Future Fuels for Difficult to Decarbonise Transport Sectors

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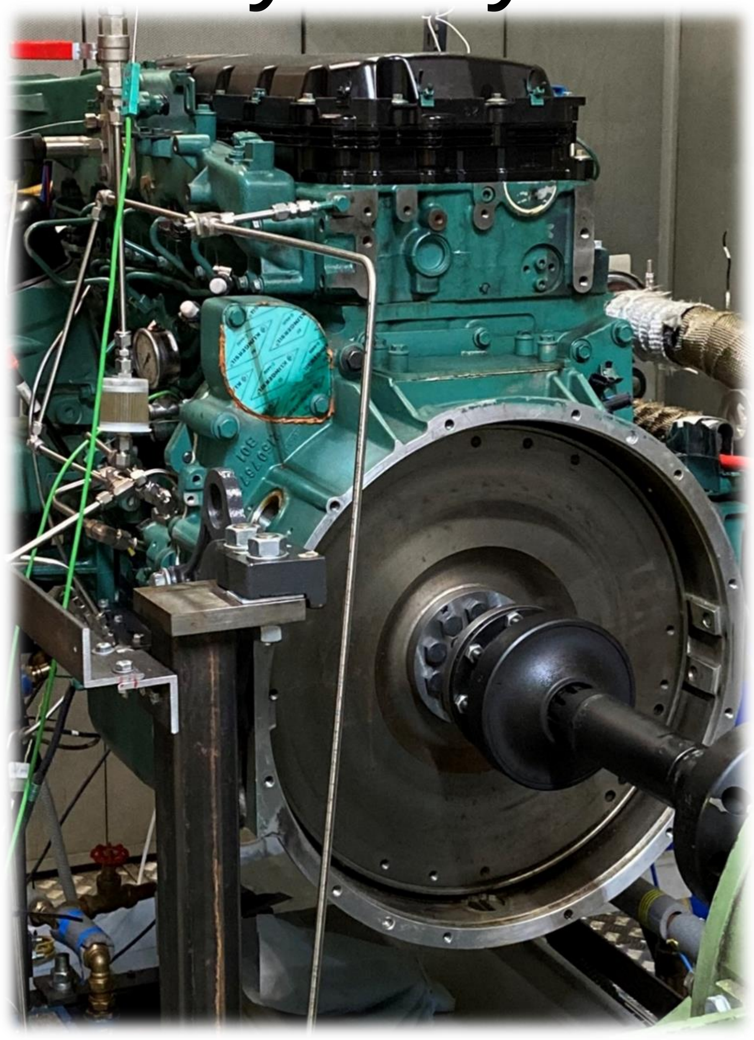
Background

- Decarbonisation of the transport sector is a necessary step to reduce CO_2 emissions in order to achieve the 2050 climate neutrality goals.
- Aviation, shipping and HGV freight are unlikely to fully move on from combustion engines using liquid fuels.[1]
- Wide adoption of biofuels is a vital goal for the decarbonisation of these transport sectors, but current biofuel research facilities do not accurately represent the engines which will remain in use by these industries.
- Combustion is initiated by free radicals, H, OH, R & O_2 and biofuels can contain structures which may facilitate unique reactions with radicals that are not available in fossil fuels.[2]

Project Overview

- The incorporation of biofuel structures receptive to new radical reactions, such as α-β unsaturation, would benefit from further research.
- We hypothesise that the inclusion of these reactive fuel structures would result in improved performance in a heavy-duty engine.

