Bio4Fuels

Norwegian Centre for Sustainable Bio-Based Fuel and Energy

Bio4Fuels
SP5 – Process Design and End Use

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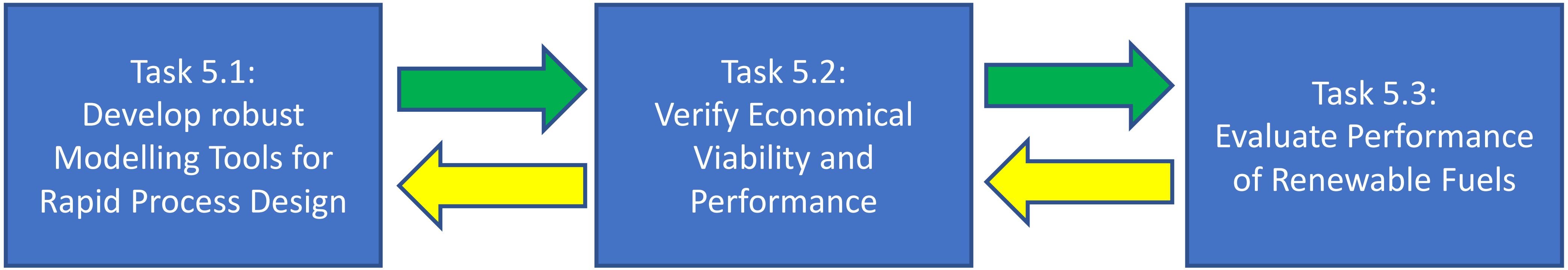
Bio4Fuels Day, Nov. 19. 2020

Bio4Fuels
SP5 – Process Design and End Use

- Task 5.1: Modelling tool for biorefineries (Prof. Heinz Preisig, NTNU)
- Task 5.2: Techno-Economic Evaluation and Scale of Economy (Sen.Adv. Bernd Wittgens, SINTEF)
- Task 5.3: End-Use (Prof. Terese Løvås, NTNU)



Task 5.1: Modelling tool for Biorefineries

Three main objectives:

1. Establish ontology*-based software for the modelling of biofuel production processes
   - includes terminology, ontology structure and equations for the entity models

2. Establish a library of basic units' simulations
   - models using the entity models

3. Establish a library of common reaction systems - biological and chemical

*Ontology: How entities are grouped into basic categories and which of these entities exist on the most fundamental level.

Task 5.1: ProMo - Status

ProMo is an ontology-based software suite for process modelling developped by the NTNU's Process System Engineering group.

It has three sections:

1) **Expert section** – for the construction and maintainance of the ontologies
   status: operational, will be periodically updated as we learn more about what we need in the other sections.

2) **Translator section** – for the generation of unit and process models
   status: main section is operational

3) **Task factory** – for the generation of executable code
   status: work required for the instantiation and code splicing. Here we lost one year due to personell issues.

