Waste biorefinery technologies for accelerating sustainable energy processes

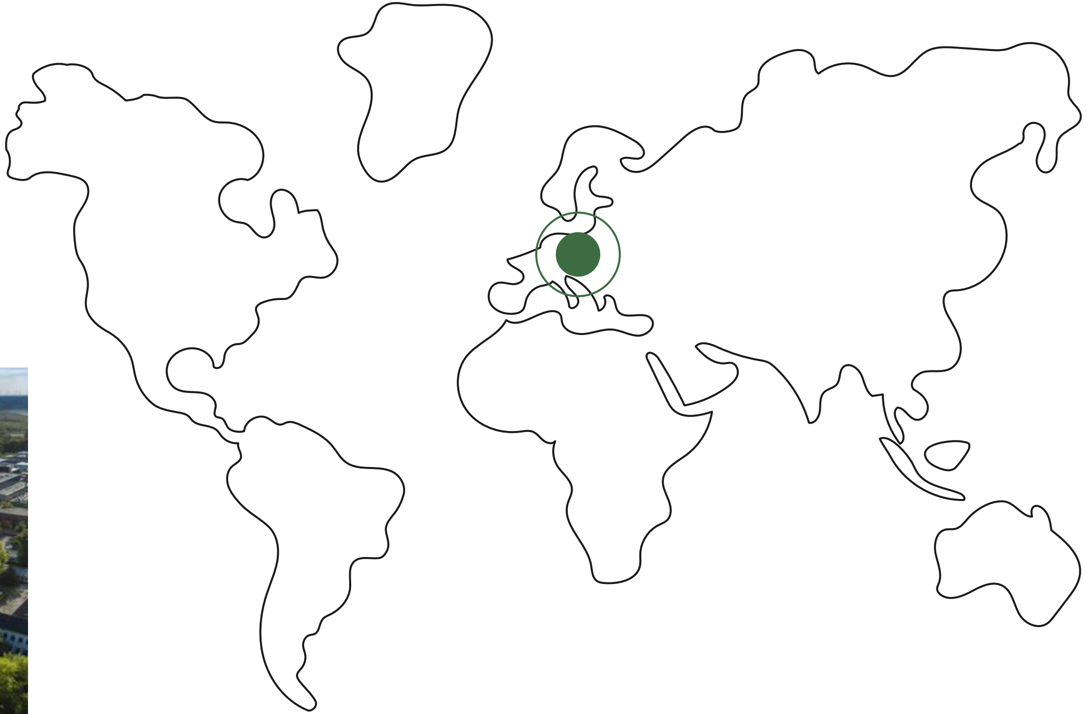
Evolutionary optimization of biofuels for highly efficient combustion engines with low exhaust emissions

Fabian Mauß, Hayat El Harrab and Tim Franken

05th October 2022

Where Are We?

- **BTU Cottbus-Senftenberg (Germany)**



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WIRE

Motivation | Method | Results | Conclusion

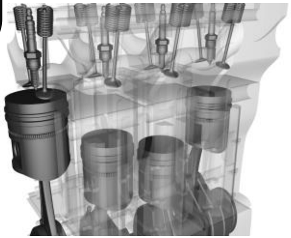
Selected biofuels and their properties

Design of biofuels

Aim: Optimization of biofuel production and combustion

From biomass to biofuels

From biofuel to propulsion

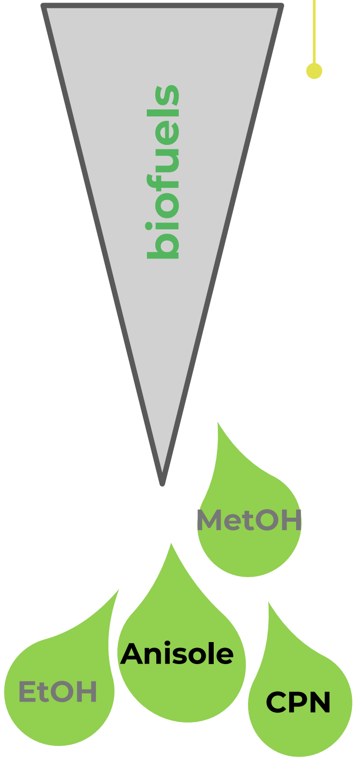


Design of biofuels

Spark ignition engine

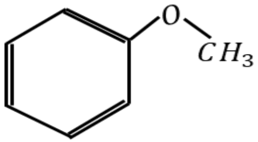
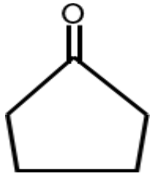
Requirements for combustion engines

- **Higher oxygen content**
- **LHV > 30 MJ/kg**
- **HoV < 60 kJ/kg**
- **Boiling point 50-210 °C**
- **RON > 95**



Source: FVV Fuel Composition for CO2 Reduction, 2022.

Properties of biofuels

Property	RON95E10	Anisole	CPN
Structure			
LHV / MJ/kg	41.6	33.3	32.1
RON	95.8	103	101
C:H:O	6.3:12.1:0.21	7:8:1	5:8:1
Density (25°C) / kg/m³	738	990	945
Boiling point (1bar) / °C	36-194	153	131
HoV / kJ/kg	25	39.8	47

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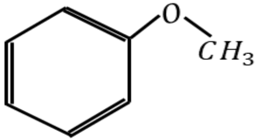
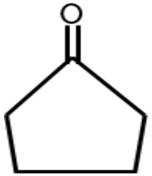
Structure			
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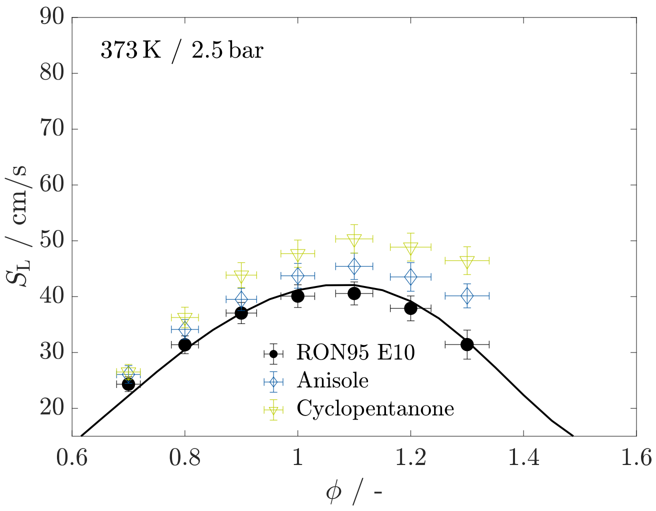

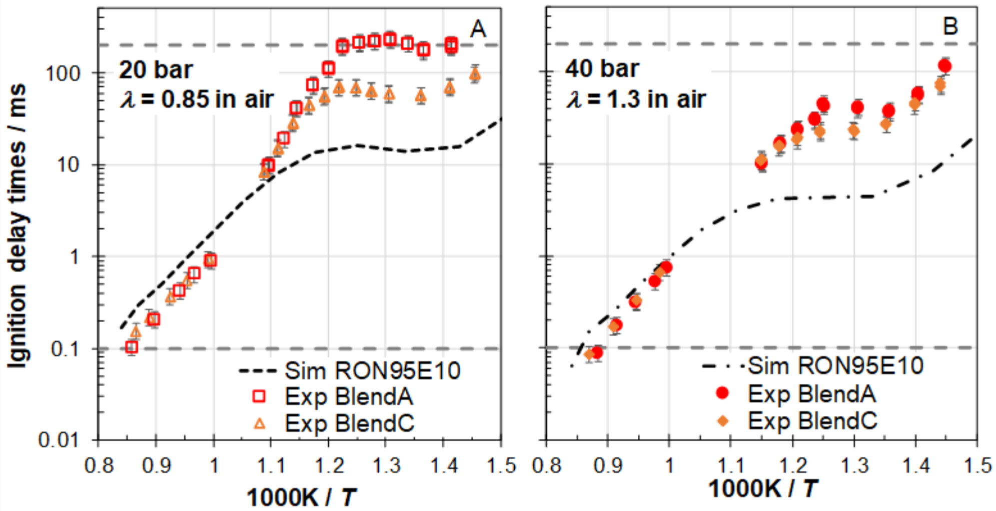

Source: FVV Fuel Composition for CO2 Reduction, RWTH Aachen ITV and HGD, 2022.

- Cyclopentanone and anisole show **higher burning velocities** over the whole ϕ-range compared to RON95E10.
- **Lower reactivity** of cyclopentanone-RON95E10 (BlendA) and anisole-RON95E10 (BlendC) blends at rich and lean conditions.

