#### Internal Combustion Engines research in the TU/e Zero Emission Laboratory

**Noud Maes** 

Mechanical Engineering, Power & Flow





#### Content

Zero Emission Laboratory

- Vision & organization
- Setups

Recent & current work

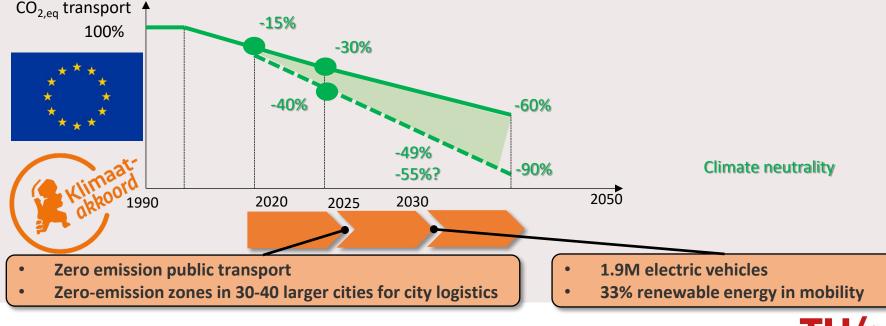
Quick reference to CFD





#### **Zero Emission Lab vision**

• EU-funded Mission D+: emission-free, future-proof mobility for people & goods by 2050



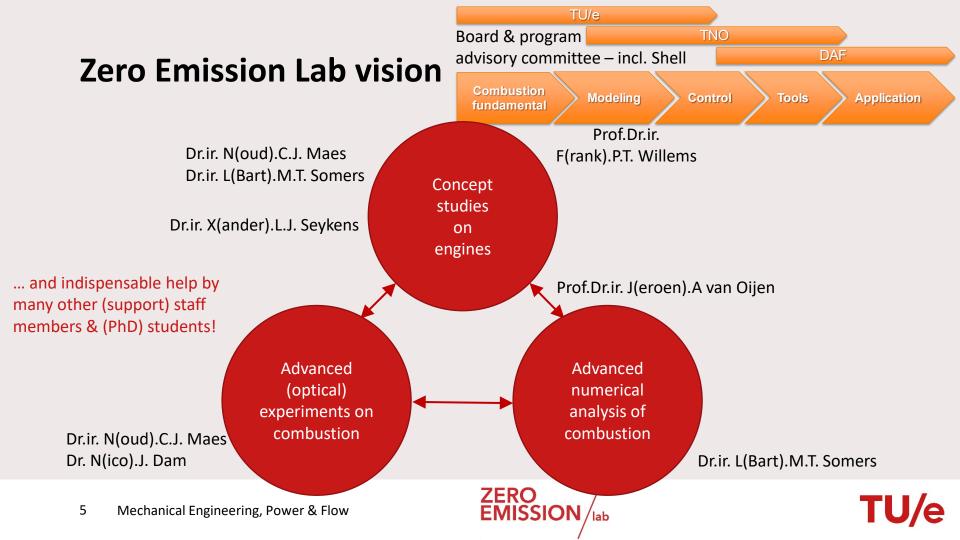
#### Zero Emission Lab vision

**ICE0.0** ۲

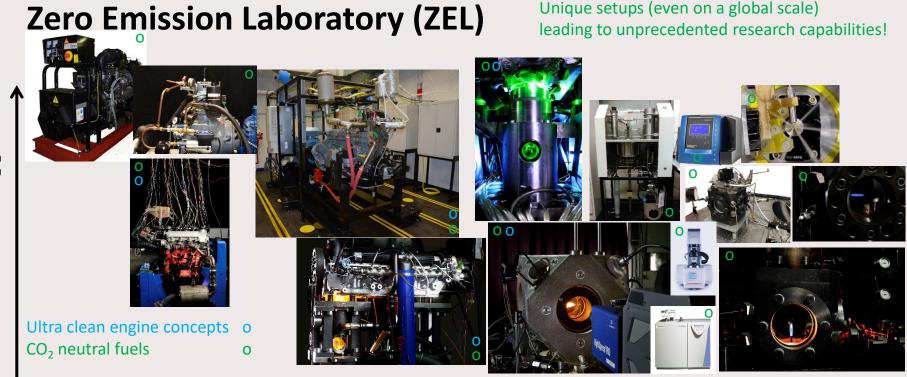


- E- and advanced bio-fuels ٠
- - UHC & CO
- **Combination of ultra-efficient internal combustion engines and sustainable** • fuels is key to accelerate GHG emission reduction in heavy-duty transport
- Key scientific challenges: •
  - In-cylinder mixture formation
  - Heat release shaping & control •
  - Fuel flexibility •
- Mechanical Engineering, Power & Flow 4









Fundamental nature of research





Lubricity, stability, & elemental composition testing

- Prior to engine tests
  - Limited batch sizes & preventing damage
  - Insight in applicability/usability





CO<sub>2</sub> neutral fuels

0





Hatz engine Generator engine with emission and in-cylinder pressure analysis Robust, cheap, fuel-flexible DI CI commercial setup

**<u>New</u>**: 3 Hatz engines on moving frames for BSc students



#### CO<sub>2</sub> neutral fuels

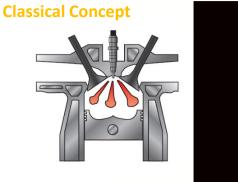


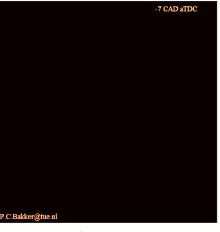
9 Mechanical Engineering, Power & Flow





Paccar MX13 single-cylinder (RCCI capable) engine Reactivity Controlled Compression Ignition Ultra clean & fuel flexible with fuels that inherently prevent soot formation!





Hot burning soot

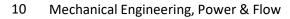


Chemiluminescence

New Concept



Ultra clean engine concepts o CO<sub>2</sub> neutral fuels o

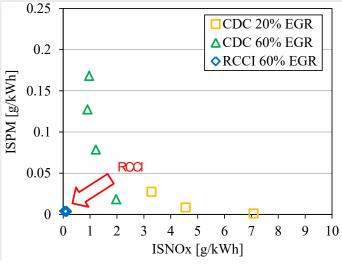


Paccar MX13 single-cylinder (RCCI capable) engine Reactivity Controlled Compression Ignition

Low emissions with combustion phasing control!