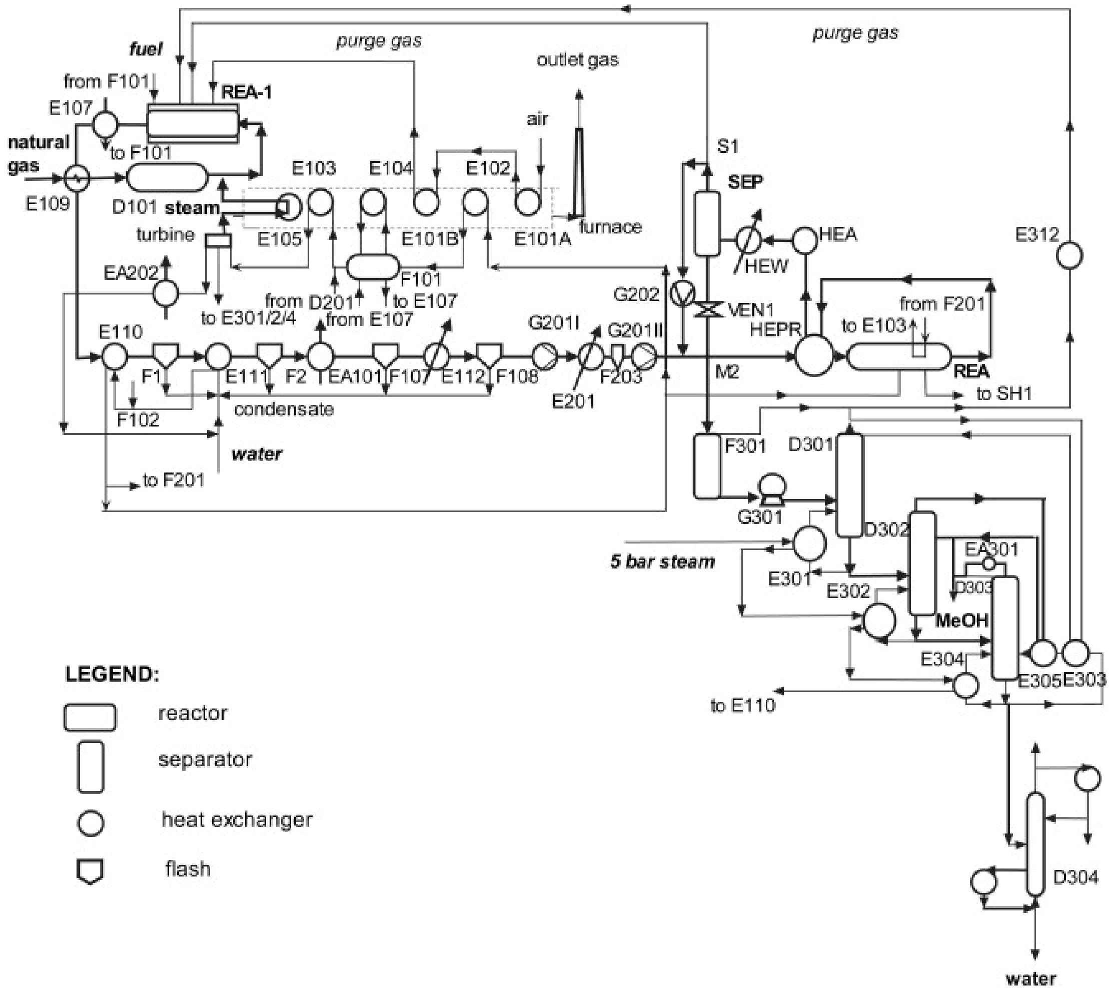
Task 5.1: Modelling Status

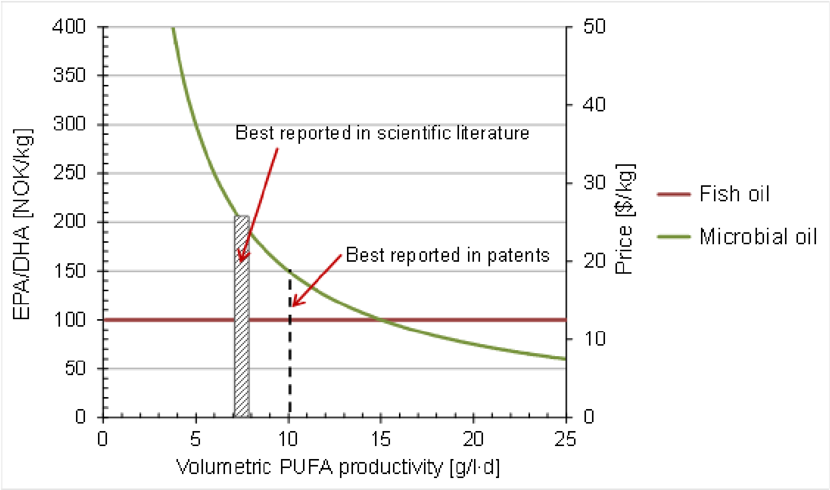
- Bio-related processes as topologies (Use Cases)
  - EcoLodge (BuOH + HBU -> BuB)
  - Distillation
  - Adsorption
  - Mass & pressure distribution in complex tanks
  - Membrane units
  - KomBiChemPRO (hydrothermal treatment of aqueous hemicellulose)
- Thermodynamics module
- Pressure distribution - a topology mapping
- Interfacial processes - a topology mapping

Task 5.1: 2021 Planning & Ongoing Work

- Software – main focus on the code generation Task Factory (ProMo section 3)
- Ontologies – continuous adjusting due to changing requirements.
- Implementations of various detailed models relating to handling thermodynamics either by compuation or interfaces to databases.
- Implementation of process-unit models for bioprocesses
- Parallel experimental continuing with EcoLodge, the new IndNor project of integrating EcoLodge into one intensive unit and adding processes from DBFZ.
- Related to other projects (Horizon2020: MarketPlace, VIPCOAT; NFR: NanoLodge)
    - Work towards an international standard for model topologies
    - Extending the European Materials & Modelling Ontology