Properties of biofuels

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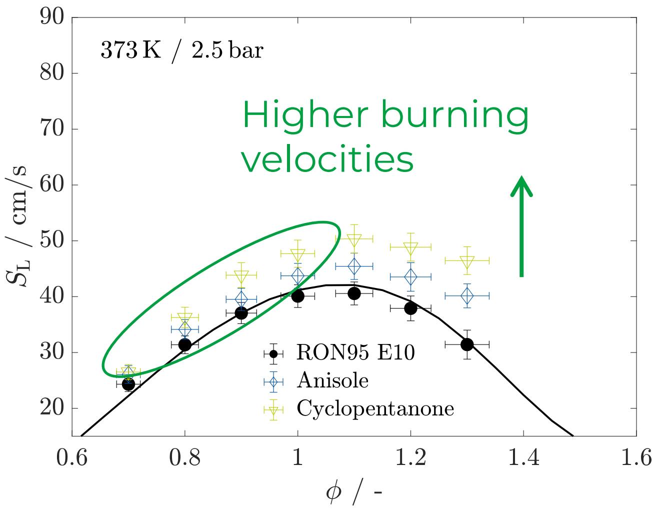

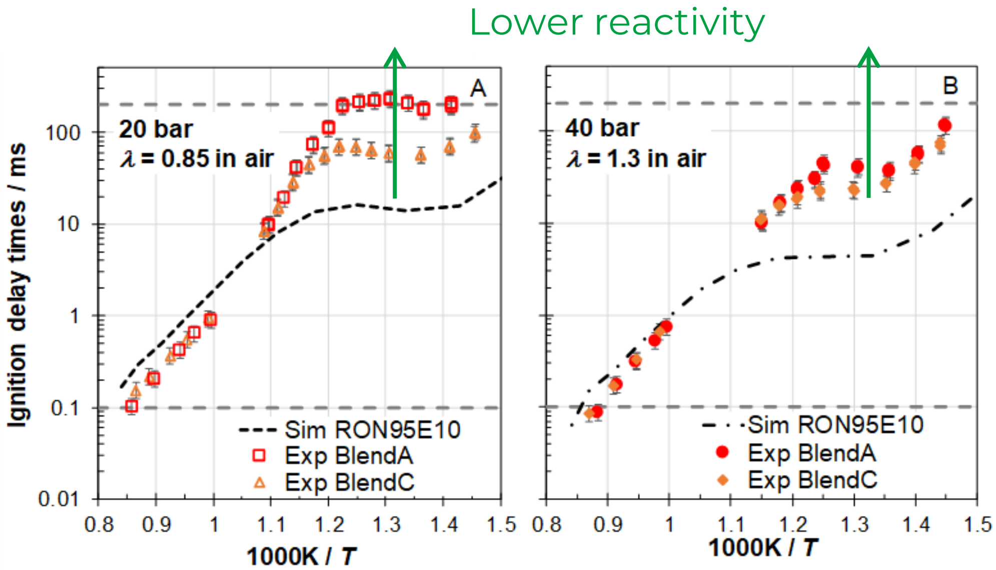

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Motivation

Method

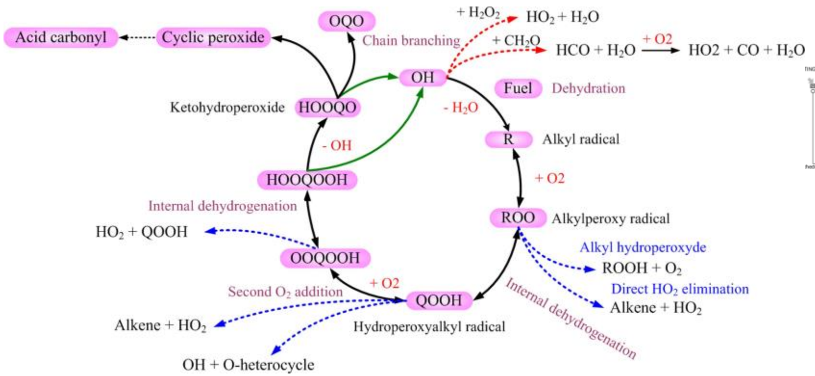
Stochastic Reactor Model and Genetic Optimization

