃ only at naturally aspirated conditions

*optimized ignition timing (around 40-35 CAD BTDC)



areNH₃a

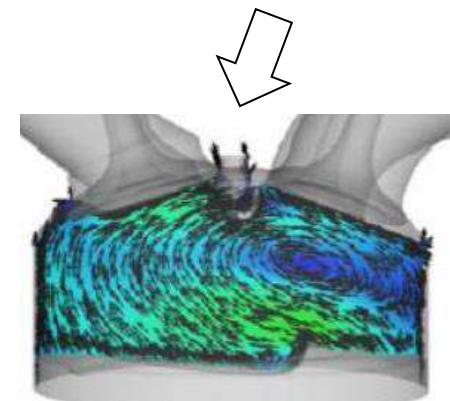
STELLANTIS

<https://arenha.eu/>

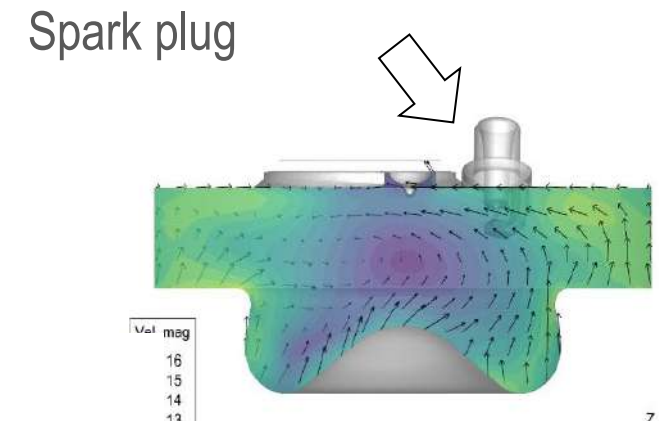
EXTENSION OF 'LOW' OPERATING LIMIT

- Solution : Increase the CR
 - Diesel Engine with Spark Ignition

Engine Type	Current PSA EP6DT	SACI PSA DV6
Displacement Volume V_{cyl}	400 cm ³	400 cm ³
Compression Ratio	10.5	14 to 17
Valves	4	2
Tumble ratio	2.4	
Swirl ratio		2



SI



SACI

*No optimization of ignition system or location



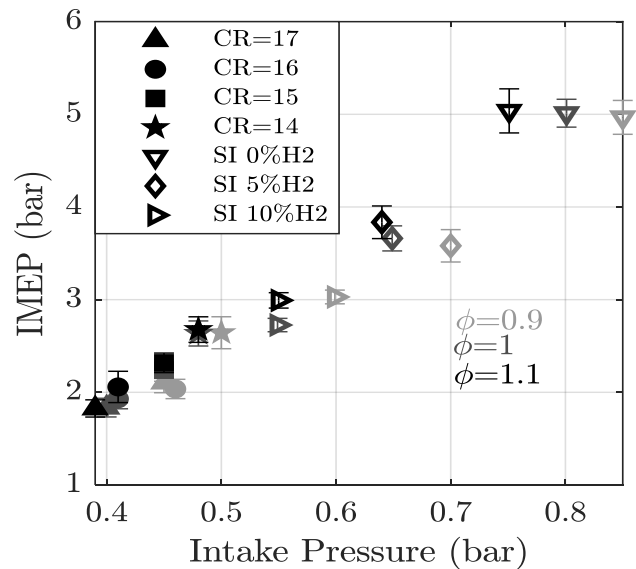
STELLANTIS

areNH₃

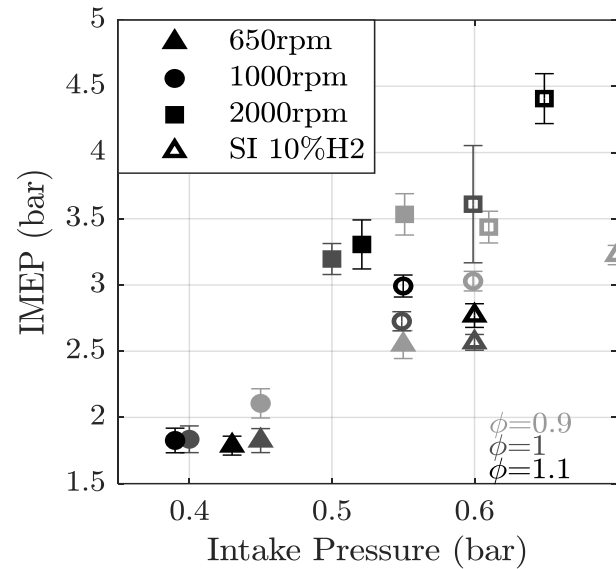
<https://arenha.eu/>

□ Increase of CR :