Task 5.2: Techno-Economic Evaluation and Scale of Economy





Task 5.2: Objectives

Fundamental science converted to commercial opportunities

More efficient processes -> reaching lower costs

- Create building blocks for sub-processes
- Models address:
  - Flexible plant and process design
  - Costing
  - Evaluation of performance
- Different design alternatives based on estimated CAPEX & OPEX
- Simplified and intensified processes
- Incorporate monetarization of side and by-products

Task 5.2: Status (Butyl-Butyrate from sugar)

- Process Design and Equipment Sizing completed
- Operational Conditions verified
- CAPEX, OPEX estimated
- Net Cash Flow Table and Sensitivity Analysis performed

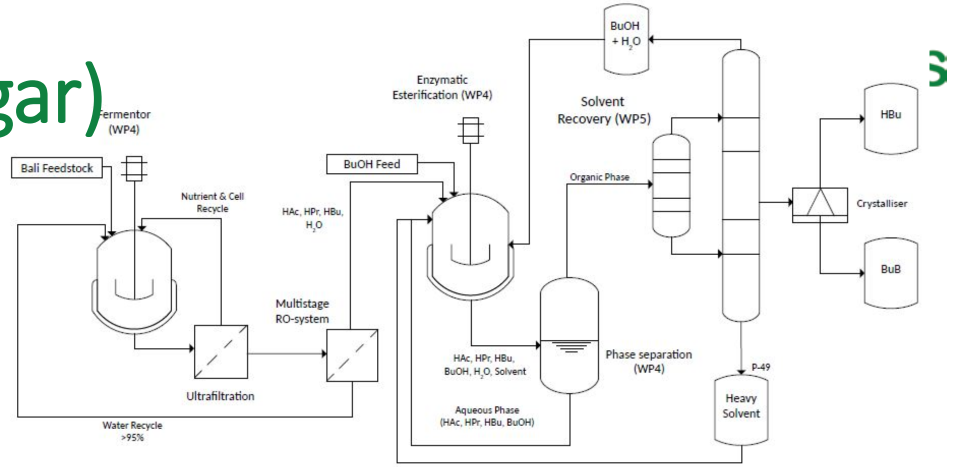


Table 3: Butanol fermentation parameters

Parameter	Value	Units
Glucose start	80	g/L
Residence time	50	h
Yield acetone	10.3	g/L
Yield etanol	1.7	g/L
Yield butanol	19.8	g/L
Yield acetic acid	0.4	g/L
Yield butyric acid	1.7	g/L
Residual glucose	0.0	g/L
Butanol glucose yield	0.41	g/g glucose
Butanol productivity	0.31	g/(L h)

Table 4: Butyric acid production parameters

Parameter	Value	Units
concentration	29.7	g/L
volumetric productivity	9.5	g/L/h
selectivity	0.94	g/g (wt HBu of total acids)
yield (glucose)	0.45	g/g
biomass concentration	35.0	g/L
cell bleed rate	0.032	1/h
feed dilution rate	0.32	1/h
acid product concentration	300.0	g/L
required production rate	2546	kg/h

Table 7: CAPEX table

Name	Unit type	Kind	Keydim	Units	Cost	Units	#	Total 100 mt/d	Total 1 mt/d	Total 10 kg/d	Notes
Hydrolyzation tank	Tank	fixed roof	2189	m3	278000	USD	2	556000	22240	890	
Hydrolyzation agitation	Pumparound	+20% on tank			55600	USD	2	111200	4448	178	
HBu-fermenter	Tank	fixed roof	285	m3	113042	USD	1	113042	4522	181	
HBu agitation	Pumparound	+20% on tank			22608	USD	1	22608	904	36	
BuOH-fermenter	Tank	Fixed roof	2072	m3	271176	USD	4	1084704	43388	1736	
Gas stripping condenser	Heat exch.	fixed tube	154	m2	317000	USD	1	317000	12680	507	(2)
Gas stripping compressor	Compressor	axial	360	kW	1861000	USD	1	1861000	74440	2978	
Esterification reactor	Vessel	horizontal	310	m2	1321000	USD	2	2642000	105680	4227	
HBu NF membrane	NF membrane		5000	m2	675000	USD	1	675000	27000	1080	(1)
Enzyme filter						USD		0	0	0	
Bub NF membrane	NF membrane		600	m2	81000	USD	1	81000	3240	130	(1)
Decanter						USD	1	0	0	0	
Esterification R/O unit	Vessel	horizontal	440	m3	1779000	USD	2	3558000	142320	5693	
Distillation boiler	Reboiler	kettle	60	m2	690000	USD	1	690000	27600	1104	(4)
Dist. side condenser	Heat exch.	multi pipe	17	m2	67000	USD	1	67000	2680	107	
Dist. top condenser	Heat exch.	multi pipe	60	m2	225000	USD	1	225000	9000	360	(3)
Dist. prefrac vessel	Vessel		9	m3	80000	USD	1	80000	3200	128	(5)
Dist. main shell	Vessel		18	m3	123000	USD	1	123000	4920	197	(6)
Sum						USD		12206554	488262	97652	