Results

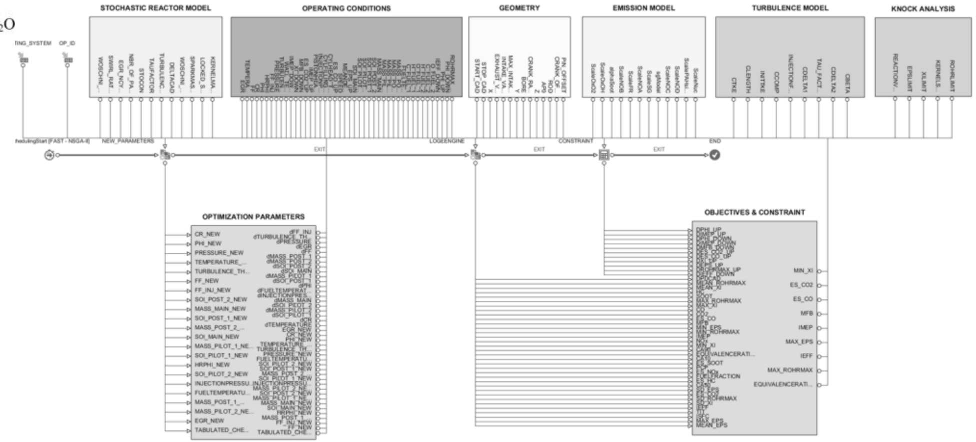
Conclusion

Optimization methodology

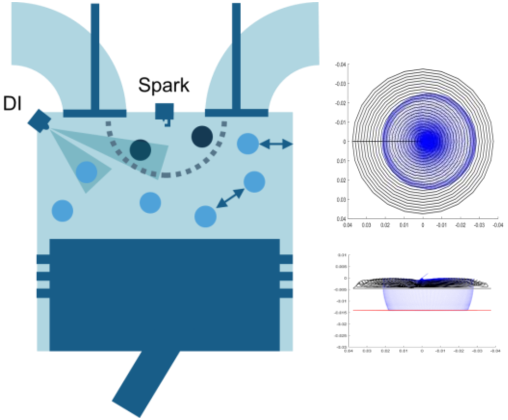
Detailed chemistry of biofuels



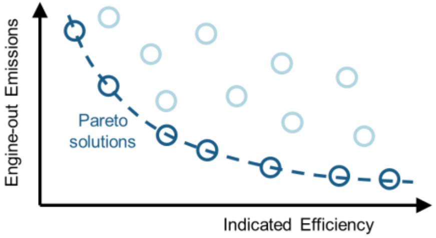
Optimization project



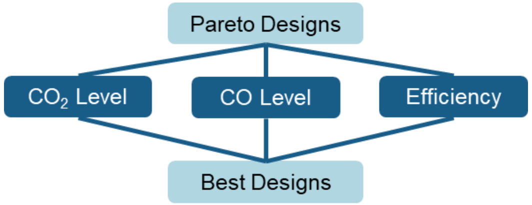
Stochastic Reactor Model



Pareto solutions

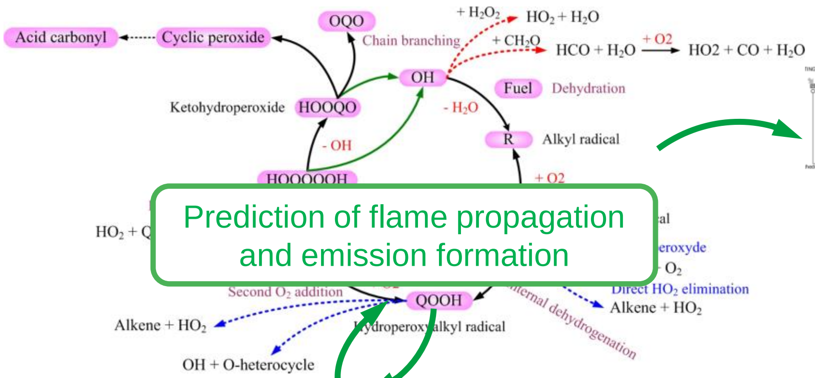


Decision making



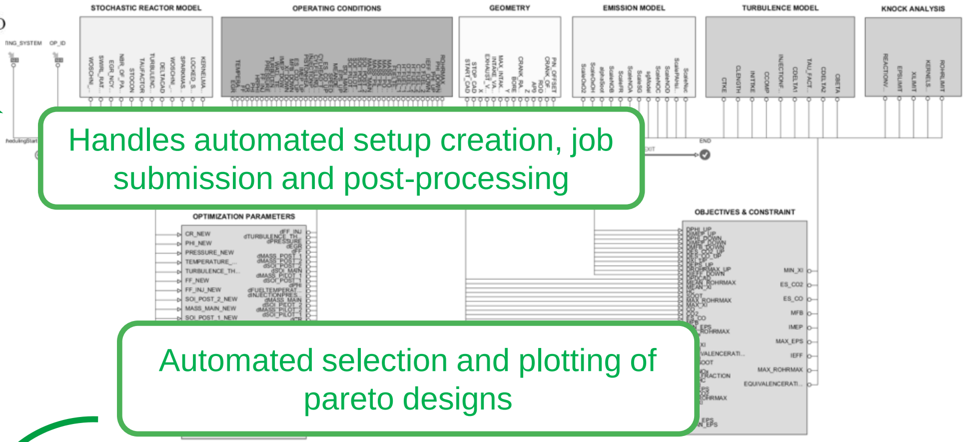
Optimization methodology

Detailed chemistry of biofuels



Prediction of flame propagation and emission formation

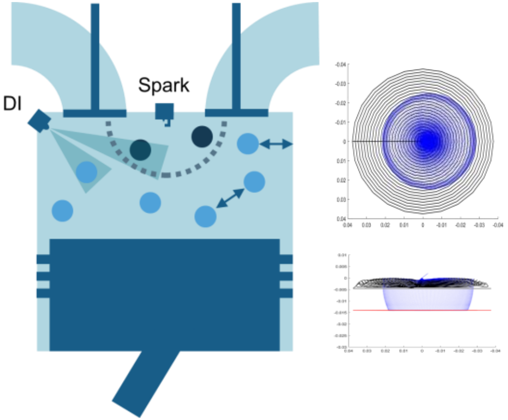
Optimization project



Handles automated setup creation, job submission and post-processing

Automated selection and plotting of pareto designs