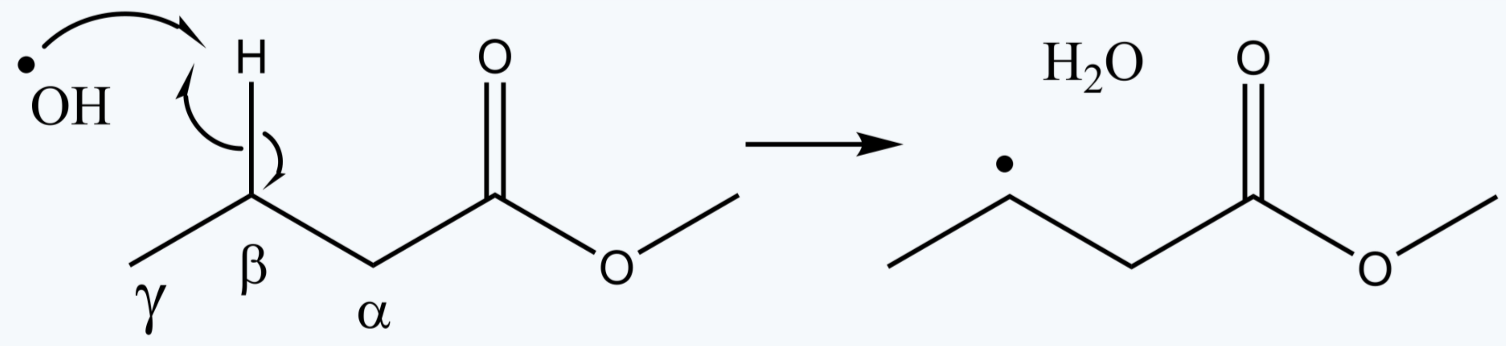
Heavy-duty Fuels Research Facility



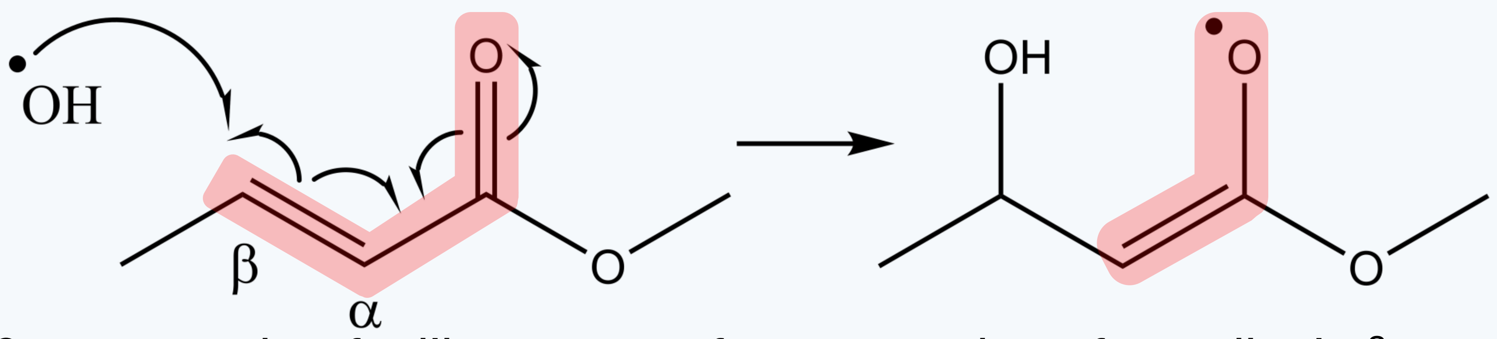
	Volvo D8k
No. of cylinders	6
Displacement	7.7 L
Stroke	135 mm
Bore	110 mm
Compression ratio	17.5 : 1
Economy revs	1,000 – 1,700 r/min

- Commercially available since 2014.
- Euro 6 compliant.
- Ideal sample of the current market.
- Better representation of engines which will remain in the transport sector.

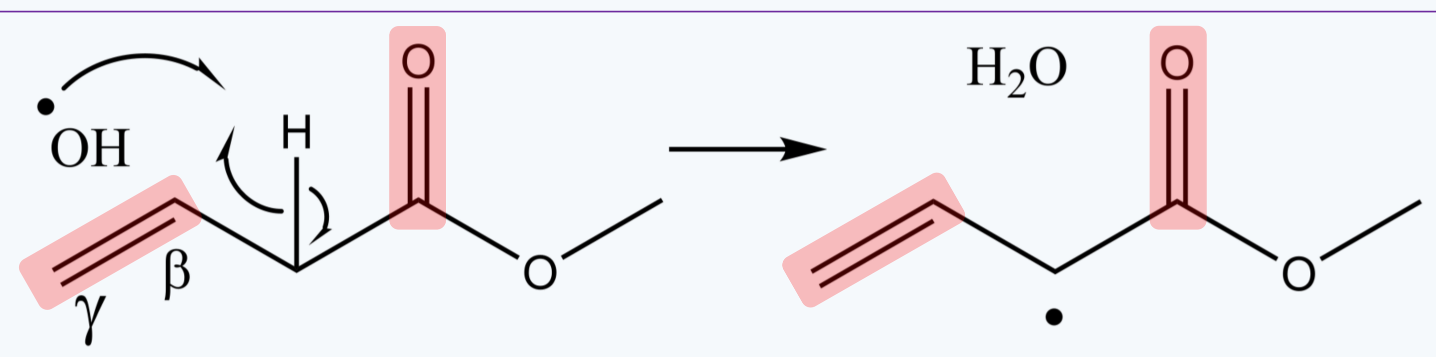
Radical Receptive Fuel Structures



- Simple reactivity – H abstraction by free radical initiates combustion.