- Change high/low octane fuel ratio
- Timing of the DI low octane fuel





Ultra clean engine concepts o CO<sub>2</sub> neutral fuels o





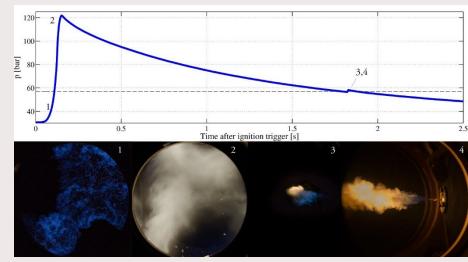
Eindhoven High-Pressure Cell (EHPC)

Pre-burn of lean charge of  $C_2H_2$ , Ar,  $N_2$ , and  $O_2$  – sequential fill!

Relatively long cool down Diesel surrogate fuel injection Engine-like conditions:

- Densities up to 40 kg/m<sup>3</sup> (350 bar)
- Peak temperatures up to 2000 K
- $O_2$  from 0 to 35 vol-%

Ø100 mm optical access – ~1.3 L

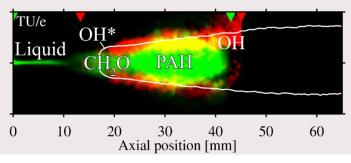


 Ultra clean engine conceptsoCO2 neutral fuelso

Eindhoven High-Pressure Cell

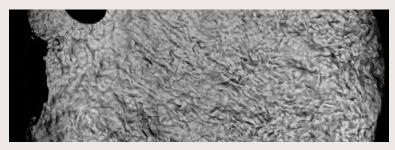
Visualization of

- Liquid/vapor-phase fuel
- Species distributions
- Soot (precursors)

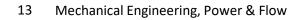














Combustion Research Unit (CRU):

Commercial ignition quality tester

Constant volume chamber ~0.4 L, pre-heating and compressed gases Engine-like conditions:

- Pressures up to 60 bar
- Peak temperatures up to 1050 K
- $O_2$  from 0 to 21 vol-%

Robust, fuel-flexible commercial setup for analyzing heat-release Optional optical access through borescope Equipped with dual-circuit heavy-fuel oil injector



CO<sub>2</sub> neutral fuels



Eindhoven Low-Pressure Cell (ELPC) Constant volume chamber ~1 L

- Filled with compressed gases (N<sub>2</sub>, He, Ar)
- Pressures up to 50 bar

- EL)e, Ar)
- Mostly used for hydrogen research fuel pressure up to 100 bar

ZERO

ISSION

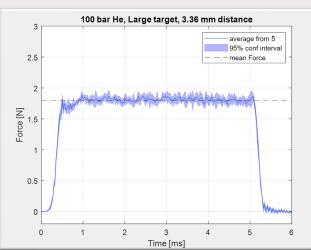
- Full optical access
- Mach-disk formation, mixing, & penetration studies

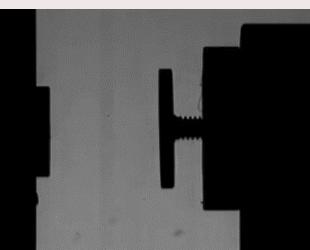


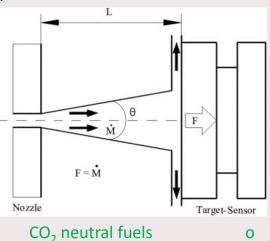


Atmospheric momentum exchange setup

- Essential parameters for modeling fuel injections!
- Syringe pump: momentum & mass flow up to 200 MPa
- Currently in use for H<sub>2</sub> injections (starting with He)
  - Up to 200 bar gas bottle pressure









#### Proteus "ICE H2.0"

- Base engine: 1-cylinder, 2L Cl
  - Proteus Ricardo base
  - DAF MX13 liner, piston, & head
  - Extended piston "Bowditch" → Optical access
  - Quartz/sapphire piston
  - Adjustable CR
  - Flexible skip-firing





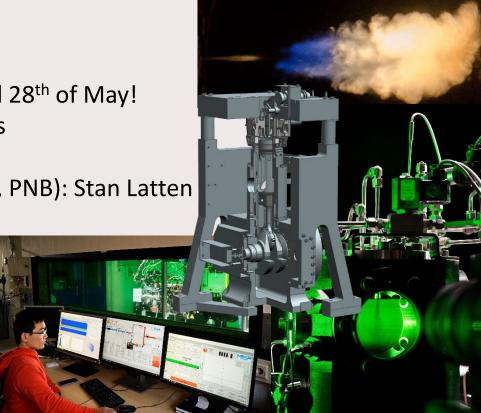
#### **Recent & current work**

SmartCHP: Yu Wang → PhD defended 28<sup>th</sup> of May! Using Fast-Pyrolysis Bio-oils in engines

**ZEL project/ACD-call** (DAF, Shell, TNO, PNB): Stan Latten (Re)building an optical H2-ICE

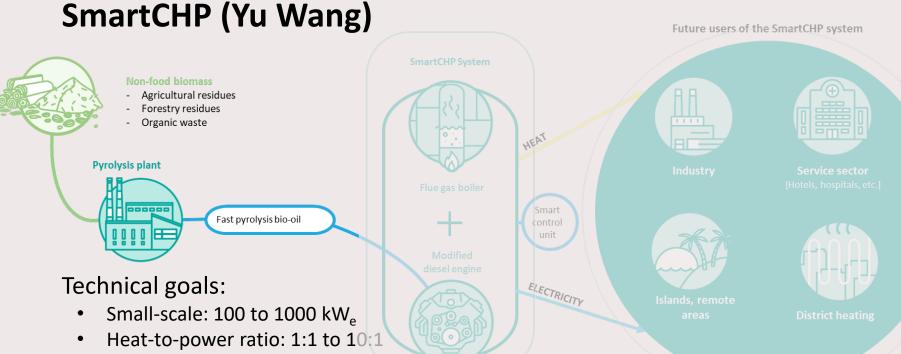
**APC** (vici prof. v. Oijen): Max Peters Hydrogen jets

**CSC** (future fuels): Zhoncheng Sun Biofuels & oxymethylene ethers





Yu Wang, "Direct application of fast pyrolysis bio-oil in combined heat and power", PhD thesis, TU/e, 2024.