Stochastic Reactor Model



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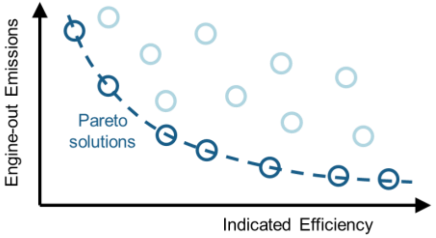
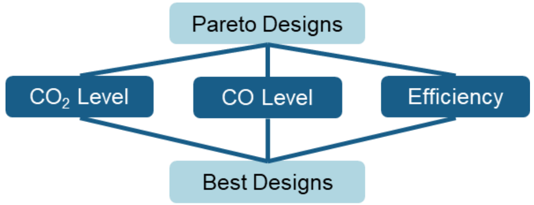
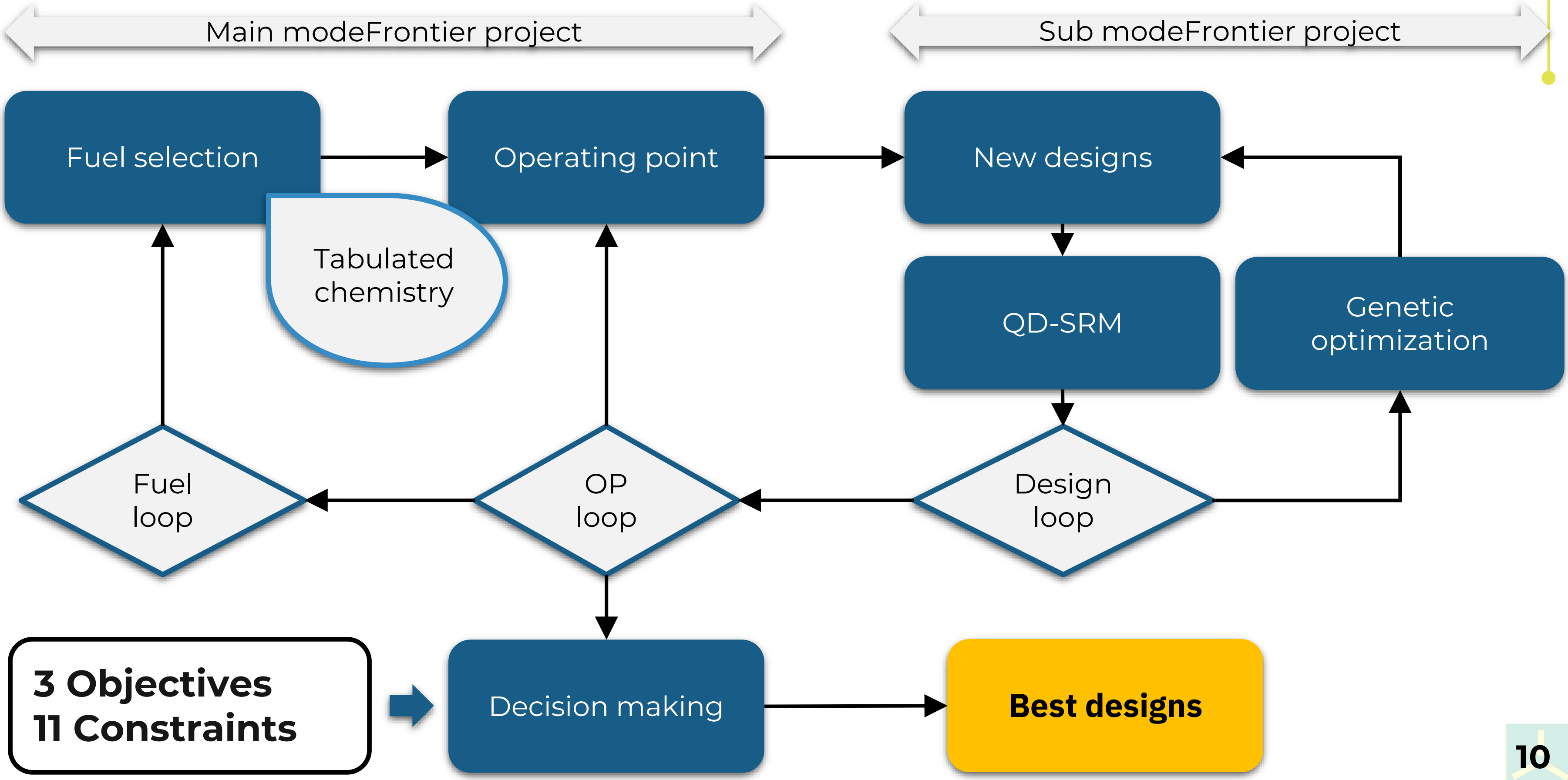


Decision making



Optimization methodology

WIRE



W I R E

Motivation

Method

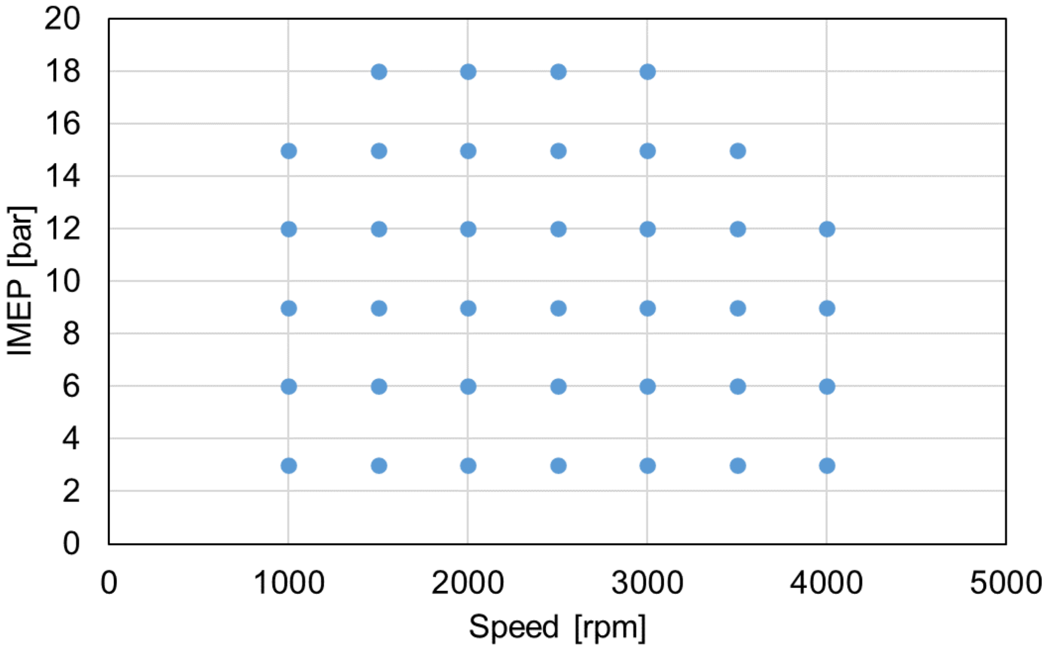
Results

Conclusion

Engine test case and optimization results

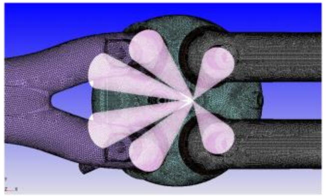
Engine specifications

Single-cylinder research engine at RWTH Aachen / Chair tme

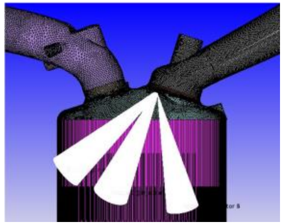


Parameter	Value
Bore / mm	75
Stroke / mm	113.2
Compression Ratio	10.8:1
s/b Ratio	1.5

Top



Front



Source: FVV Fuel Composition for CO2 Reduction, 2022.