➤ SACI versus SI engine



Engine speed :1000 rpm

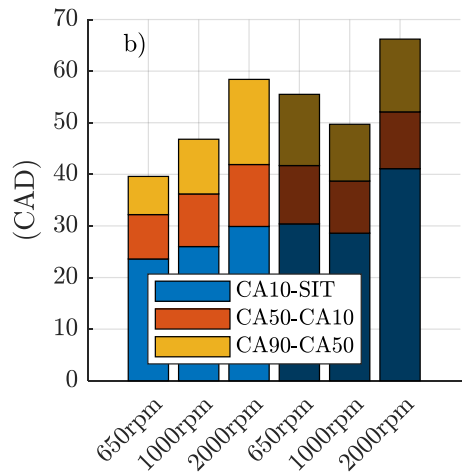


SACI CR: 17, SI :CR=10.5

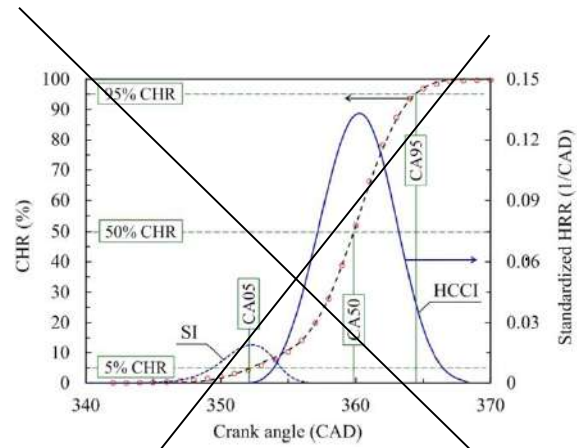
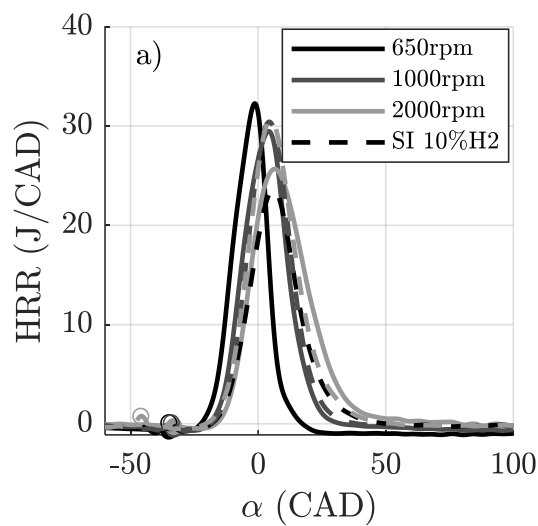
- Good improvement of NH₃ combustion with CR increase despite of flow field
- No H₂ needs
- Extension of low load limits
 - 1.7 b IMEP (as Koike et al. with Reformer)
 - CR 17, 650 rpm,
 - lower limit with slightly rich



FLAME DEVELOPMENT : SACI VERSUS SI



$\phi = 1$



- SACI combustion mode :
 - Without H2
 - Not 2 identified phases of HRR
- Faster first phase than SI engine
 - Pressure effect

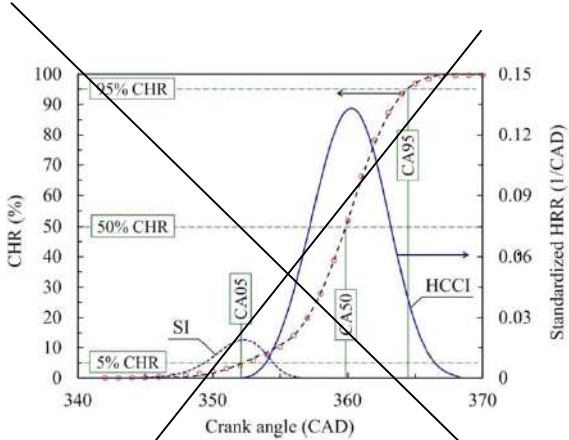
FLAME DEVELOPMENT : SACI VERSUS SI

-40 CAD to 27 CAD ATDC



Spark timing : -40 CAD

ER NH3 = 0.9 - IMEP = 6.7 b



- SACI combustion mode :
 - Without H2
 - Not 2 identified phases of HRR
- Faster first phase than SI engine
 - Pressure effect
 - FULLY PREMIXED PROPAGATION