- Overall CHP efficiency > 85%
- GHG emission reduction > 80%

FPBO properties (compared to diesel)

- High viscosity (×15)
- Low energy density (~37%)
- High oxygen and water content
- Impurity particles
- Strong acidity

#### Challenges in engine application:

- Unknown ignition & combustion characteristics
- Corrosivity, nozzle clogging, poor ignitability

FPBO



Diesel







PAH

Ambient gas

FLOL

Nozzle

Ċ –

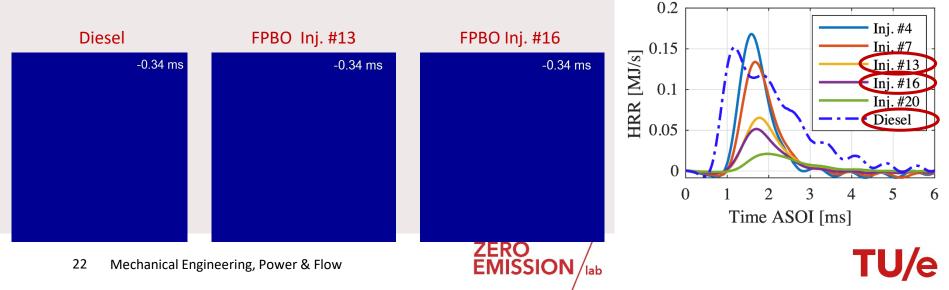
- Ignition
- Combustion
- Fuel recipe

# Fundamental research → Engineering practice

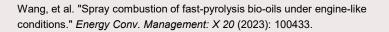
CVCC Durability ٠ Emission ٠ Engine Efficiency ٠ Fuel switching system FPBO storage Tank (50 L) 3 tanks (10 L) Modeling Ignition . Soot **Fuel composition** ٠ Emission Engine control & data Engine analyzer acquisition system Core reactor (CORE) †m. TU/e Flame-sheet ower & Flow eactor (FLAM † m

Natural luminosity (soot) of diesel & neat FPBO at 300 bar P<sub>ini</sub>

- Nozzle clogging
- Poor atomization
- Shorter burn duration



Heat release rate



Neat FPBO at 300-bar P<sub>ini</sub>

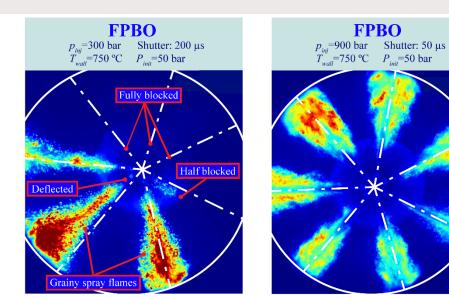
- Nozzle clogging
- Poor atomization
- Shorter burn duration

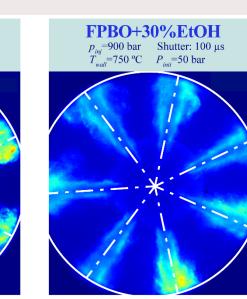
#### Neat FPBO at 900-bar P<sub>ini</sub>

- Improved nozzle durability
- Improved atomization

FPBO with addition of 30% EOH

- Further improved atomization
- Reduced sooting tendency
- Slightly shortened ignition delay





Wang, et al. "Spray combustion of fast-pyrolysis bio-oils under engine-like

conditions." Energy Conv. Management: X 20 (2023): 100433.

TU/e

Two-stage Lagrangian model

- Simulates mixing-limited spray combustion
  - Minimalistic flow model (1D entrainment model)
  - 2 perfectly stirred reactors with transport
  - Detailed chemistry

Multiple-step ignition process

Transport between spray core and periphery regions  $\frac{2}{29}$  0.8

FLOL

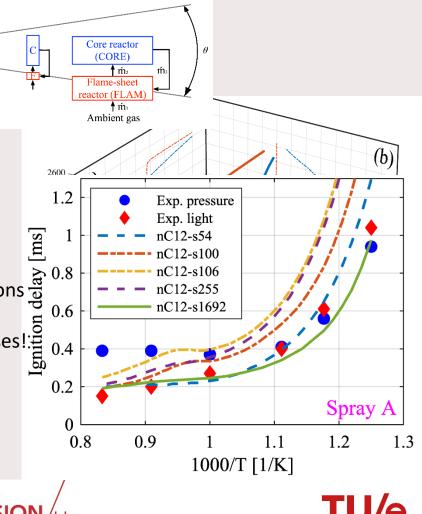
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und

Nozzle

- Validated at Spray A conditions •
- Validated at Spray A conditions Powerful tool to investigate spray ignition processes plication to FPBO and blends Application to FPBO and blends
- High T<sub>amb</sub> is required (>1000 K)
- Ethanol addition promotes the 2<sup>nd</sup>-stage ignition •

Wang, et al. "Evaluation of fuel spray ignition delay behavior using a twostage Lagrangian model." Combustion and Flame 265 (2024): 113449.



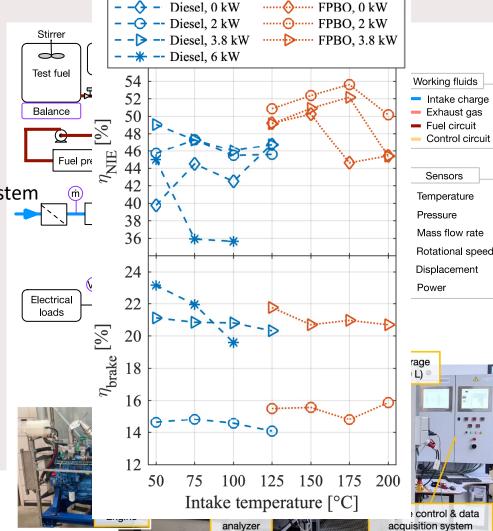
Dedicated engine modifications

- Intake preheating & elevated CR
- Fuel switching & dual-circuit injection system
- Unattended engine operation system 500-hour durability test
- For the first time ever in the world

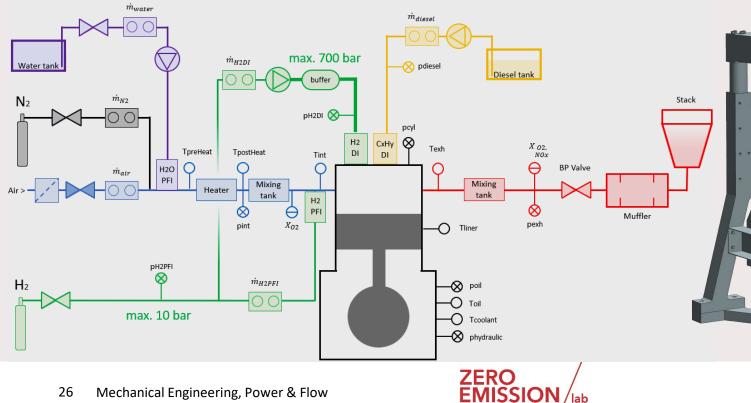
Efficiencies & emissions

- Improved  $\eta_{\text{NIE}}$  due to faster burning rate
- Lower NO<sub>x</sub> but higher CO than diesel

Wang, et al. "Application of fast pyrolysis bio-oil in a genset engine for combined heat and power generation.", *under review*.