Engine specifications

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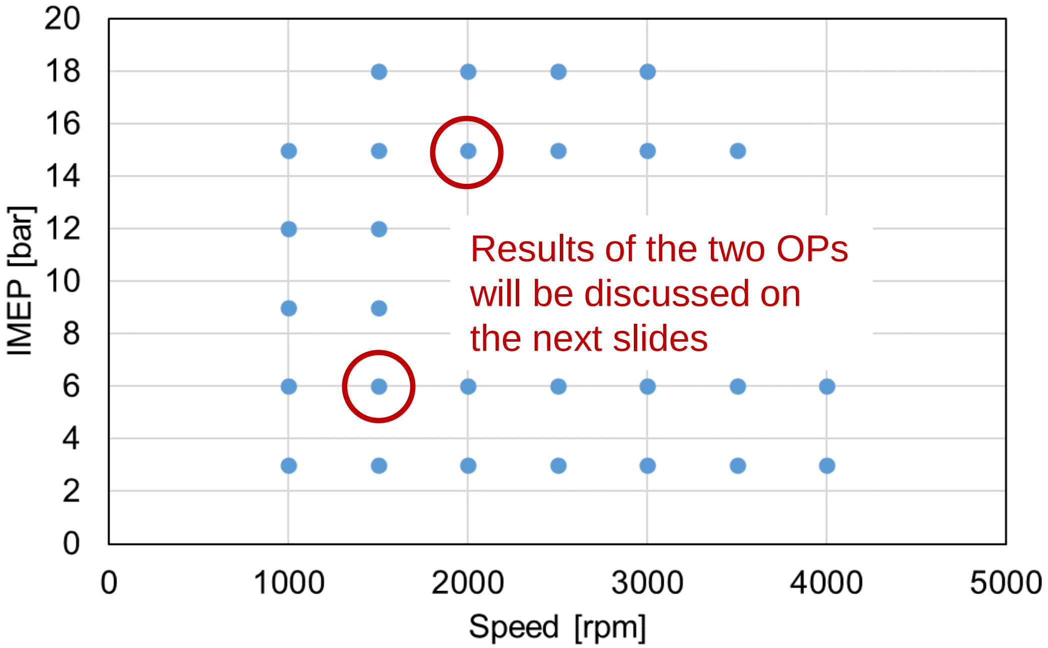

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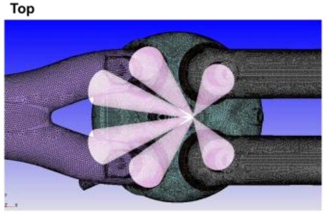
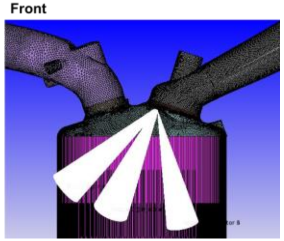
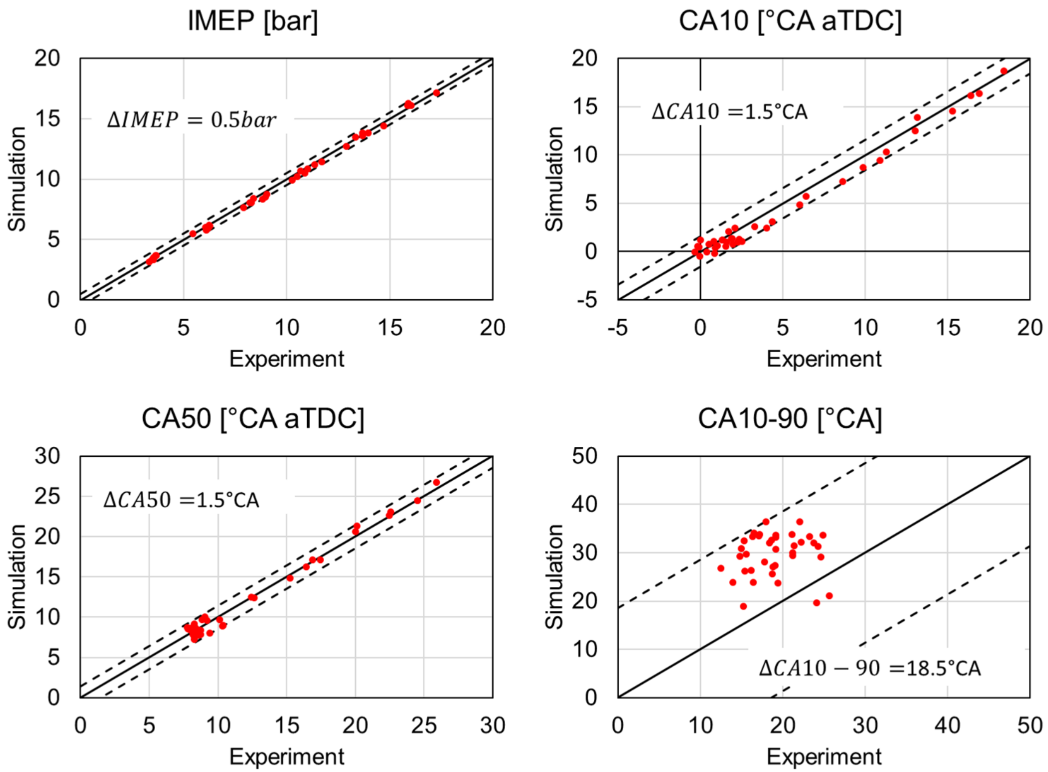




Source: FVV Fuel Composition for CO2 Reduction, 2022.

QD-SRM results

Model parameters are trained for RON95E10 base engine map



QD-SRM parameters	
Number of particles	500
Time step size / °CA	0.5
Number of Cycles	30

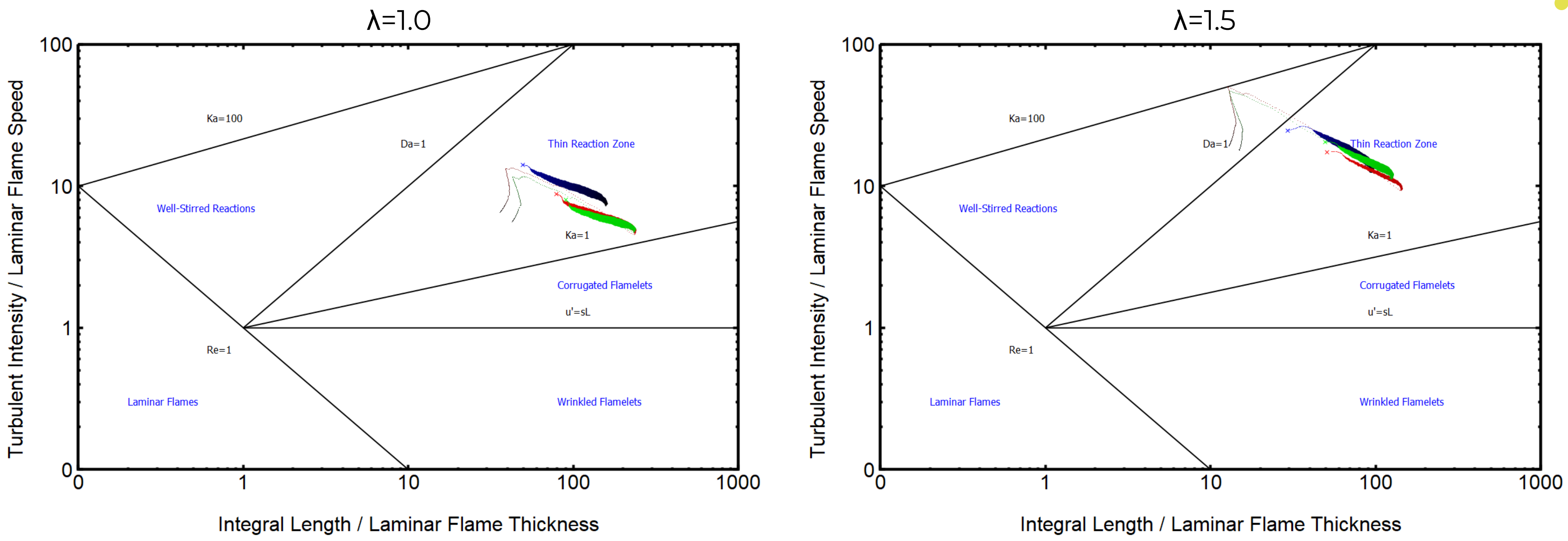
Reaction mechanism	
Number of species	500
Number of reactions	3429

Source: FVV Fuel Composition for CO2 Reduction, RWTH Aachen ITV and HGD, 2022.

QD-SRM results

X RON95E10 X Anisole X Cyclopentanone

Stroke/bore = 1.5; CR = 10.8
n = 2000 1/min; $IMEP_{net}$ = 6 bar



- Anisole and cyclopentanone burn at **higher Damkoehler numbers** and **lower Karlovitz numbers** compared to RON95E10.
- Combustion regime shifts to **well-stirred reactions at lean conditions**.