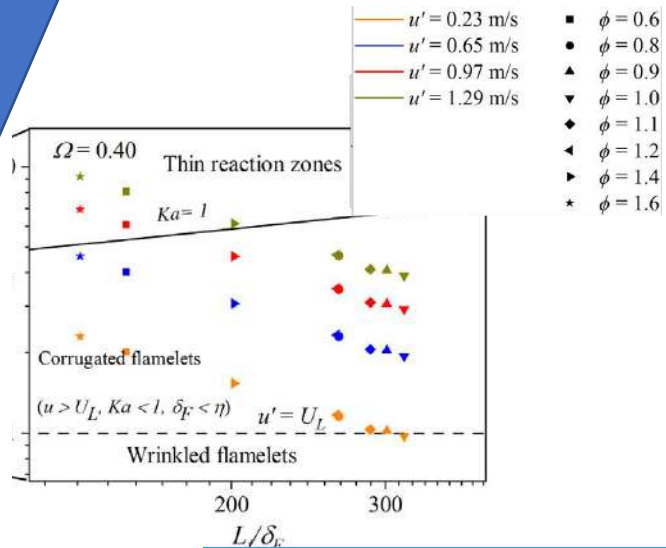
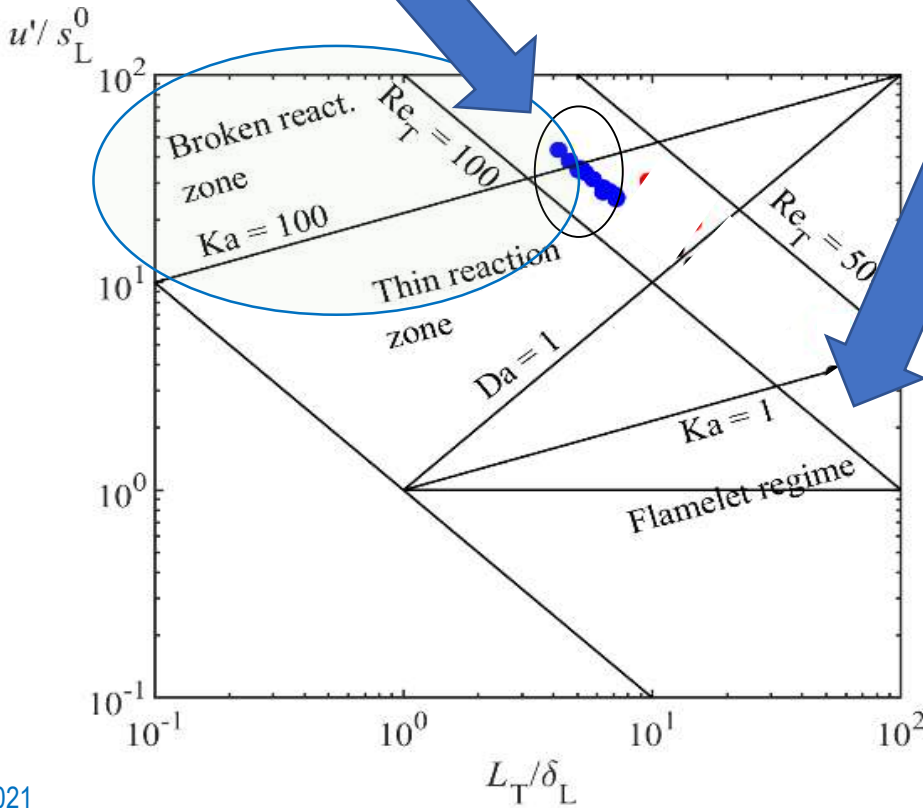
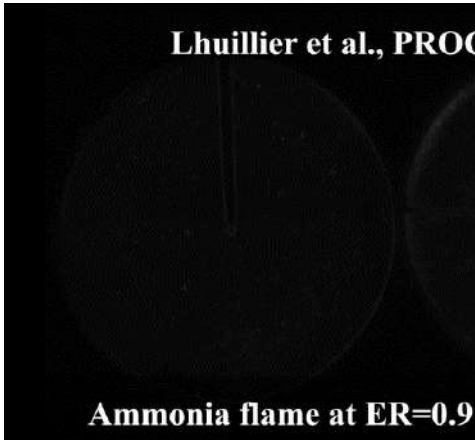
PREMIXED TURBULENT FLAMES

SI engine

- $s_L \ll U'/s_L$
- $\delta_L \gg L_T/\delta_L$???

SACI engine : HT/HP

- $s_L \nearrow U'/s_L \searrow$
- $\delta_L \searrow L_T \nearrow L_T/\delta_L$???



▪ SACI combustion mode :