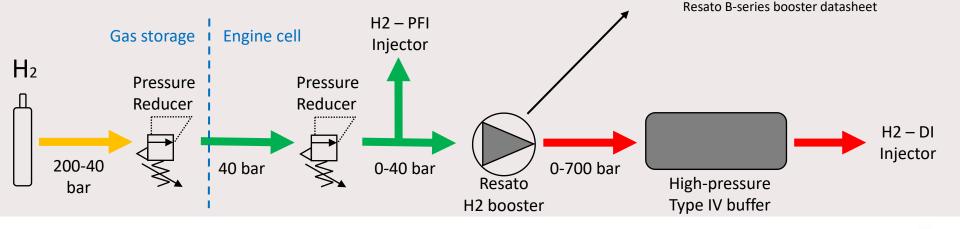
/lab





- 200 bar H<sub>2</sub> pack, reduced to 40 bar before entering lab
- In engine cell further reduced to  $\sim$ 7 bar for PFI operation
- For DI: reducer set to 40 bar to feed H<sub>2</sub> booster
- Up to 700 bar achievable for H<sub>2</sub>-DI applications
- Just 3 bar H<sub>2</sub> inlet pressure required for booster → allows for emptying H<sub>2</sub> pack!





Stepwise approach  $\downarrow$ 

#### Input parameters:

- Injection mode (PFI/DI) •
- Ignition mode (CI, SI, TJI) •
- Boost pressure / temperature Mixing / flame evolution •
- Load point (IMEP/RPM) •
- Diesel/H<sub>2</sub> ratio
- EGR rate
- Etc.

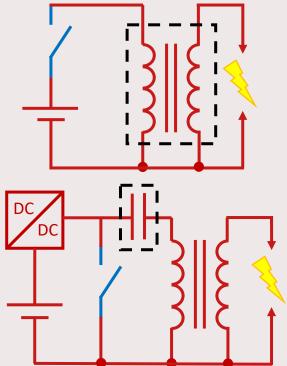
#### Output parameters:

- Efficiency
- $NO_{v}$  (and CO, CO<sub>2</sub>, HC, PM) emissions

Phase	Strategy	Diesel fuel	H <sub>2</sub> fuel	Ignition method	Compression ratio
1	Diesel	Yes	No	Compression Ignition	High
2	Diesel-H2 DF	Yes	Yes, various quantities PFI	Compression Ignition	Low/High
3	H2 PFI SI	No	Yes, through PFI	Spark Ignition	Low
4	H2 LPDI SI	No	Yes, through early DI (partially premixed)	Spark Ignition	Medium
5	H2 HPDI SI	No	Yes, through late DI (diffusion flame)	Turbulent Jet / prechamber assisted spark-ignition	High

- H<sub>2</sub>: lower minimum spark energy than gasoline
- In some ignition systems, residual energy may remain after spark
- Additional, low-energy spark during exhaust / intake stroke
- Spark breakdown voltage scales with pressure
- Spark energy too low to ignite gasoline, but will ignite  $H_2$ !
- Ignition system without residual energy required!

- Transistor Controlled Ignition (TCI)
  - Conventional method (contact-breakers)
  - Energy stored in coil (as magnetic field)
  - Charges while switch is closed, discharges upon opening
  - Residual energy may remain after spark extinguishes!
- Capacitor Discharge Ignition (CDI)
  - Supply voltage boosted to 400V
  - Energy stored in capacitor (as electric field)
  - Charges continuously, discharges upon closing switch
  - No residual energy after switch opening!

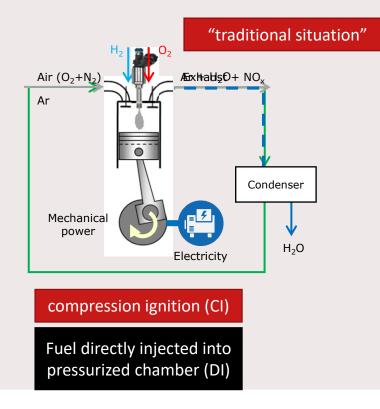


Both schematics are highly simplified!

- EGR control
  - Skip-firing makes conventional EGR impossible
  - Exhaust gases are diluted by intake air
  - Solution: simulated EGR by pre-mixing air, N<sub>2</sub>, and H<sub>2</sub>O using mass flow controllers
- EGR measurements
  - $H_2$  combustion  $\rightarrow$  No CO<sub>2</sub> formation
  - Using O<sub>2</sub> concentration instead
  - Wideband O<sub>2</sub> sensors in intake + exhaust (verified by IAG/Horiba emission analyzer)

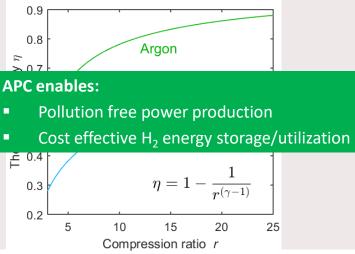


#### **Argon Power Cycle (Max Peters)**



#### **Revolutionary power cycle**

Use argon (Ar) instead of air (N<sub>2</sub>) Affordable, non-toxic gas Recirculate in closed loop Monoatomic: Theor. Efficiency  $55\% \rightarrow 80\%$ Only water formed