Notes to CAPEX table

1. 30-60 USD/m2, Unit cost is 3x membrane cost
2. 1.9 MW, 1000 W/(m2 K)
3. 340 kW, 1000 W/(m2 K)
4. 1.2 MW, 1000 W/(m2 K)
5. 5m height, 1.5m Ø
6. 10m height, 1.5m Ø, 0.5 m/s superficial velocity

A scaling to 1/10 and 1/100 of nominal production (1 metric ton per day) is given by using scaling factor exponent of 0.7.

Table 5: Esterification parameters

Parameter	Value	Units
Feeding HBu conc.	300	g/L
Feeding BuOH conc.	810	g/L (pure)
Organic phase volume-fraction	0.33	volume
Novozym 435 conc.	20	g/L
Residence time	2	h
Aqueous phase BuOH conc.	15	g/L
Aqueous phase HBu conc.	8	g/L
Organic phase BuOH conc.	82	g/L
Organic phase BuB conc.	60	g/L
Butyl butyrate productivity	30	g/(L h) pr. liter organic phase
Enzyme recycle factor	0.8	

Table 6: BuB-esterification calculations

Parameter	Value	Units
Total liquid volume	833	m^3
Organic phase volume	278	m^3
Aqueous phase volume	556	m^3
Replenish rate of enzyme	556	kg/h
Hexadecane circulation rate	139	m^3
Butanol circulation rate	11390	kg/hr
Water produced in esterification	520	kg/h
Water to be removed	11392	kg/h
Power requirement for water removal	80	kW

Task 5.2: Challenges

- Process Design and cost estimation is in general an iterative process
- NEED the proper mass and energy balances
- **Industrial Verification of Costing Needs to be performed**
- Degree of detail depends on application (Short cut to investment decision: NCF, NPV, IRR)
- Derived data are vital for
  - LCA and LCC
  - Up-scaling

Task 5.2: On-going Experimental Work

Ecolodge reactor in operation

- Raman spectrometer for process monitoring
- Hydrozyclone to remove cells in measurement cell

Butanol reactor operates with gas stripping to recover products

Butyric acid system

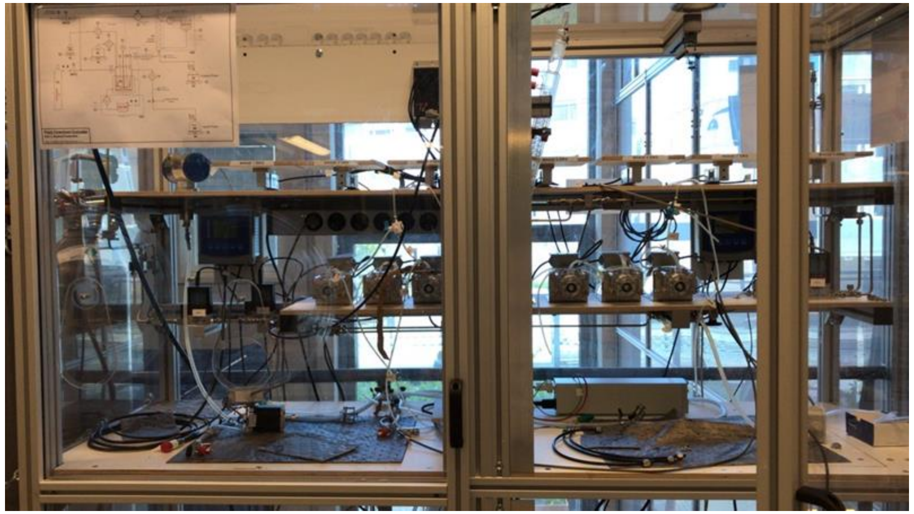
- Evaluation of a cross-flow system to retain cell mass in reactor
- Electro-dialysis to recover butyri acid