- Turbulent scale size ? Flamelet regime ?
-

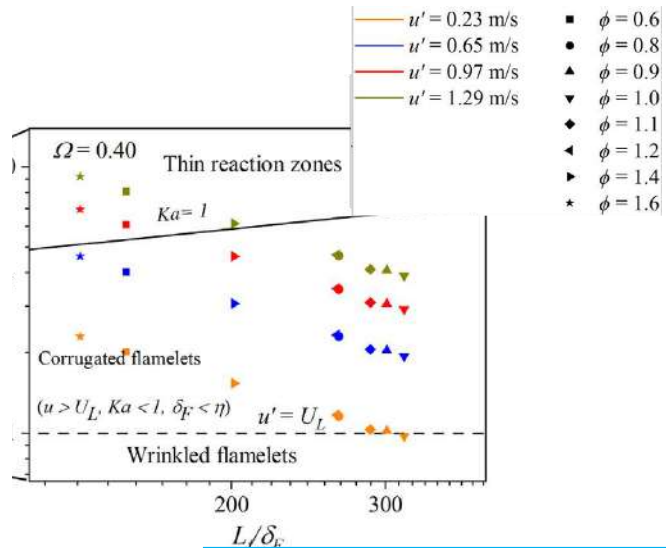
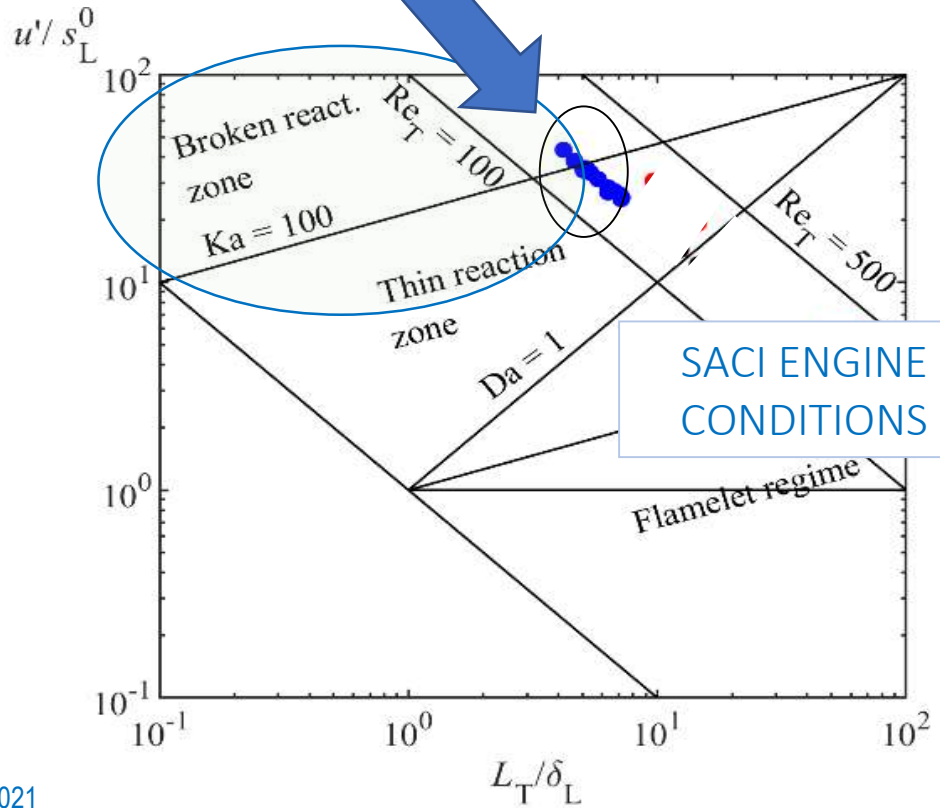
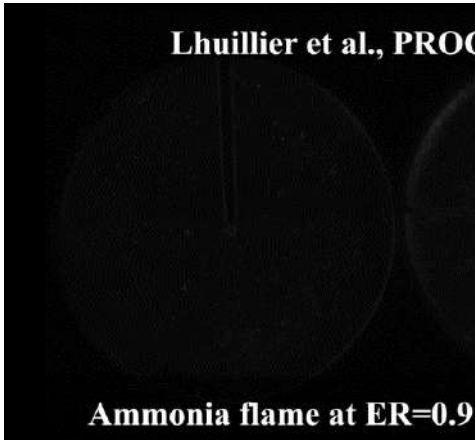
PREMIXED TURBULENT FLAMES

SI engine

- $s_L \ll U' / s_L \gg$
- $\delta_L \gg L_T / \delta_L ???$

SACI engine : HT/HP

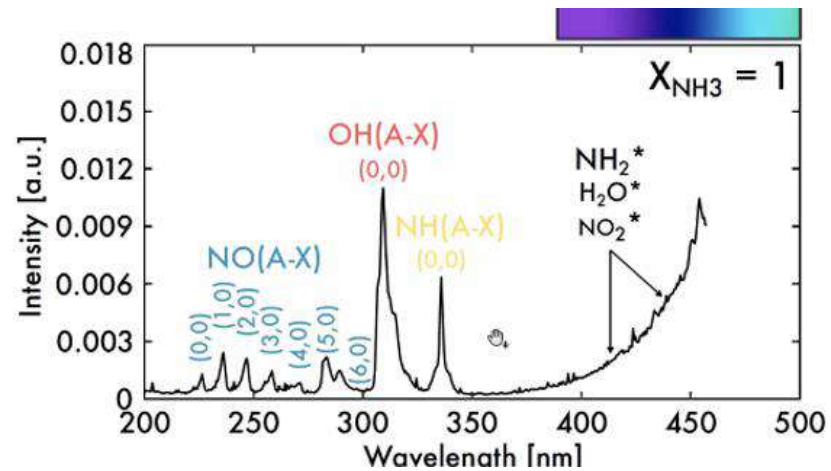
- $s_L \nearrow U' / s_L \searrow$
- $\delta_L \searrow L_T \nearrow L_T / \delta_L ???$



▪ SACI combustion mode :