Resolution: 0.87 µm/pixel Frame rate: 100 kHz

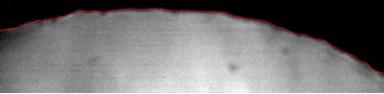
#### **Needle lift measurement**



Additional measurement credits Vincent Fontijn

35

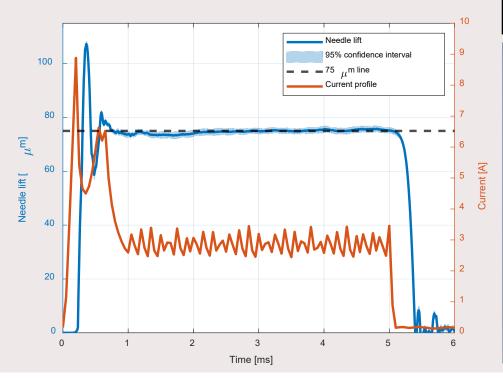
Max Peters: APC & high-pressure H2 jets





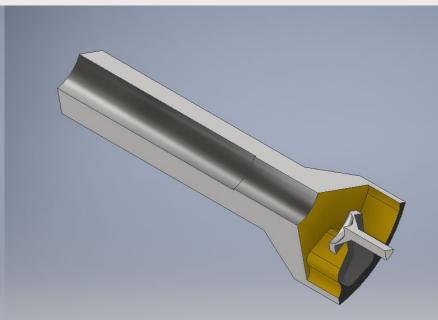
TU/e

### **Final geometry**

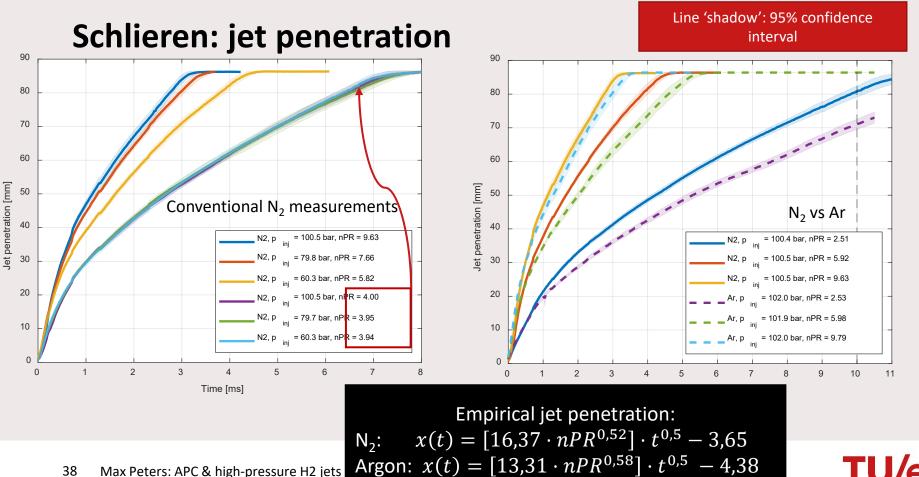


#### Conclusion: Smallest flow area around needle due to small lift!

+ Experiments validated with Laser Doppler Vibrometer!





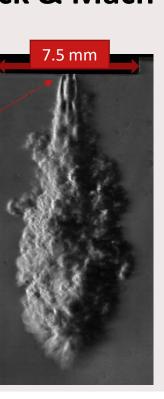


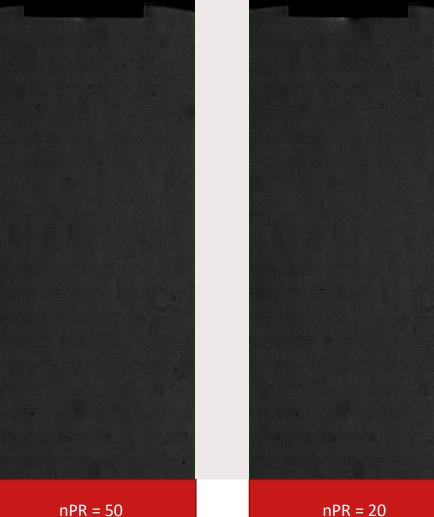
38 Max Peters: APC & high-pressure H2 jets TU/e

#### **Barrel shock & Mach disk**



Barrel shock are small! (max.  $\sim 5 \cdot d_e$ ) At very high nPR





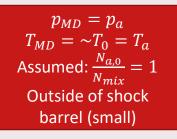
nPR = 50

# **Rayleigh scattering**

What do we need?  $\frac{\sigma_f}{\sigma_a}$  (Rayleigh cross section for H<sub>2</sub> and ambient)

 $\frac{N_{a,0}}{N_{mix}}$  (density field inside the jet)

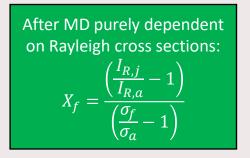
Tsujimura [2003] & Ewan and Moody [1986] for number density



Barrel-shaped	shock	Reflec	ted sho	ock
Flow boundary	<u> </u>		$\sim$	
	$\rightarrow$		73	ilip line
	Expansio	n wave	Mąch	disc
M = 1	M >	>1		M < 1
			5	~
			$\succ$	_
				_

	Nozzle exit	Barrel-shaped shock	Mach disc
Pressure	$p^*$	$p^*$	$p_{MD} = p_{\alpha}$
Density	$\rho^*$	<< <i>p</i> *	$\rho_{MD} = P_a/R_0 T_{M0}$
Temperature	$T^{*}$	-	$T_{MD} = T_0$
Velocity	u*	>> u*	$u_{MD} = \sqrt{\kappa R_0 T_{ND}}$
Mach number	1	>> 1	1

Figure 6. Schematic diagram of underexpanded jet behavior just downstream of nozzle exit [17].

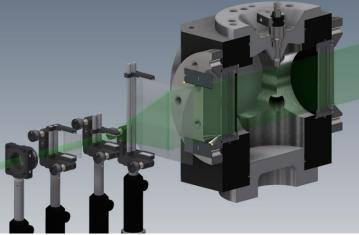


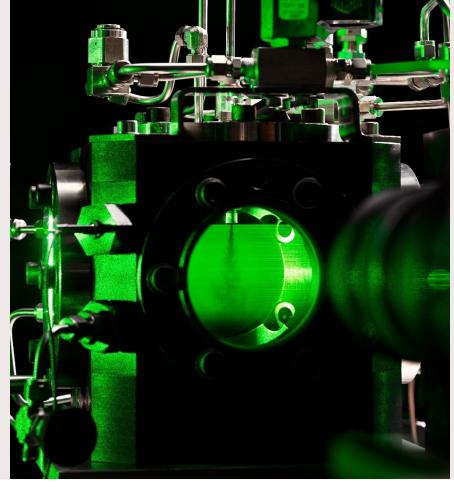
Rayleigh cross section $\sigma_i \ [10^{-27} cm^2]$ at 532 nm.			
N <sub>2</sub>	Ar	<i>H</i> <sub>2</sub>	n – heptane
5.23	4.56	1.13	309.8

Reduced signal in the H<sub>2</sub> jet vs. ambient!





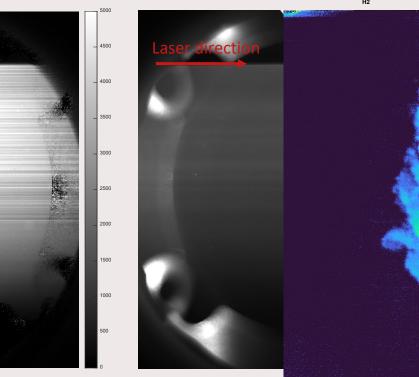


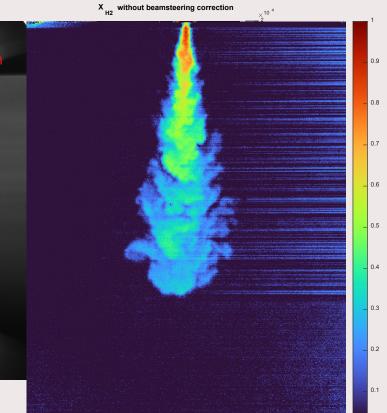




# Pixis, 50-mm f/1.2, 3-nm filter @532, & 0.5-µm particle filters

flatfielded and vacuum flared begin image





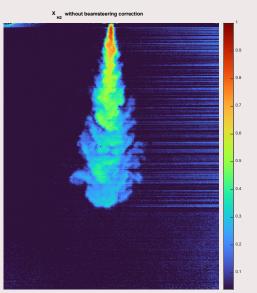
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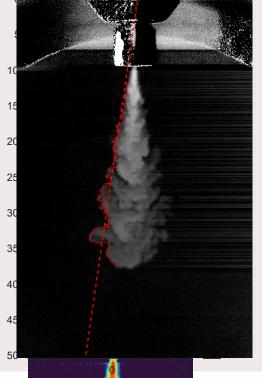
Result: Image - 'Vacuum' image @ 0,03 bar (for flare correction)