Implementation of Esterification under evaluation

Master studenter:

Yvonne Amponsah, University of Bologna, IT

Henri Steinweg, KIT, D



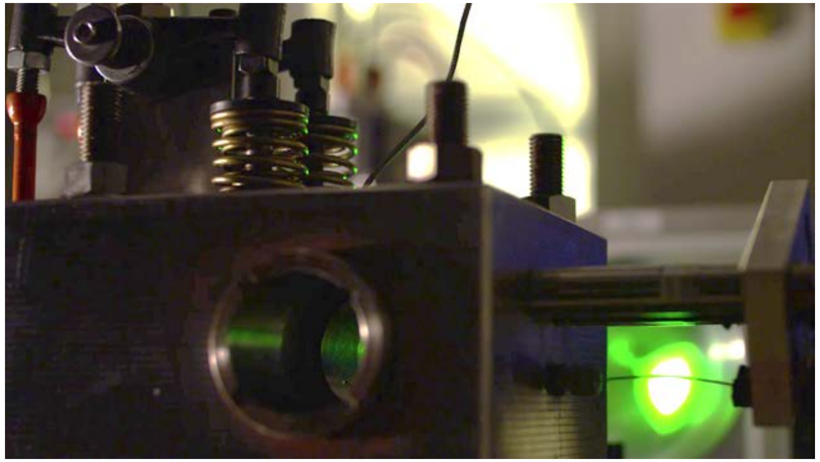
Task 5.2: Governing plans for 2021

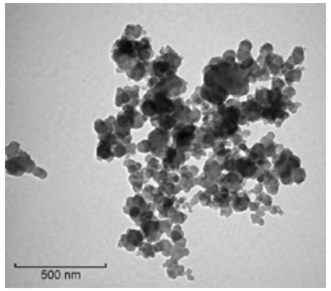
- Evaluation of core technologies relevant for Bio4Fuels
  - Biochemical conversion
    - Enzymatic Pre-treatment
    - Butyl- Butyrate (almost done)
  - Thermochemical Conversion
    - Up-grading of pyrolysis oils
    - Electrochemical conversion of pyrolysis oils
    - Electrochemical Degradation of lignin

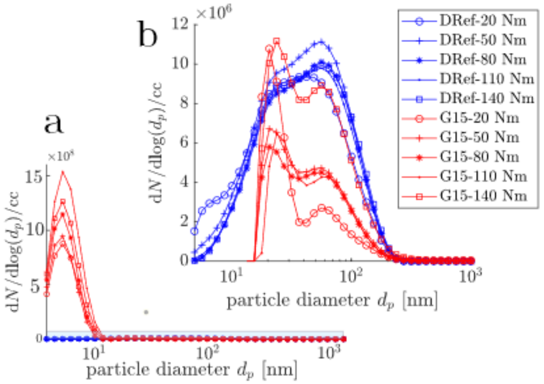
Create scientific foundation:

- Try to replace opinions with facts.
- Identify economical attractive value chains.
- Understanding where and how to reduce costs?
- "Toolbox" for rapid process costing.
- **Verification of costing with industrial partners**.
- Stakeholder involvement needs re-consideration to get "data"
- Develop "evaluated process data" for LCA / LCC.

Task 5.3: Product quality & End Use







Particle size distribution of soot from studies of bio-based glycerol emulsion compared to reference diesel. The study shows increase of the smallest particles from glycerol emulsion, although total particle mass emissions are lower.

Objective:

- Study of current and new biofuels under relevant combustion conditions
- Focus on fuel conversion (to power) and emission control
- Focus on regulated and unregulated emission

Task 5.1.3: Combustion tests in optical engine - Status

- Laboratory operative
- Experimental campaigns ongoing for various biofuel blends and surrogates

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Diffuse Back-Illuminated Extinction Imaging of Soot: Effects of Beam Steering and Flame Luminosity

Karl Oskar Pires Bjørgen, David Robert Emberson, and Terese Lovas
Norwegian University of Science & Technology

Citation: Bjørgen, K.O.P., Emberson, D.R., and Lovas, T., "Diffuse Back-Illuminated Extinction Imaging of Soot: Effects of Beam Steering and Flame Luminosity," SAE Technical Paper 2019-01-0011, 2019, doi:10.4271/2019-01-0011.