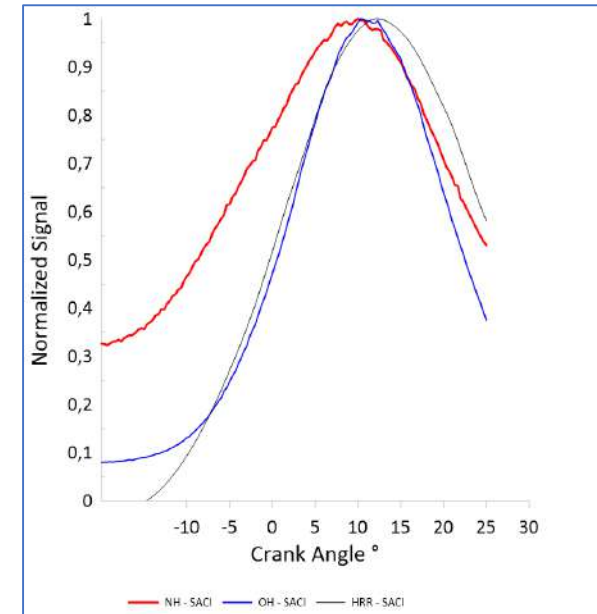
- Turbulent scale size ? Flamelet regime ?
-

OH (blue) + NH (red) chemiluminescence



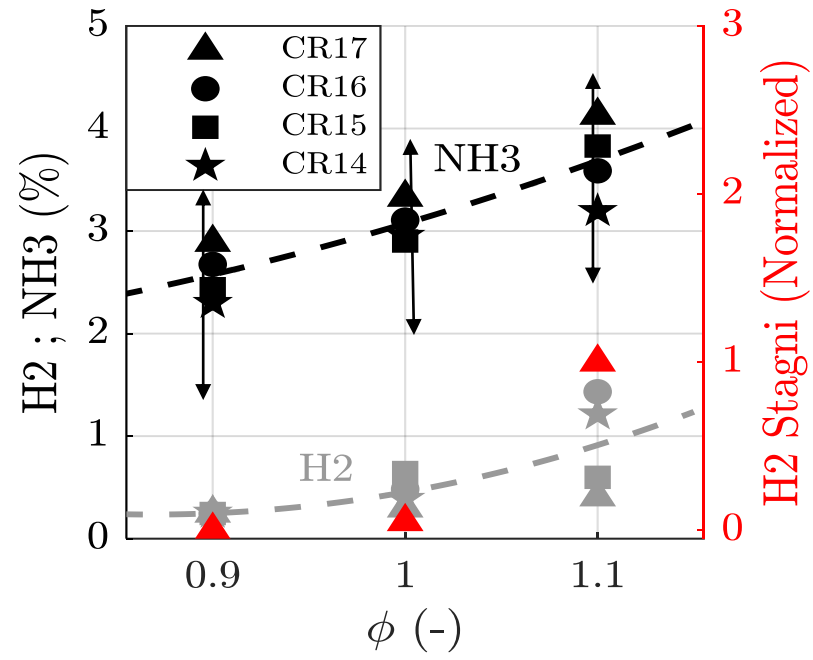
T. Guiberti, NH₃ event, 2021

FLAME DEVELOPMENT : SACI VERSUS SI



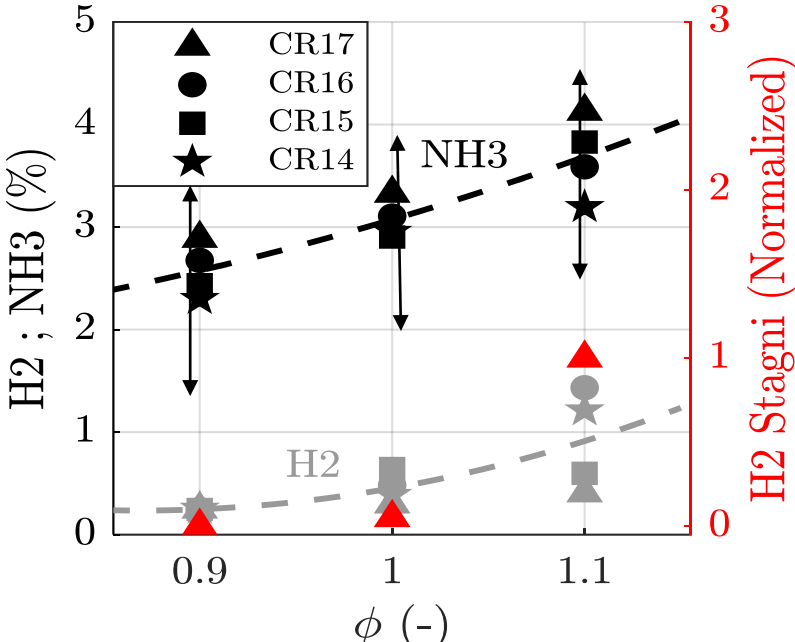
- SACI combustion mode :
 - HT/HP + Turbulent flow field = Flamelet regime ?