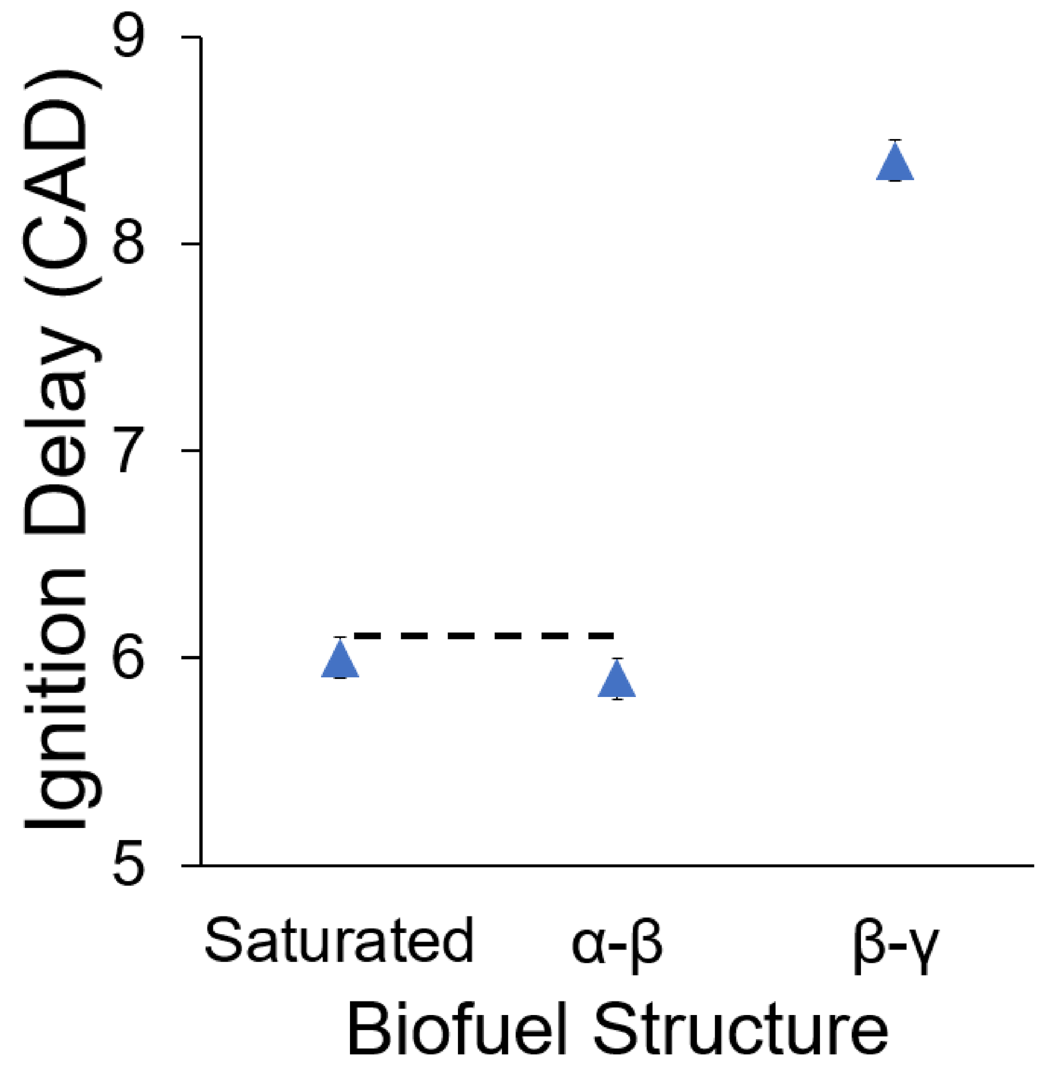


- α-β unsaturation facilitates new, faster reactions for radicals.[3] Free radical addition to the double bond can initiate combustion.
- Faster reactivity improves the autoignition process, which is necessary for efficient release of energy during combustion.