QD-SRM results

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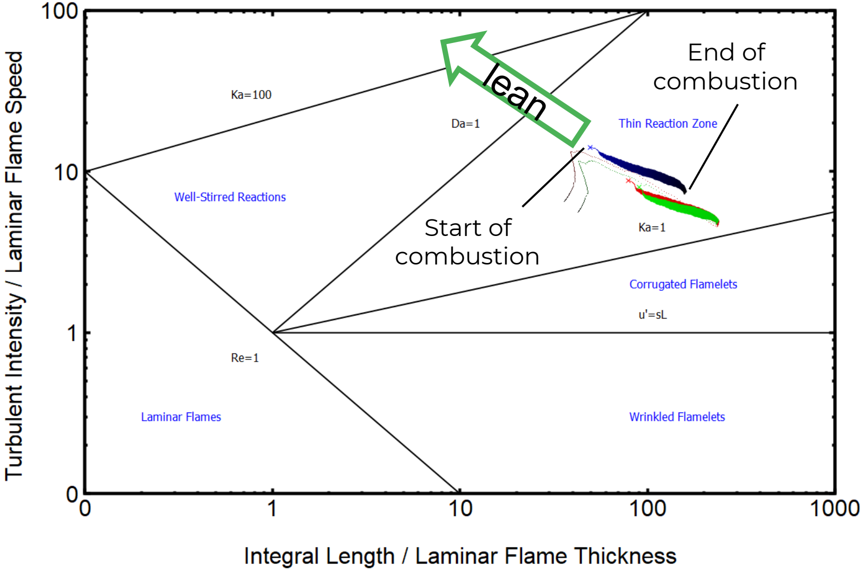
λ=1.0



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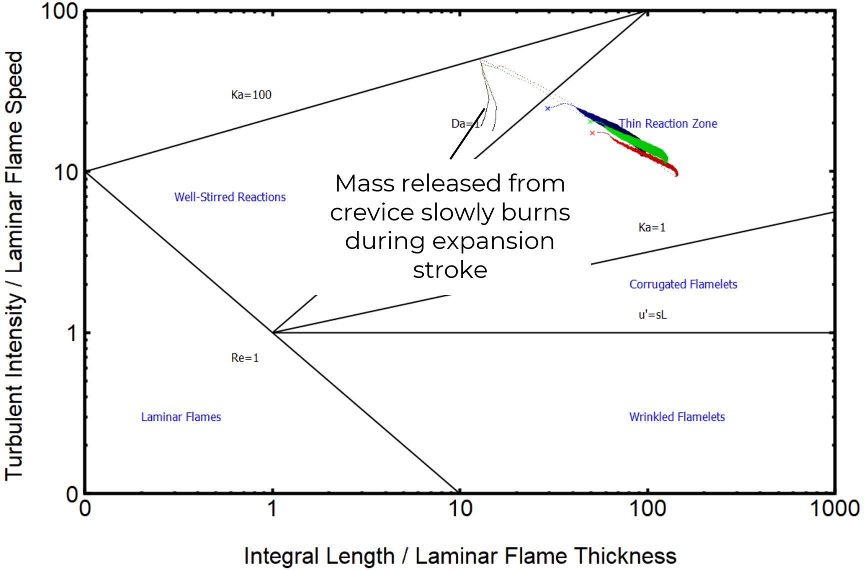


- Anisole and cyclopentanone burn at **higher Damkoehler numbers** and **lower Karlovitz numbers** compared to RON95E10.
- Combustion regime shifts to **well-stirred reactions at lean conditions**.

Biofuel blend matrix

Fuel blends investigated

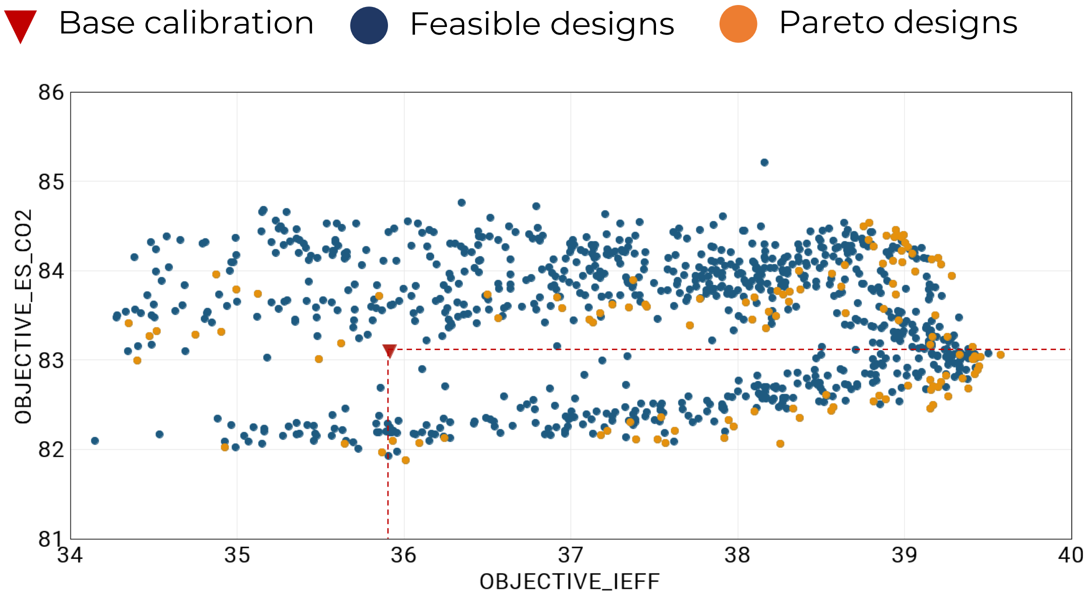
Fuel 1	**Fuel 2**	**Vo-%:Vo-%**	**Ma-%:Ma-%**	**Mo-%:Mo-%**
RON95E10	-	100:0	100:0	100:0
Anisole	-	100:0	100:0	100:0
Cyclopentanone	-	100:0	100:0	100:0
RON95E10	Anisole	91:9	88:12	90:10
RON95E10	Anisole	57:43	50:50	54:46
RON95E10	Cyclopentanone	93:7	91:9	91:9
RON95E10	Cyclopentanone	56:44	50:50	48:52

- The **91:9 and 93:7 blends** represent the **maximum possible oxygen concentration** in the fuel blend fulfilling the EN228 legislation.

Optimization parameters

WIRE

Stroke/bore = 1.5; CR = 10.8
n = 1500 1/min; $IMEP_{net}$ = 6 bar

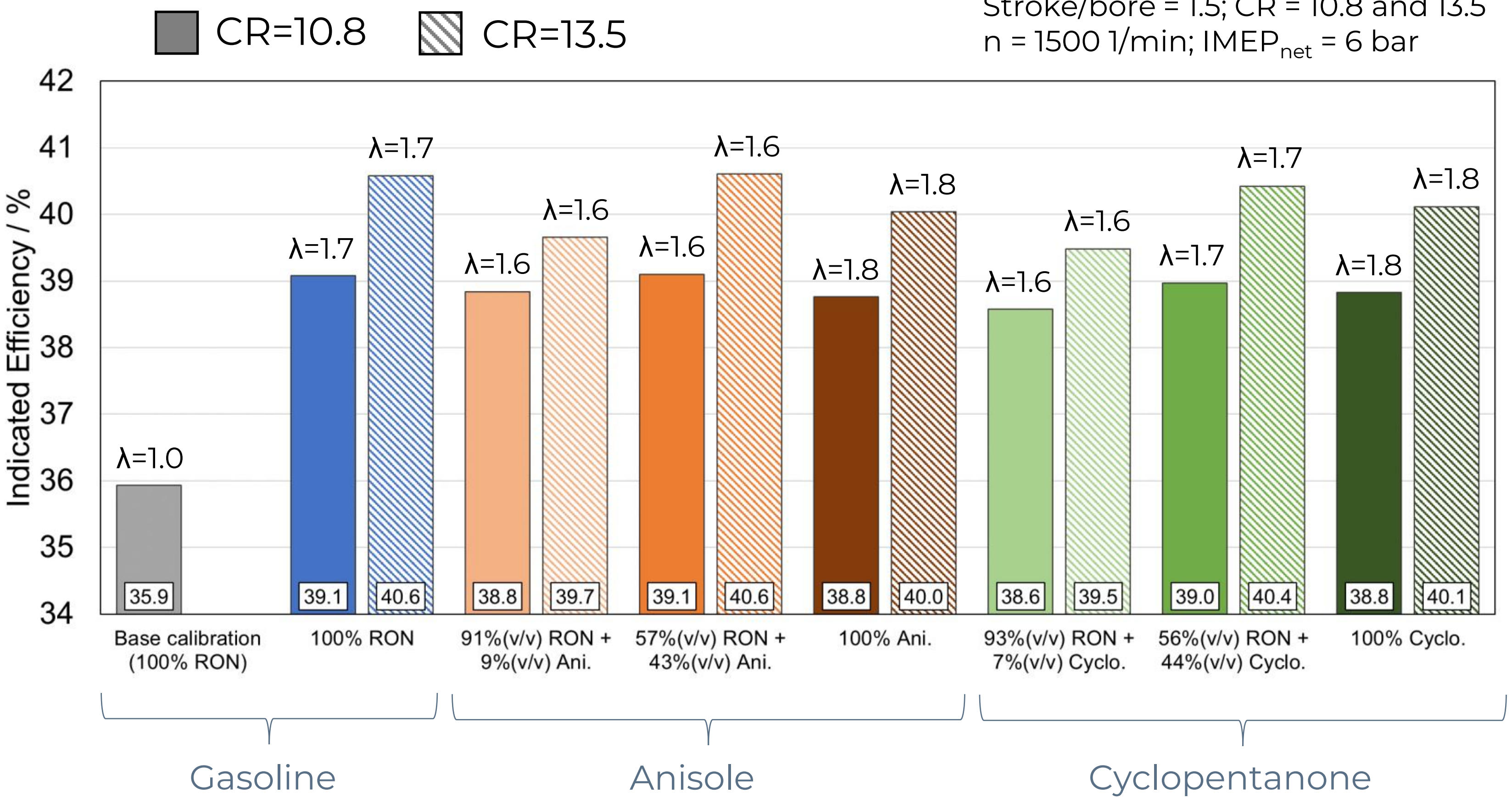


Optimization parameters	Lower bound	Upper bound
Fuel mass / mg	-50%	+0%
Boost pressure / bar	-0.5	+1.0
Spark timing / °CA	-15.0	+15.0
Compression ratio	10.8:1 and 13.5:1	

- **Decision making** is applied to select designs from the pareto front. The importance weights of the objectives are changed to select the desired designs.