FLAME DEVELOPMENT : SACI VERSUS SI

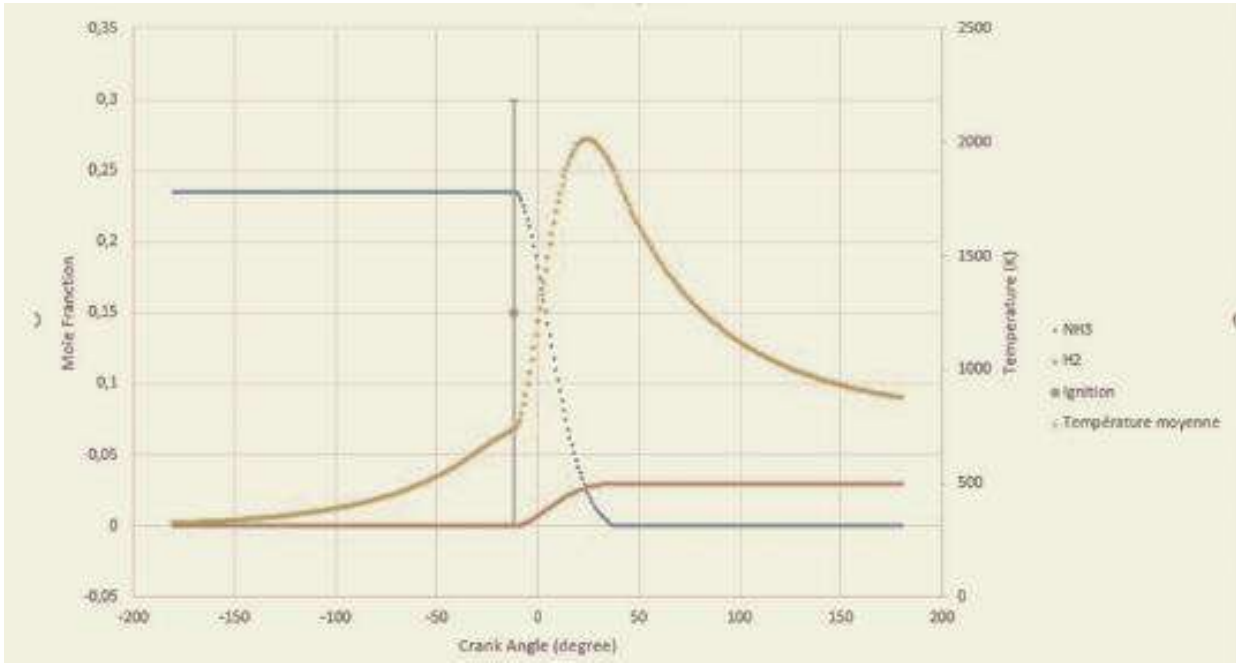


- SACI combustion mode :
 - HT/HP + Turbulent flow field = Flamelet regime ?