Abstract

This study presents diagnostic development of diffuse back-illuminated extinction imaging of soot. The method provides high temporal and spatial resolution of the line-of-sight optical density of soot (*KL*) in compression-ignited fuel sprays relevant to automotive applications. The method is subjected to two major sources of error, beam steering effects and broadband flame luminosity effects. These were investigated in detail in a direct injection combustion chamber with diesel fuel, under high and low sooting conditions. A new method for correcting flame luminosity effects is presented and involves measuring the flame luminosity using a separate high-speed camera via a beam splitter. The new method and existing methods are applied and the resulting flame luminosity correction errors are compared. The new method yields 50% lower errors than the most promising method (optical flow method). The impact on *KL* was investigated, showing that the *KL* uncertainty when using the optical flow method is unbounded for *KL* values above 2.7, while the new method has an uncertainty of 0.5 for the maximum *KL* value of 3.8. The new method yields overall lower uncertainties and is more suited to measuring *KL* in optical thick conditions. Large refractive index gradients in the path of the incident light cause false attenuation, resulting in ambiguity of the measured *KL*, referred to as beam steering. A detailed investigation of the beam steering effects caused by the non-uniformities in the diffused light source was performed. A beam steering model was made and qualitatively validated from experiments. The results from the beam steering model showed the importance of having a large collection angle, in order to average out small-scale non-uniformities in the light source. The model also showed that large-scale non-uniformities in the light source could affect the measurement even if the collection angle is large.

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Optical Measurements of In-Flame Soot in Compression-Ignited Methyl Ester Flames

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ABSTRACT: This study investigates in-flame sooting characteristics of biodiesel surrogates in compression-ignited spray flames. The aim of the study is to produce reliable experimental data on in-flame soot for validation of kinetic mechanisms and soot models. A rapeseed oil biodiesel [rapeseed oil methyl ester (RME)] was compared to neat methyl oleate (MO) and methyl decanoate (MD). In addition, neat *n*-heptane was chosen as a baseline fuel and the effect of blending *n*-heptane and MD on soot production was investigated. The study was performed in a single-cylinder research engine with optical access to a single spray for varying ambient gas temperatures (825−990 K). The in-flame soot was measured by a high-speed diffuse back-illuminated extinction imaging system, and the flame lift-off length (FLOL) and the corresponding estimated equivalence ratio at FLOL was measured from high-speed OH* chemiluminescence imaging. Results show that RME has the highest tendency to soot, closely followed by MO, independent of the FLOL equivalence ratio. Having almost identical fuel properties, this is likely due to the higher degree of unsaturation in RME compared to MO. When comparing MD to *n*-heptane, a much lower in-flame soot production rate is observed despite the fact that MD has a higher number of carbon−carbon bonds, concluding that the high fuel oxygen ratio in MD is effectively reducing in-flame soot production. Generally, for FLOL equivalence ratio leaner than ~2, no in-flame soot was produced for all ambient gas temperatures. The in-flame soot production rate also showed a clear ambient gas temperature dependence for constant FLOL equivalence ratios, where the soot production rate increased with increased gas temperatures.

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Combustion and soot characteristics of hydrotreated vegetable oil compression-ignited spray flames

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Keywords:
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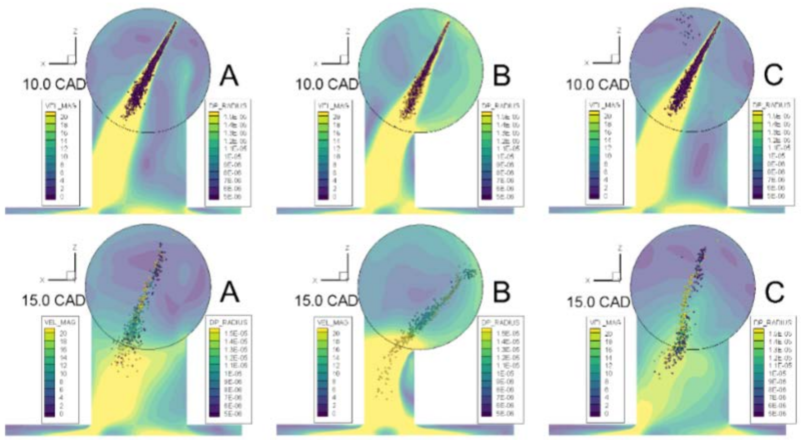
ABSTRACT