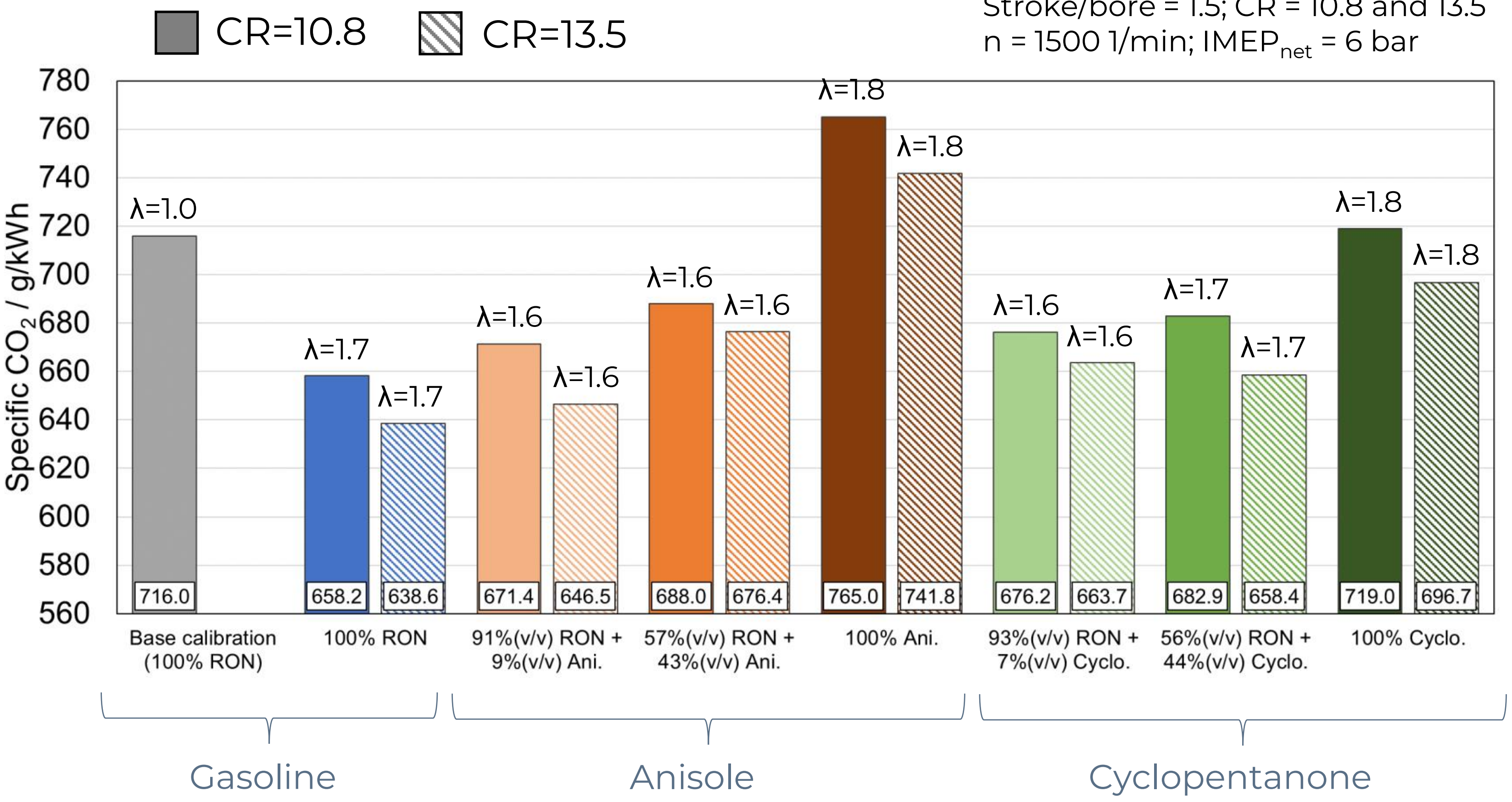
Optimization results | η_{eff}

Stroke/bore = 1.5; CR = 10.8 and 13.5
n = 1500 1/min; $IMEP_{net}$ = 6 bar

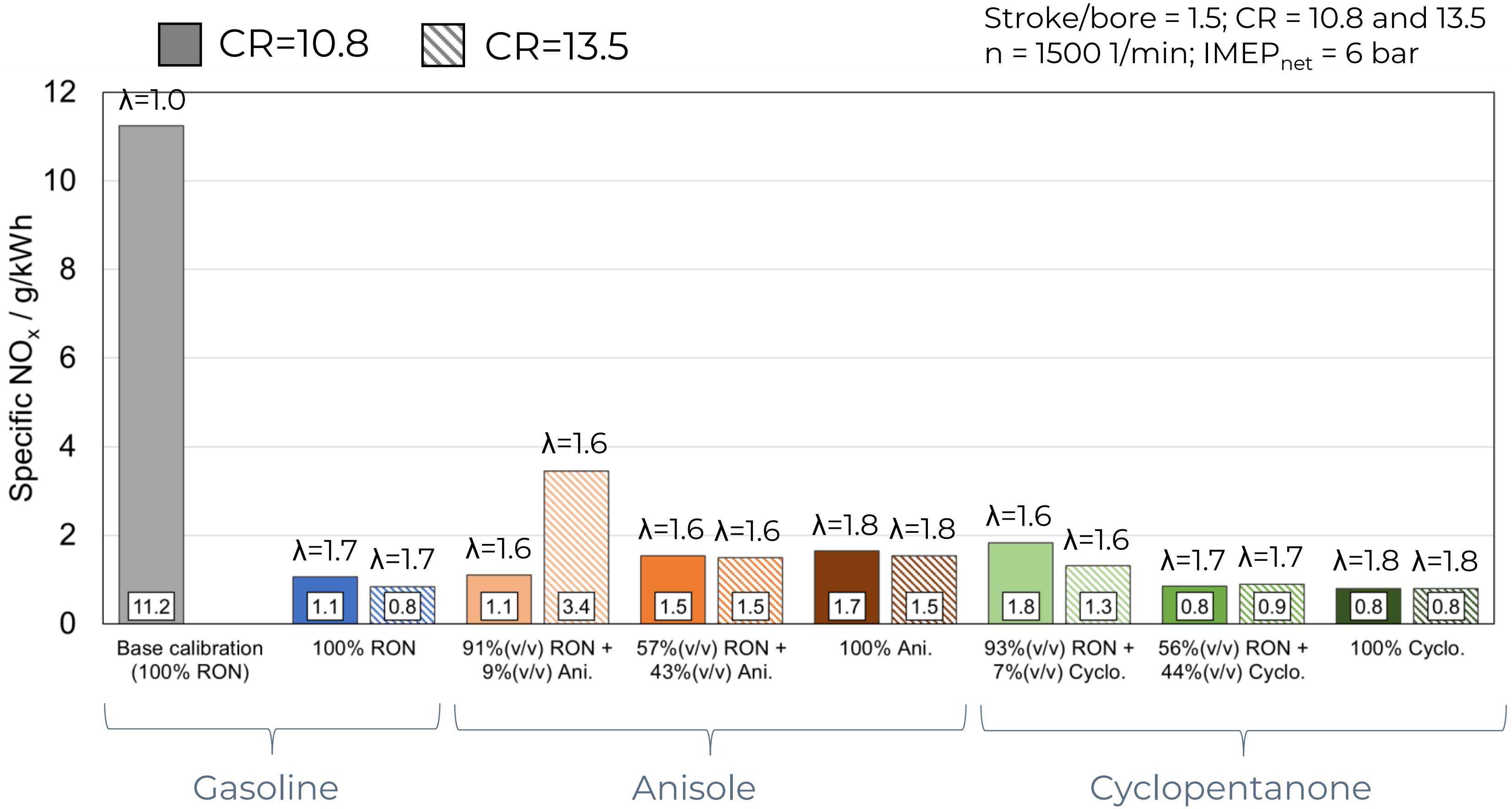


Optimization results | CO_2

Stroke/bore = 1.5; CR = 10.8 and 13.5
n = 1500 1/min; $IMEP_{net}$ = 6 bar



Optimization results | NO_x

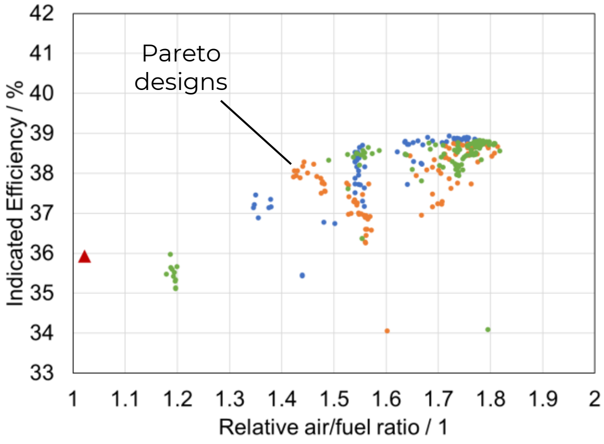


Optimization results

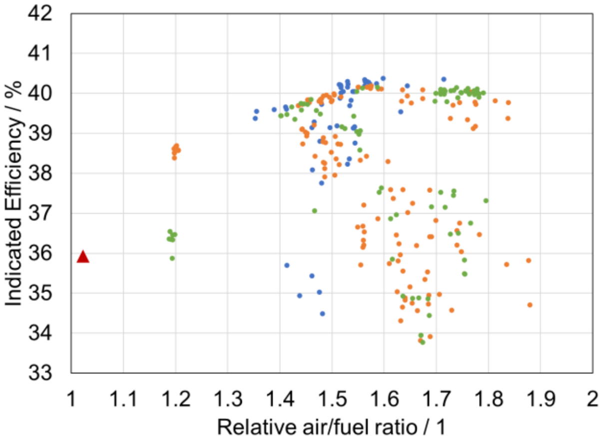
Stroke/bore = 1.5; CR = 10.8, 13.5 and 15.0
n = 1500 1/min; $IMEP_{net}$ = 6 bar

▲ Base calibration (100% RON) ● 100% RON (Pareto front) ● 100% Ani. (Pareto front) ● 100% Cyclo. (Pareto front)

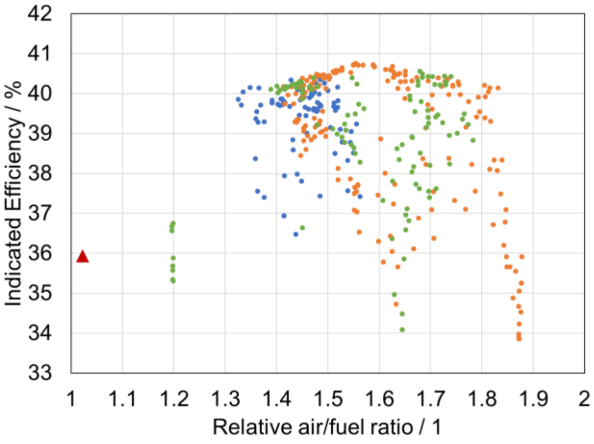
Model-based optimization results of CR = 10.8



Model-based optimization results of CR = 13.5



Model-based optimization results of CR = 15.0



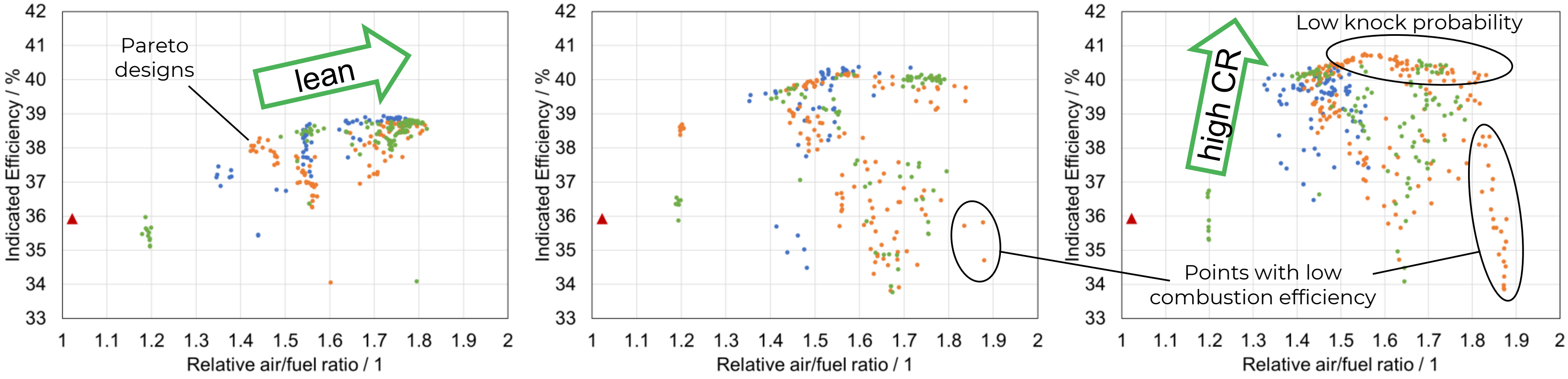
- For **neat anisole and neat cyclopentanone** a higher compression ratio of 15:1 is possible without knocking combustion.

Optimization results

Stroke/bore = 1.5; CR = 10.8, 13.5 and 15.0
n = 1500 1/min; $IMEP_{net}$ = 6 bar

Base calibration (100% RON) | 100% RON (Pareto front) | 100% Ani. (Pareto front) | 100% Cyclo. (Pareto front)

Model-based optimization results of CR = 10.8 | Model-based optimization results of CR = 13.5 | Model-based optimization results of CR = 15.0