FLAME DEVELOPMENT : SACI VERSUS SI



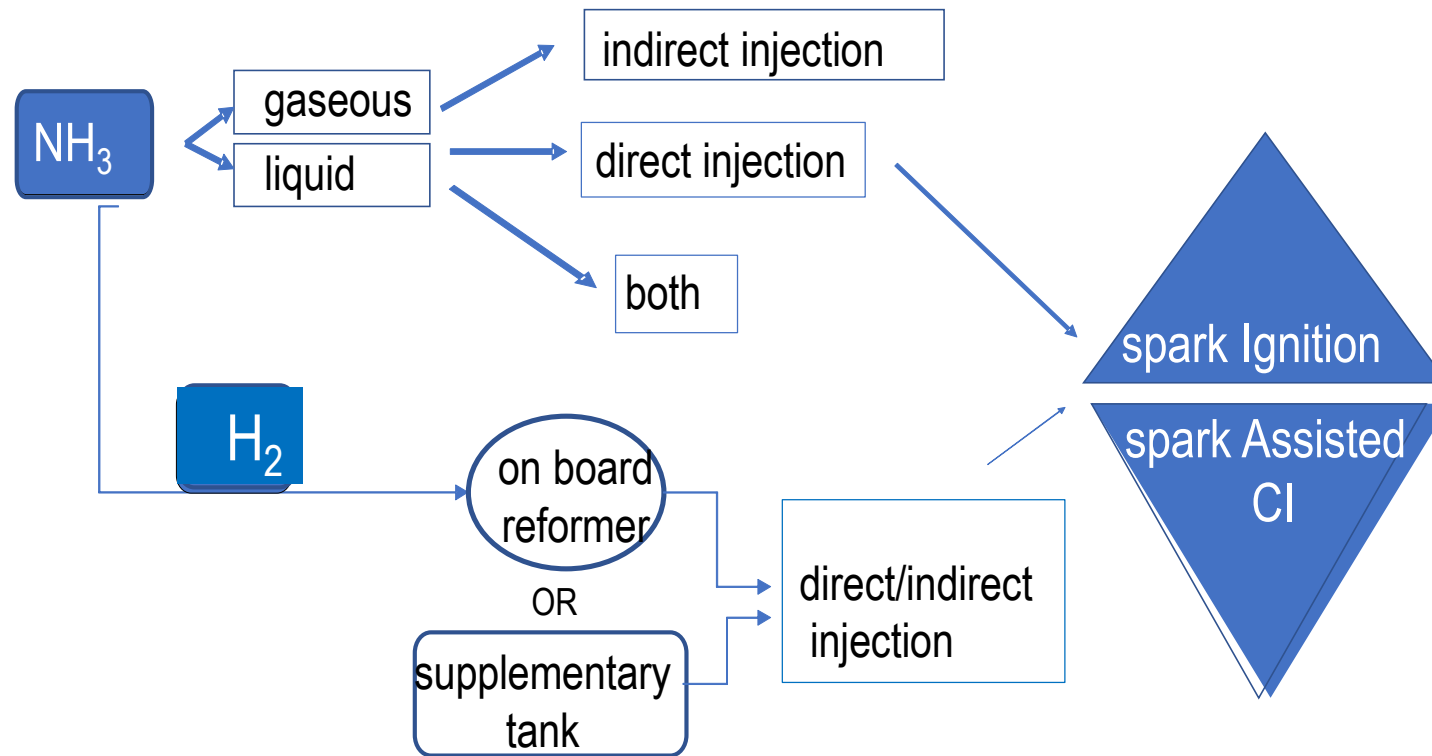
Kinetics mechanism Stagni et al. 2020



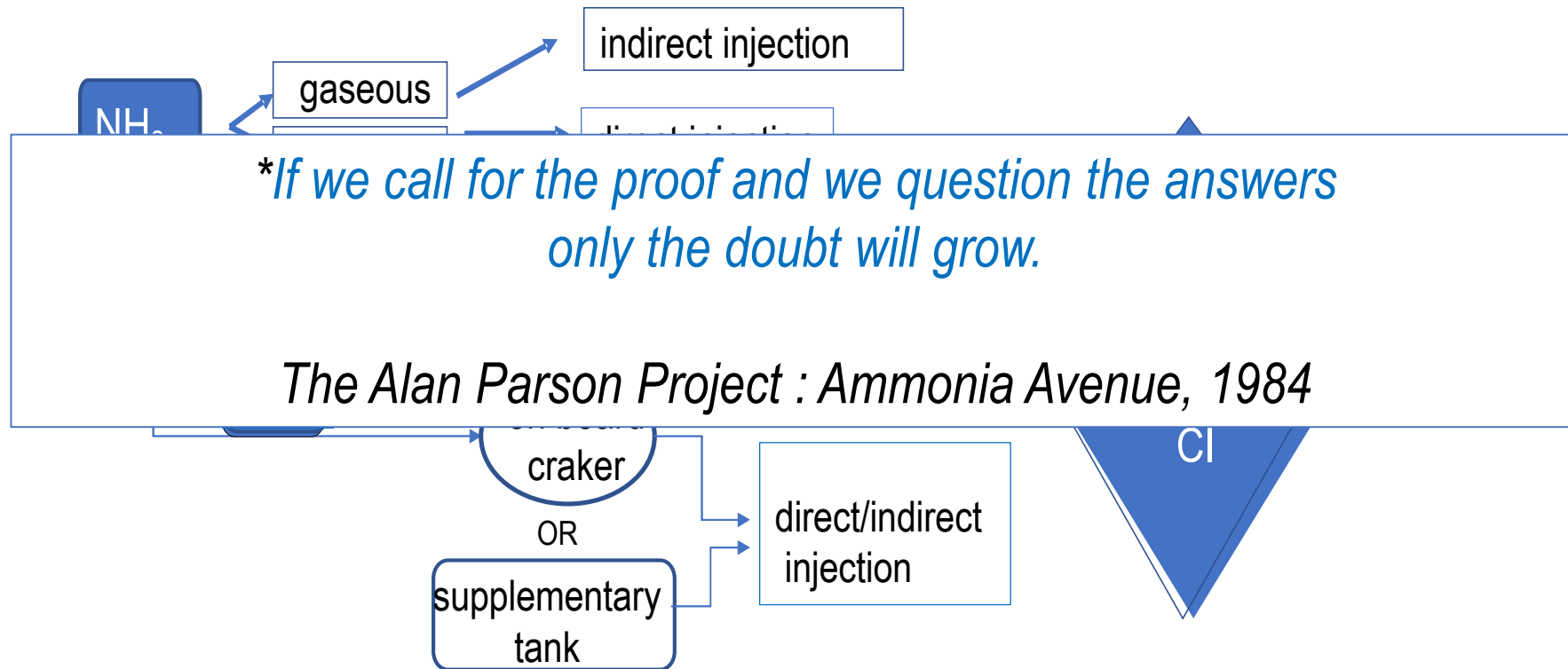
- SACI combustion mode :
 - HT/HP + Turbulent flow field = Flamelet regime ?
 - HT/HP = in situ NH₃ decomposition in H₂

For zero-carbon footprint : how ignite ammonia-air mixture,

How obtain complete combustion without any use of conventional fuels ?