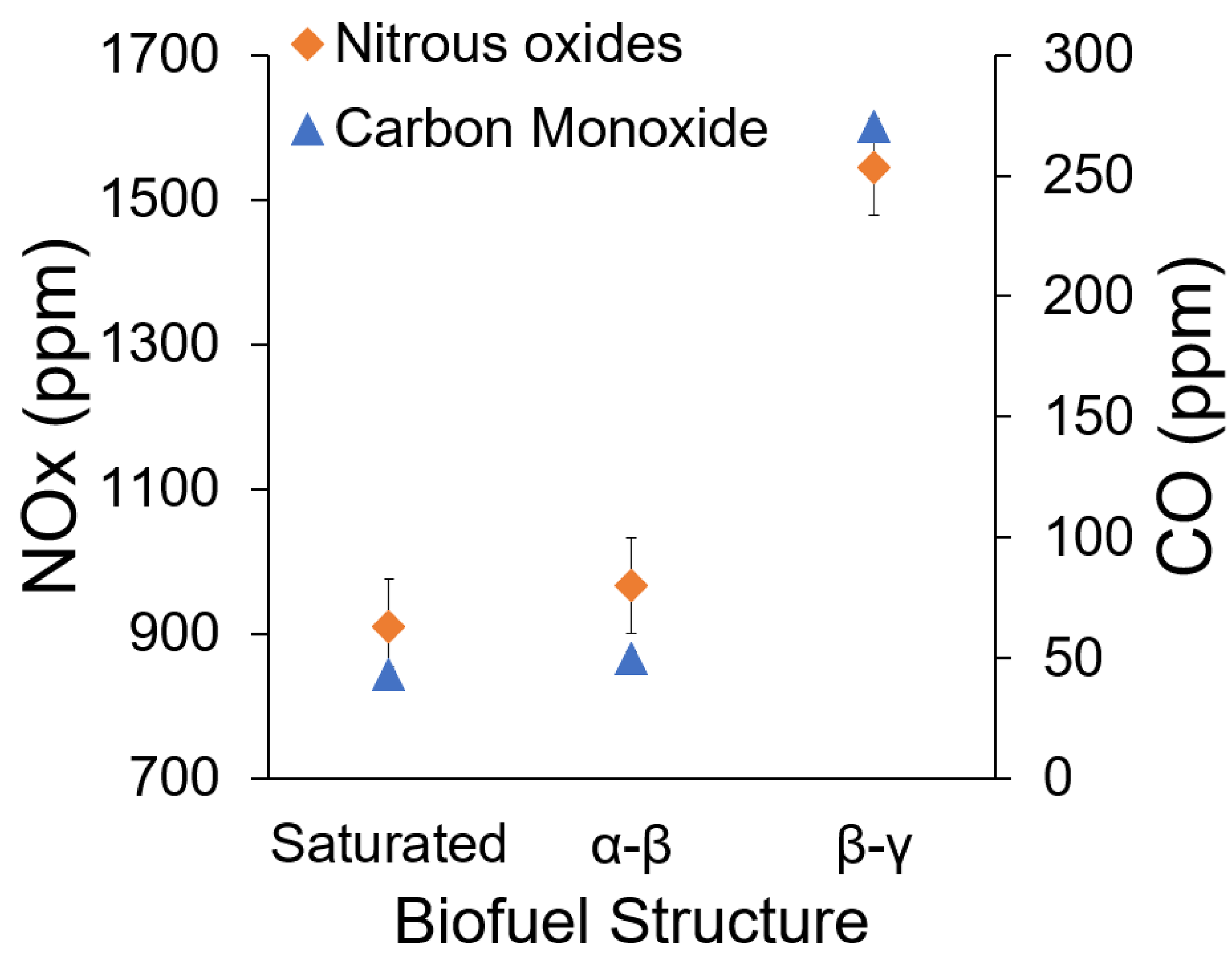


- Unsaturated β-γ carbons do not create a unique structure.
- Simple reactivity – H abstraction by free radical initiates combustion.