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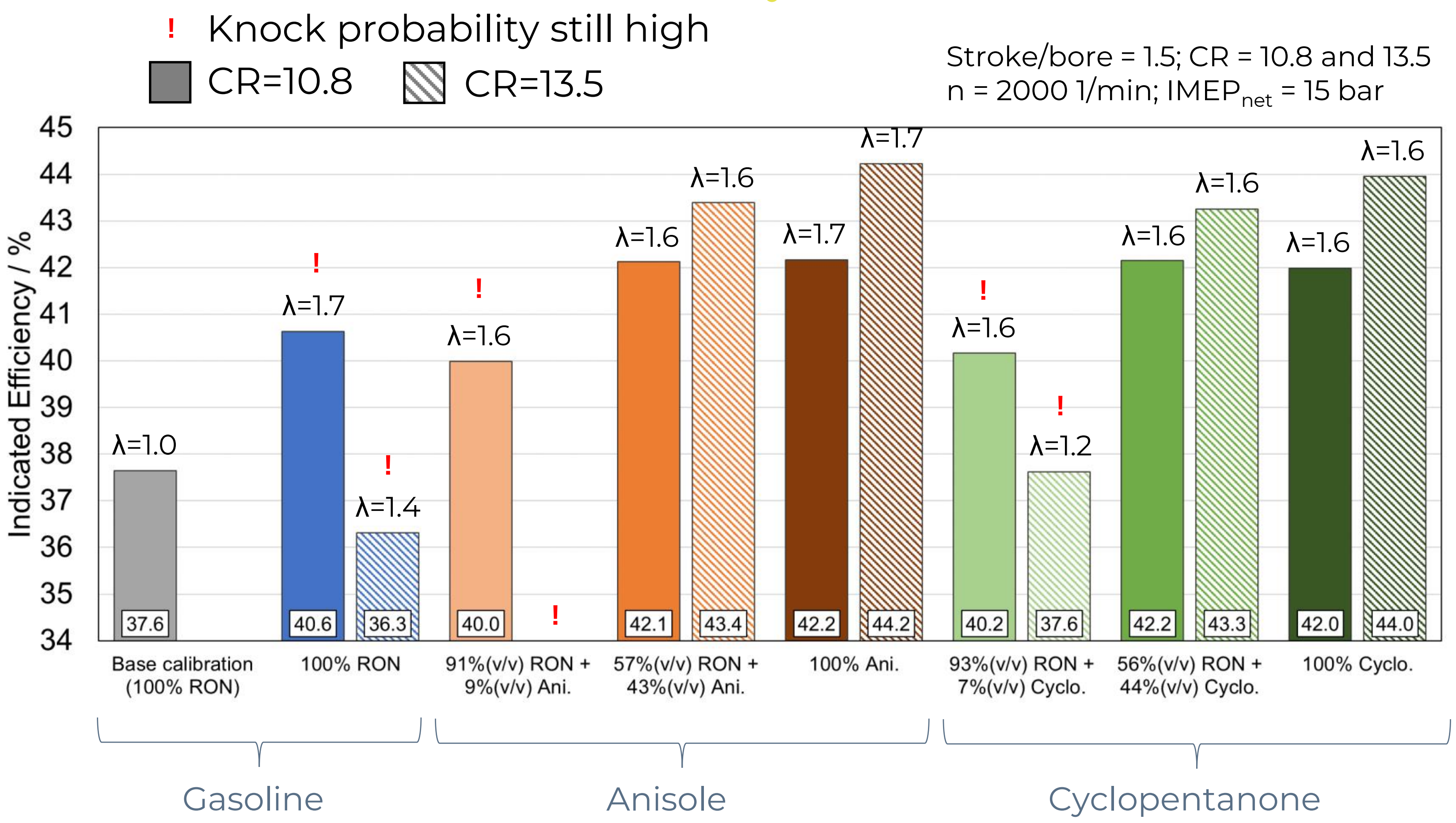
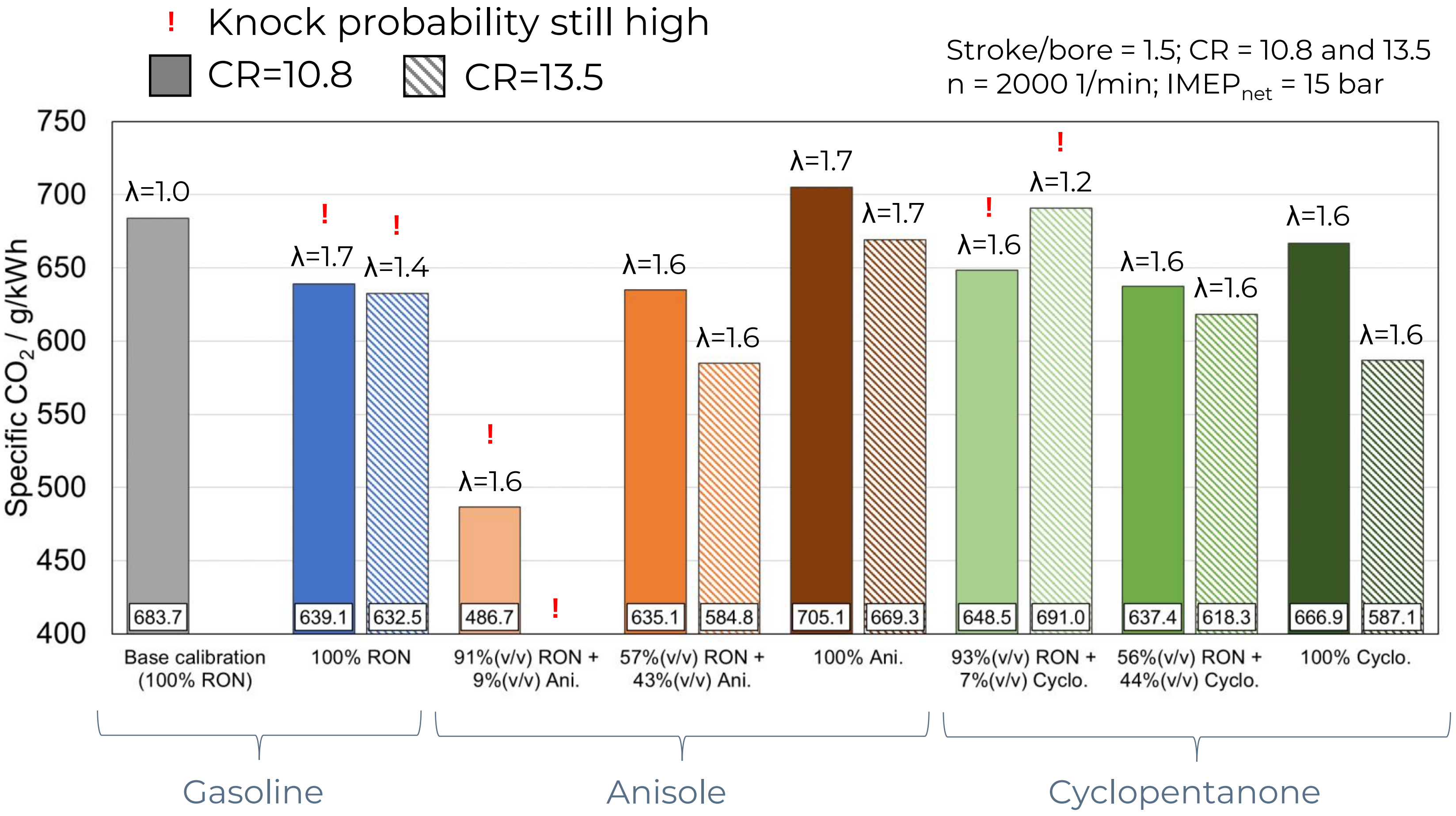
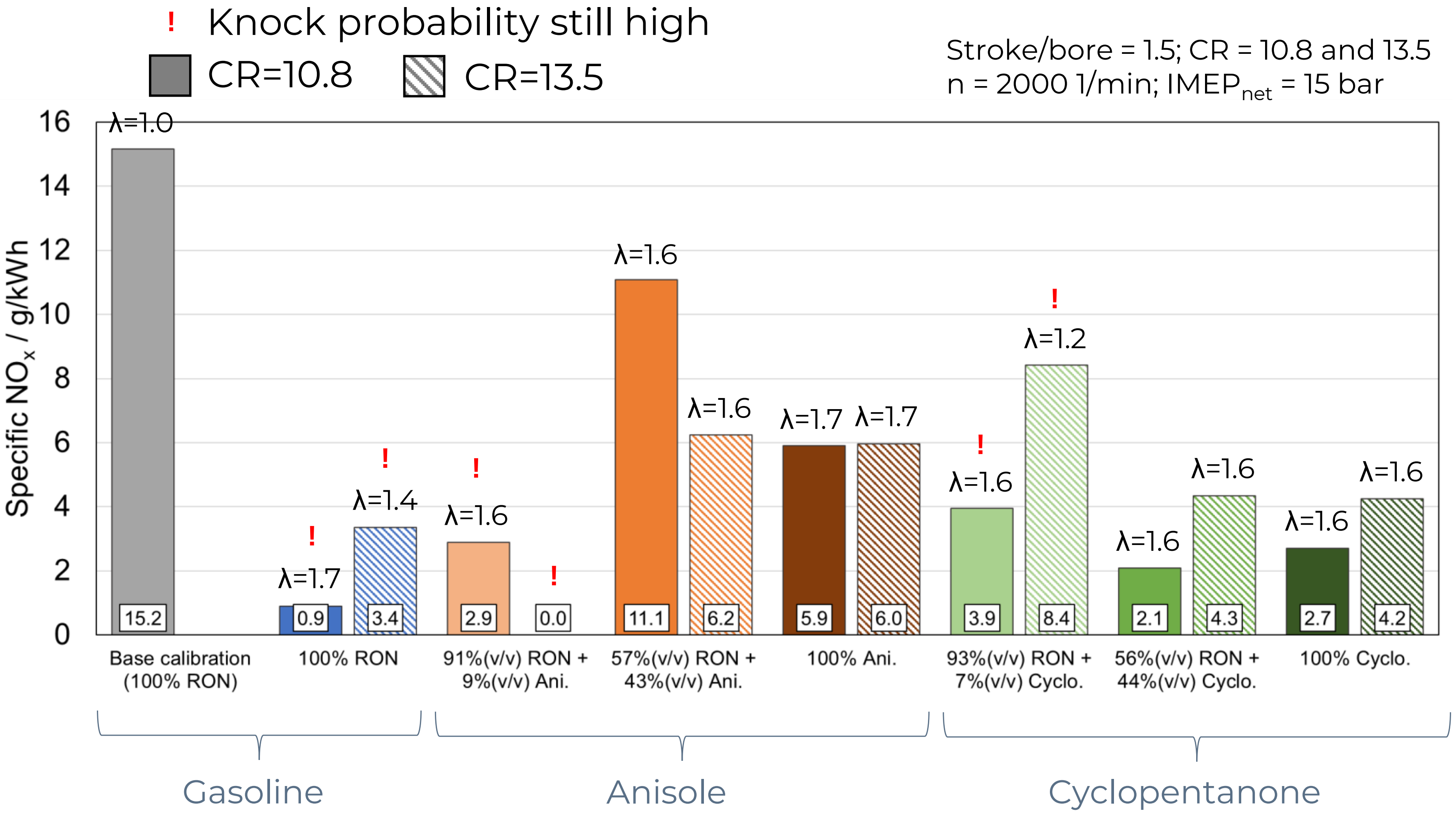
Optimization results | η_{eff}



Optimization results | CO_2



Optimization results | NO_x



WIRE

Motivation

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Results

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Evaluation of the biofuel performance

Conclusion

- The QD-SRM was extended for **biofuel combustion** and **lean conditions** and showed good agreement with experimental results.
- At part- and high-load operating conditions, **lean operation was extended** with high fraction of anisole or cyclopentanone in the blend.
- **Highest indicated efficiencies** are obtained at high-load operating conditions with high fraction of anisole or cyclopentanone in the blend.
- Further increase of indicated efficiency due to **increase of compression ratio**. Fraction of anisole or cyclopentanone must be increased to reduce knock probability.
- **NO_x emissions** are significantly reduced for lean conditions.

Thanks

Chair of Thermodynamics / Thermal Process Engineering

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https://www.b-tu.de/fg-tdtvt/