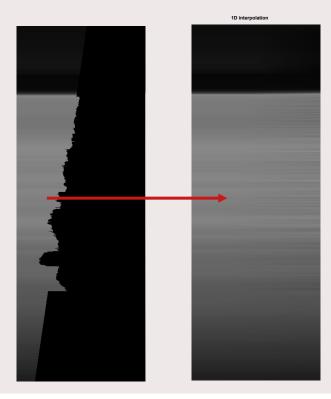
42 Max Peters: APC & high-pressure H2 jets

100 bar  $H_2$  in 10 bar  $N_2$ 

# Beam steering improvements

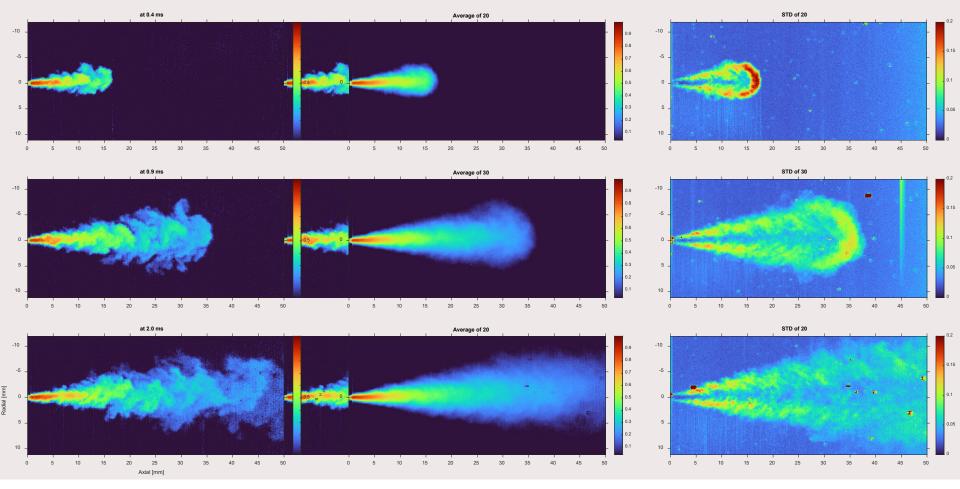






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43 Max Peters: APC & high-pres



44 Max Peters: APC & high-pressure H2 jets

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# **Argon Power Cycle**

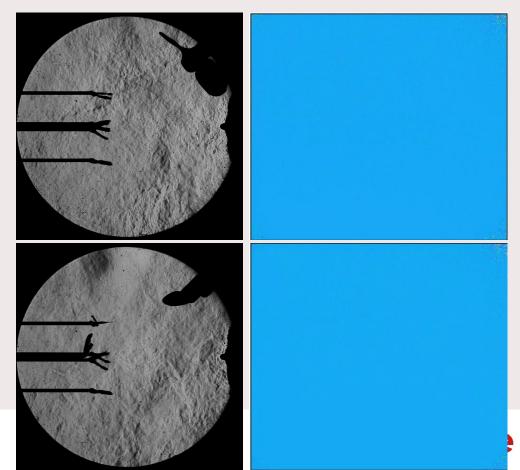
Next: combustion!

Tcore ≠ Tbulk

High-speed 50-µm bare-wire TC measurements for core T

### Schlieren

### **OH\*** Chemiluminescence



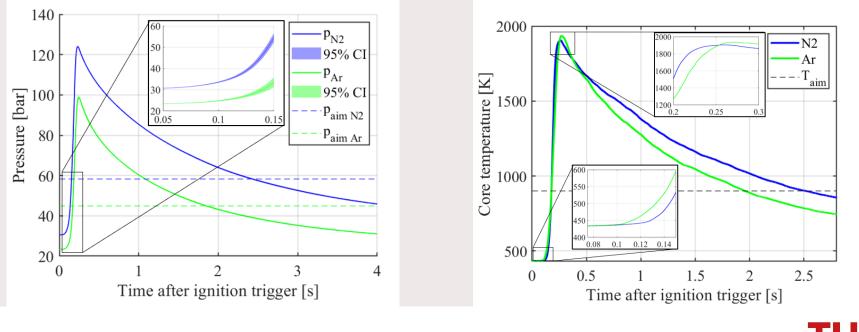
Ar

 $N_2$ 

45 Mechanical Engineering, Power and Flow Additional measurement credits Steef Licher

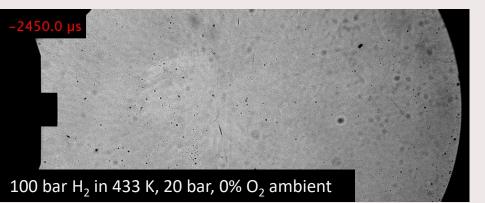
### **Argon Power Cycle**

Target: 22.8 kg/m<sup>3</sup> & 900 K @ inj., peak 2000 K  $\rightarrow$  50% of the C<sub>2</sub>H<sub>2</sub> in Ar!