Quantitative measurements of combustion and in-flame soot in hydrotreated vegetable oil (HVO), biodiesel (rapeseed methyl ester [RME]) and diesel fuel spray flames are presented in this study. The measurements were performed in a compression ignition chamber with optical access having engine-like thermodynamic conditions. The simultaneously employed optical techniques were high-speed diffuse back-illuminated light extinction imaging for measuring the optical depth (*KL*) of in-flame soot, and OH* chemiluminescence for imaging high temperature reaction zones. The results show that diesel produces a considerably higher amount of in-flame soot compared to RME and HVO, which is likely due to the aromatics present in diesel, while RME and HVO produce similar levels. RME was found to produce slightly less soot, which is likely due to the fuel-bound oxygen, since HVO and RME have a similar number of carbon-carbon bonds. The soot production during the premixed and mixing-controlled period were found to have similar trends. The time lag between start of ignition and soot formation was found to be constant for varying ambient temperatures for individual fuels, where soot was detected earliest after ignition for diesel, followed by HVO and RME, matching the measured sooting tendencies. The stabilised flame lift-off length of HVO was found to be shorter than that of diesel, while RME had the shortest of them all.

Task 5.1.2: Trained engine simulations of combustion including emissions- Status

- Trained engine simulations operative (based on a machine learning module)

In this work, we present a numerical study of the flow in a combustion chamber which is dedicated and designed to investigate different fuel types under compression ignition conditions.



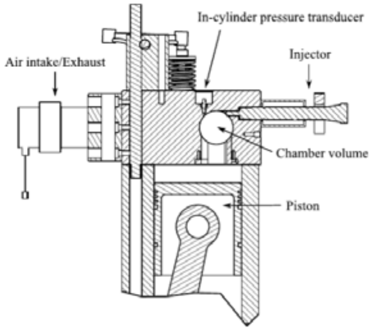


Figure 1: Schematic representation of the cross section of the OACIC [19].

Numerical investigation of optimal flow conditions in an optically accessed compression ignition engine, M. Lewandowski, C. Netzer, D. Emberson and T. Løvås, Accepted for publication in Transport Engineering.

Task 5.1: 2021 Planning and Ongoing Work

- A new PhD has been recruited in WP5.3 who will work alongside the PD already involved in the project.

- Continued focused on detailed experimental and numerical investigations of 2nd generation type biofuels in compression ignition engines.
- Various combustion parameters will be investigated with a focus on emissions of NOx and soot.
- Matching the experimental data with results from detailed kinetic simulations using a stochastic reactor model will be an important part of the PhD project.

- We will continue with more complicated fuels which are focus fuels within Bio4Fuels. Discussions with Silva Green Fuels based on HTL based fuels have been initiated.

Associated Projects

- *ACTIVATE:* Ammonia as carbon free fuel for internal CombusTion engIne driVen AgriculTural vEhicle, EEA-Grant. Partner.
- *LowEmission Centre*: Norwegian Centre for innovation (SFI) on low emission technologies for off-shore industry, Co-funded by the Norwegian Research Council and industrial partners. Partner.

Summer newsletter SP5, WP5.3 End Use

New PhD student

We welcome Zhongye Xue, a new PhD student recruited at the Department of Energy and Process Engineering NTNU, who will work alongside researcher Dr. David Emberson and Prof. Terese Løvås on investigating the use of biofuels in modern combustion engines.

This project is focused on a detailed experimental and numerical investigation of 2nd generation type biofuels in compression ignition engines. Various combustion parameters will be investigated with a focus on emissions of NOx and soot. Fundamental experimental research on combustion of the biofuels will be carried out in collaboration with the current research team, employing a well-equipped engine laboratory and specially designed combustion rig with optical access for optical measurements. This enables detailed studies of the ignition and flame structure in the combustion chamber as well as particle formation. Matching the experimental data with results from detailed kinetic simulations using a stochastic reactor model will be an important part of the PhD project.

Zhongye Xue has a master degree from Tongji University, China, majoring in Power Machinery and Engineering. He has also three years of work experience working with engine management systems in Delphi Technologies and Porsche Engineering.

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