Ammonia only or Ammonia+H₂

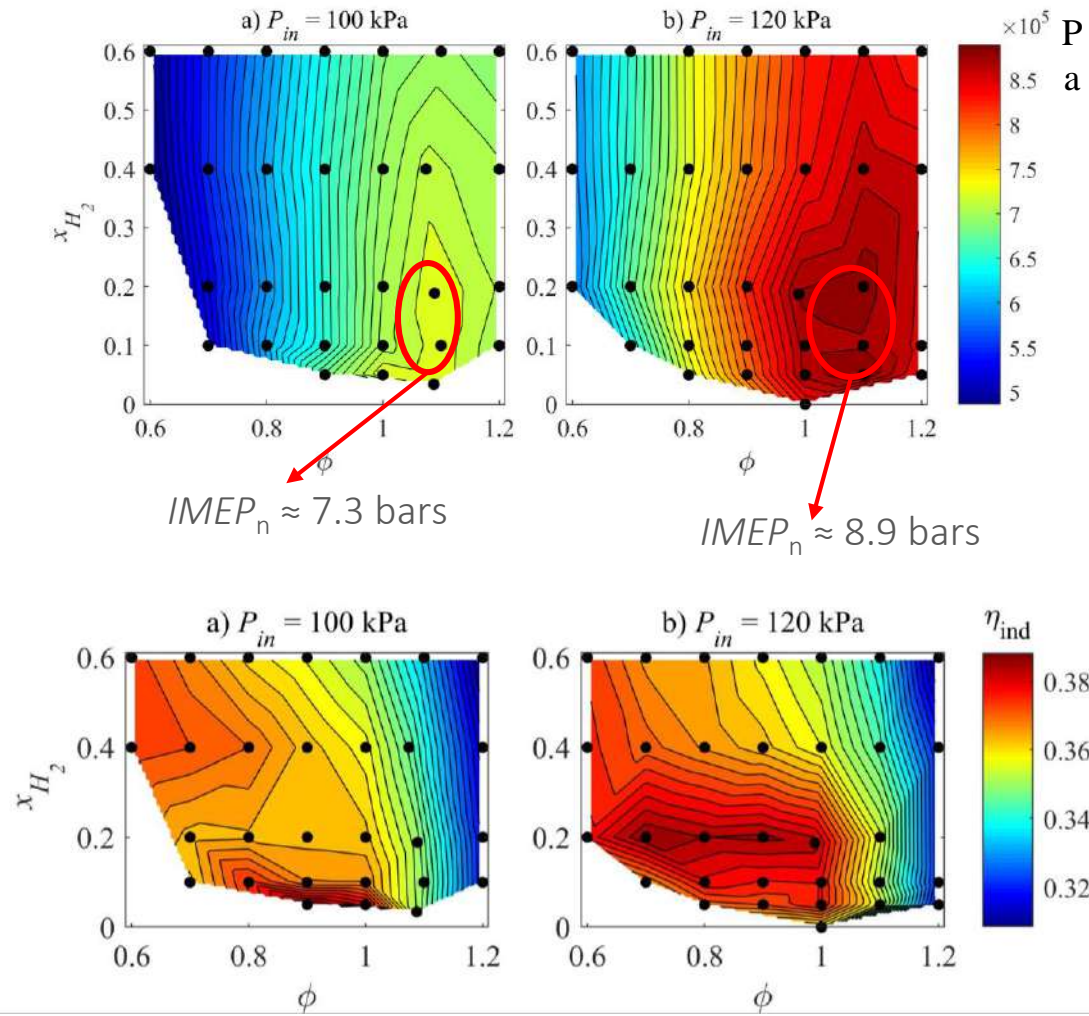


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- K.H.R. Rouwenhorst, O. Elishav, B. Mosevitzky Lis, G.S. Grader, C. Mounaïm-Rousselle, A. Roldan, A. Valera-Medina, Techno-Economic Challenges of Green Ammonia as an Energy Vector , Book chapter : Chapter 13 - Future Trends, Editor(s): Agustin Valera-Medina, Rene Banares-Alcantara,, Academic Press, 2021, Pages 303-319
- A. Valera-Medina, F. Amer-Hatem, A. K. Azad, I. C. Dedoussi, M. de Joannon, R. X. Fernandes, P. Glarborg, H. Hashemi, X. He, S. Mashruk, J. McGowan, C. Mounaïm-Rousselle, A. Ortiz-Prado, A. Ortiz-Valera, I. Rossetti, B. Shu, M. Yehia, H. Xiao, and M. Costa, A review on ammonia as a potential fuel: from synthesis to economics,, *Energy & Fuels*, DOI: 10.1021/acs.energyfuels.0c03685
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Ammonia with H₂

- IMEP and Indicated Efficiency for mid-load



- Highest output energy
 - with H₂ content < **20%** as Koike et al.
 - slightly rich
 - Similar output energy than with **CH₄/air**, $\phi = 1.0$
 - 20% Intake Pressure increase
= 22% IMEP increase

- Highest efficiencies
 - lean mixtures (no excess fuel)
 - **$5\% \leq x_{H_2} \leq 20\%$**
 - $\eta_{ind} \lesssim 40\%$ → similar to conventional fuels