Fuel Performance Results

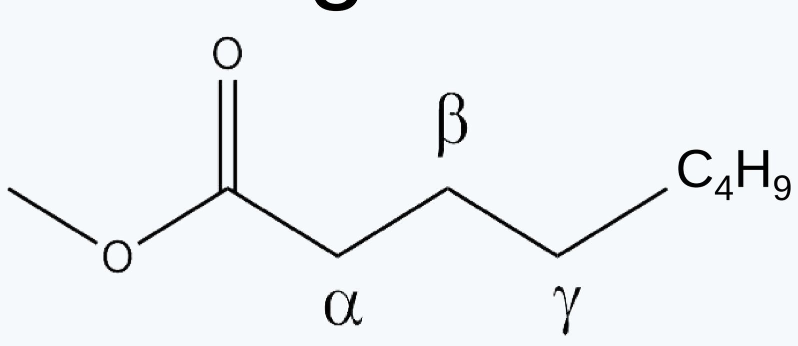


- α-β has the shortest ignition delay – easiest fuel to ignite.
- β-γ significantly longer ignition delay – very poor ignitability.



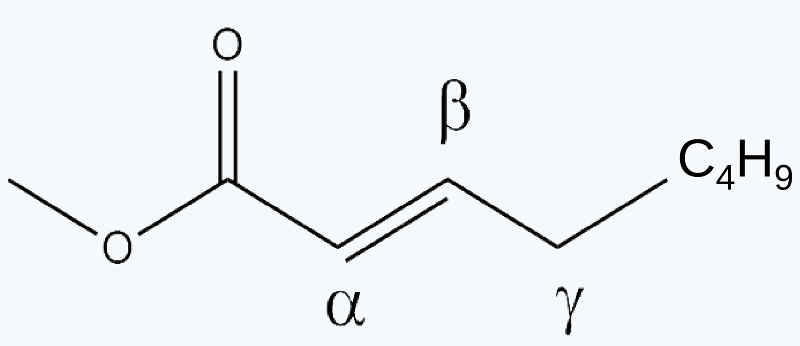
- β-γ emits far more pollutants than α-β, despite near identical structure.
- α-β emits similar pollutants to Saturated – goes against literature predictions which do not consider higher order of reactivity.[2]

Investigated Biofuel Targets



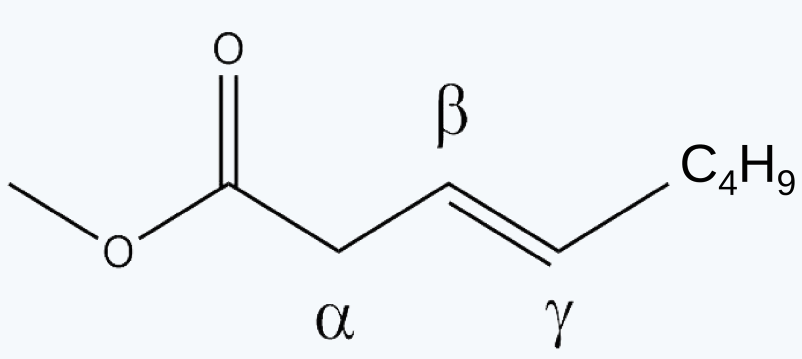
Saturated fuel

- Represents current biodiesel.
- Initiates via H abstraction.
- Simplified reactivity.



α-β unsaturated fuel

- Contains fuel structure which facilitates faster radical reactions.
- Can initiate via free radical addition.
- Enhanced reactivity.



β-γ unsaturated fuel

- Almost identical to the previous α-β fuel, but lacks a unique structure.
- Simplified reactivity.

Conclusions and Impact

- Unsaturated fuels typically exhibit higher pollutant emissions than saturated fuels, but the α-β fuel behaved similarly to the saturated fuel.
- The α-β fuel's shorter ignition delay and lower pollutant emissions points to significantly improved combustion over the β-γ fuel, despite their near identical structure which supports our hypothesis that the radical reactions limited to the α-β fuel can improve fuel performance.
- We have shown that even minor changes in chemical structure will have large impacts on fuel behaviour in heavy-duty engines.
- We have further shown that research into unique biofuel structures is vital for all transport sectors to efficiently move past fossil fuels.

References

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2. Fridlyand, A. et al. (2015). Chemical Kinetic Influences of Alkyl Chain Structure on the High Pressure and Temperature Oxidation of a Representative Unsaturated Biodiesel: Methyl Nonenoate. *Journal of Physical Chemistry A*, *119*(28), 7559–7577.
3. Atkinson, R. et al. (1983). Kinetics of the gas-phase reactions of OH radicals with a series of α,β-unsaturated carbonyls at 299 ± 2 K. *International Journal of Chemical Kinetics*, *15*(1), 75–81.