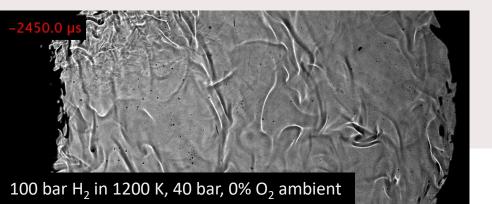


46 Mechanical Engineering, Power and Flow Additional measurement credits Steef Licher

### **Argon Power Cycle – non-reacting, high temperature**

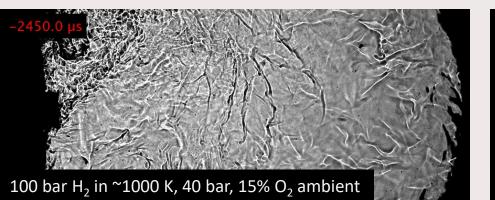




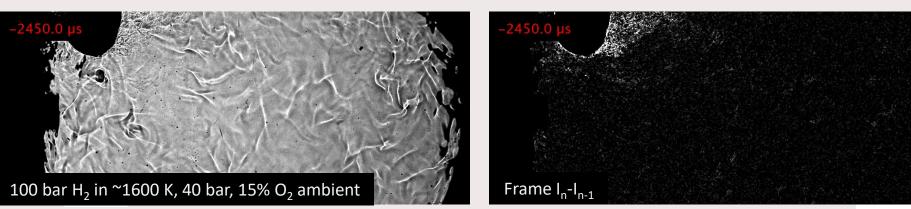




### **Argon Power Cycle – reacting conditions**

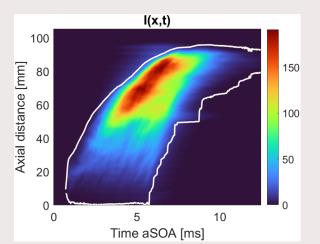


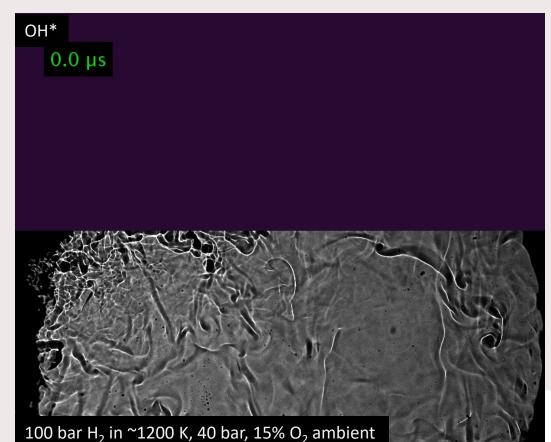




### **Argon Power Cycle – reacting conditions**

OH\* top view Schlieren side view





# **Argon Power Cycle**



### Some true-color recordings

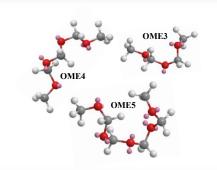
8	

50 Mechanical Engineering, Power and Flow Additional measurement credits Giliam van der Wielen



### Renewable "drop-in" fuel research by Zhongcheng Sun (GTL $\rightarrow$ GTLB30 $\rightarrow$ OME<sub>n</sub>)

- From short- to long-term solutions
- Gas to liquid (GTL)
- GTL blends with 30 vol% FAME (GTLB30)
- Oxymethylene dimethyl ether (OME<sub>n</sub>)





Zhongcheng Sun

#### Mechanical engineering, Power & Flow group

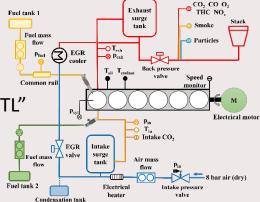


### Background

- GTL: EN 15940 compliant, higher CN, negligible sulfur & aromatics
  - Note: similar properties as HVO/HEFA → can be regarded as "XTL"
- OME<sub>n</sub>: no C-C bonds, high oxygen content, & high CN

		[]]	7					<u></u>
	Density			Viscosity			Oxygen mass%	(A/F) <sub>st</sub> ratio
	[kg/m <sup>3</sup> ]	[-]	[MJ/kg]	[mm²/s]	[°C]	[°C]	[-]	[-]
OME <sub>x</sub> *	1067.1	82.2	19.4	1.18	64.5	-20.5	48.01	5.84
GTL	777.1	74	44	2.58	72	-19	0	14.98
GTLB30	808.3	65.8	42	2.97	66	-23	3.2	14.24
Diesel	836.1	52.2	43	2.76	66	-24	0.60	14.46
								1
		1						

<sup>\*</sup> OME<sub>x</sub> (47.65% OME<sub>3</sub>, 29.7% OME<sub>4</sub>, 16.98% OME<sub>5</sub>, 5.67% OME<sub>6</sub>)

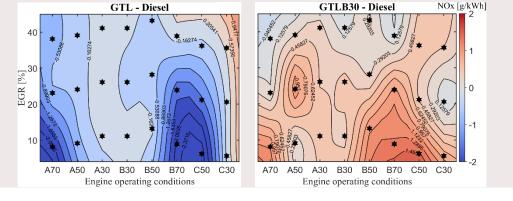


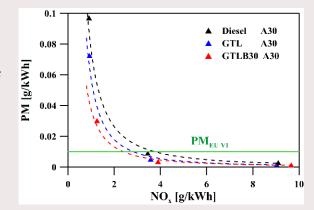
#### MX13 specification

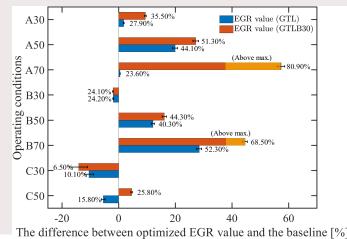
MX 13	Parameter
Number of cylinder	1
Displaced volume	2.15 L (single)
Bore	130 mm
Stroke	162 mm
Compression ratio	17.2
Piston bowl shape	Double step
Cylinder head	Low swirl

### GTL & GTLB30 engine research

- + Both GTL & GTLB30 illustrate potential in improving the PM-NO<sub>x</sub> trade-off
- NO<sub>x</sub> emissions impact on weighted average across the engine map:
  - GTL ↓ 16.1% & GTLB30 ↑8.3%
- Potential EGR optimization strategy for minimizing  $NO_x$  while adhering to Euro VI PM limits for both GTL & GTLB30
- Drop-in optimization means different EGR calibration!

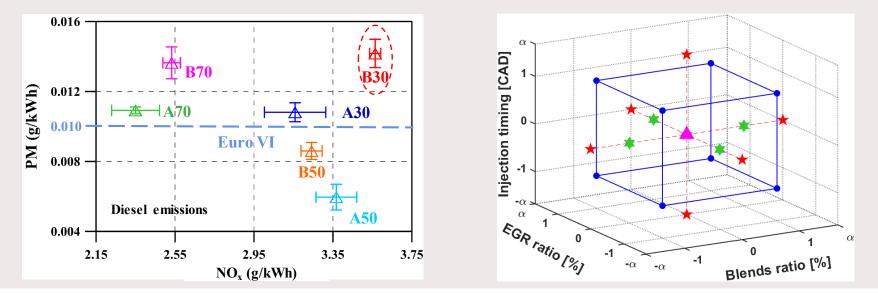






### OME<sub>x</sub> optimized research on heavy-duty engine

- OME = expensive, how much do you need? If you have x amount, fuel one or fuel many?
- Case selection: commercial B7 diesel worst emissions @ B30 (1425 RPM, 30% load)
- Design of Experiments (DOE) approach to provide a comprehensive global emissions map <sup>[1]</sup>



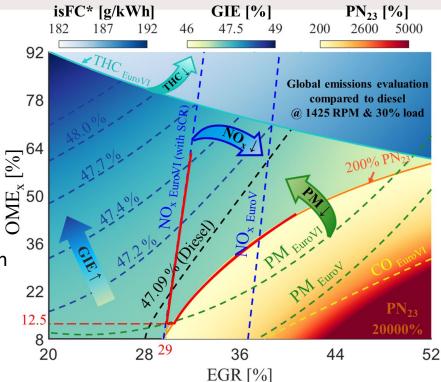
### Comprehensive emissions map @B30

- Soot emissions  $\propto$  to  $\mathsf{OME}_x\%$  in blends
- OME<sub>x</sub>: slightly negative effect on NO<sub>x</sub> emissions
  - Significantly mitigated with increasing EGR!
- CO effectively reduced with OME<sub>x</sub> addition
- MX13 @ B30: EUV NO<sub>x</sub> & EUVI PM compliant when \_

• OME <sub>x</sub>	>40%		
• FGR	>37.2%		

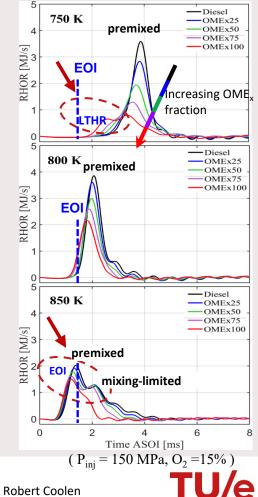
MX13 @ B30: EUVI with SCR & DOC compliant when

• <u>OME<sub>x</sub></u>	>12.5%	
• EGR	>29%	



# $OME_x$ ignition research on CRU (15 $O_2$ %)

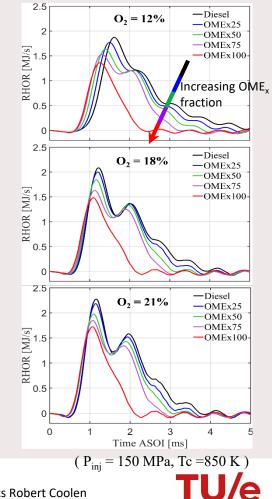
- @ 750 K, two noticeable ROHR peaks (LTHR & HTHR) of pure  $OME_x$  leads to a longer burn duration <sup>[2]</sup>
- 800 K as a transition point for blends (different combustion regime)
  - ROHR peak first increases with T, and then reduces ( $\propto$  BD)
- @ 850 K, now OME has the shortest burn duration



# OME<sub>x</sub> ignition research on CRU (O<sub>2</sub>% impact)

- At lower O<sub>2</sub>% (high EGR to simultaneously reduce NO<sub>x</sub>)
  - Modest impact on OME<sub>x</sub> ID & burn duration

(high fuel-oxygen content)



# OME<sub>x</sub> natural luminosity characteristics

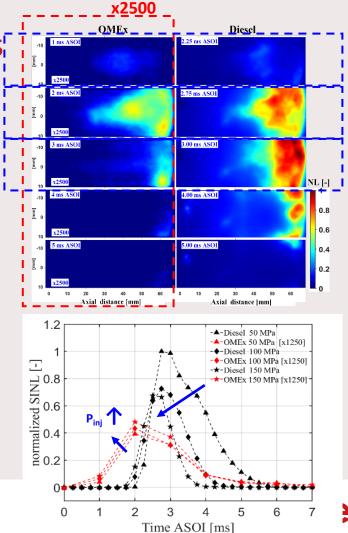
Optical diagnostics: natural luminosity (NL) imaging

- NL signal of OME<sub>x</sub> occurs earlier (1 ms < 2.25 ms)</li>
- NL intensity of OME<sub>x</sub> much lower

(chemiluminescence vs soot radiation)

Diesel NL peak ~ combustion recession timing of OME<sub>x</sub>

- Spatially integrated NL peak of OME<sub>x</sub> occurs before diesel
- With increasing P<sub>inj</sub>
  - OME SINL increases (more fuel)
  - Diesel SINL decreases (less soot, net)



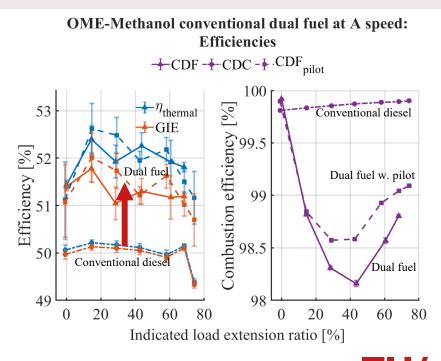
# OME – Methanol dual-fuel/RCCI

Idea pitch: potential future on-board production of OME out of MeOH

Dual-fual/RCCI operation with minimal OME

OME @ 30% load, but A70 conditions

- Adding methanol in steps using PFI
- Extending load up to 59% (reaching max (PRR))
- Small additional extension to 61% with a 7% pilot injection
- 1.5% GIE improvement with dual fuel



60 Collaboration w. Peter de Vos (Delft), graduation project work Joel Arendsen

# **Numerical simulations**

CFD

- LES
- RANS

#### **Combustion Model**

• FGM

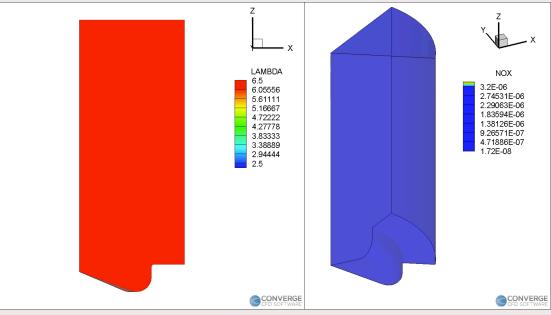
#### Software

- OpenFOAM
- Converge

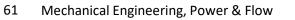
#### DME/Methanol RCCI in HD engine

ZERO

**EMISSION**/lab



**ΓU/**e



# **Numerical simulations**

CFD

- LES
- RANS

#### **Combustion Model**

• FGM

#### Software

- OpenFOAM
- Converge

#### LES of spray A (combustion in the EHPC)

n-dodecane formaldehyde carbondioxide

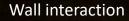
time: 0.01 ms





# **Questions?**

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Low-temperature chemistry

Liquid fuel

Single-orifice injector

Fuel vapor

Soot

High-temperature diffusion flame periphery

10 mm

 $\longleftrightarrow$ 

Diesel engine conditions: 630 °C 60 bar Hot thermocouple wires