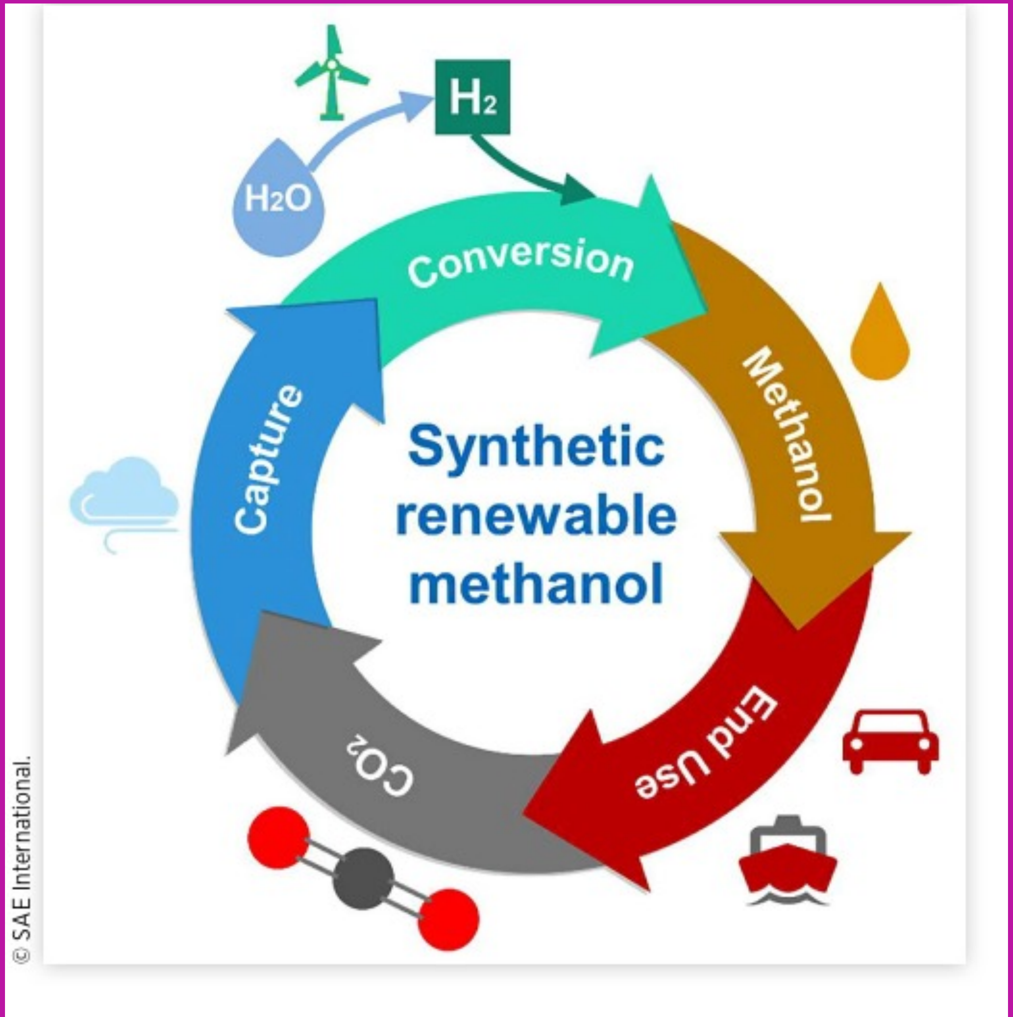
Aalto ENG

Methanol combustion modelling - engineering approach



Prof Martti Larmi

October 27, 2021

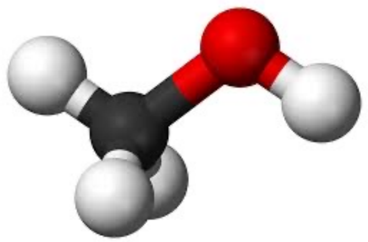
Aalto University
School of Engineering

Methanol combustion modelling – engineering approach

1. **Methanol properties**
2. Combustion strategies
3. Flow and turbulence modelling
4. Lagrangian Particle Tracking
5. Combustion modelling
6. Validation and results
7. Discussion

Methanol properties

CH_3OH



Key properties affecting end-use:

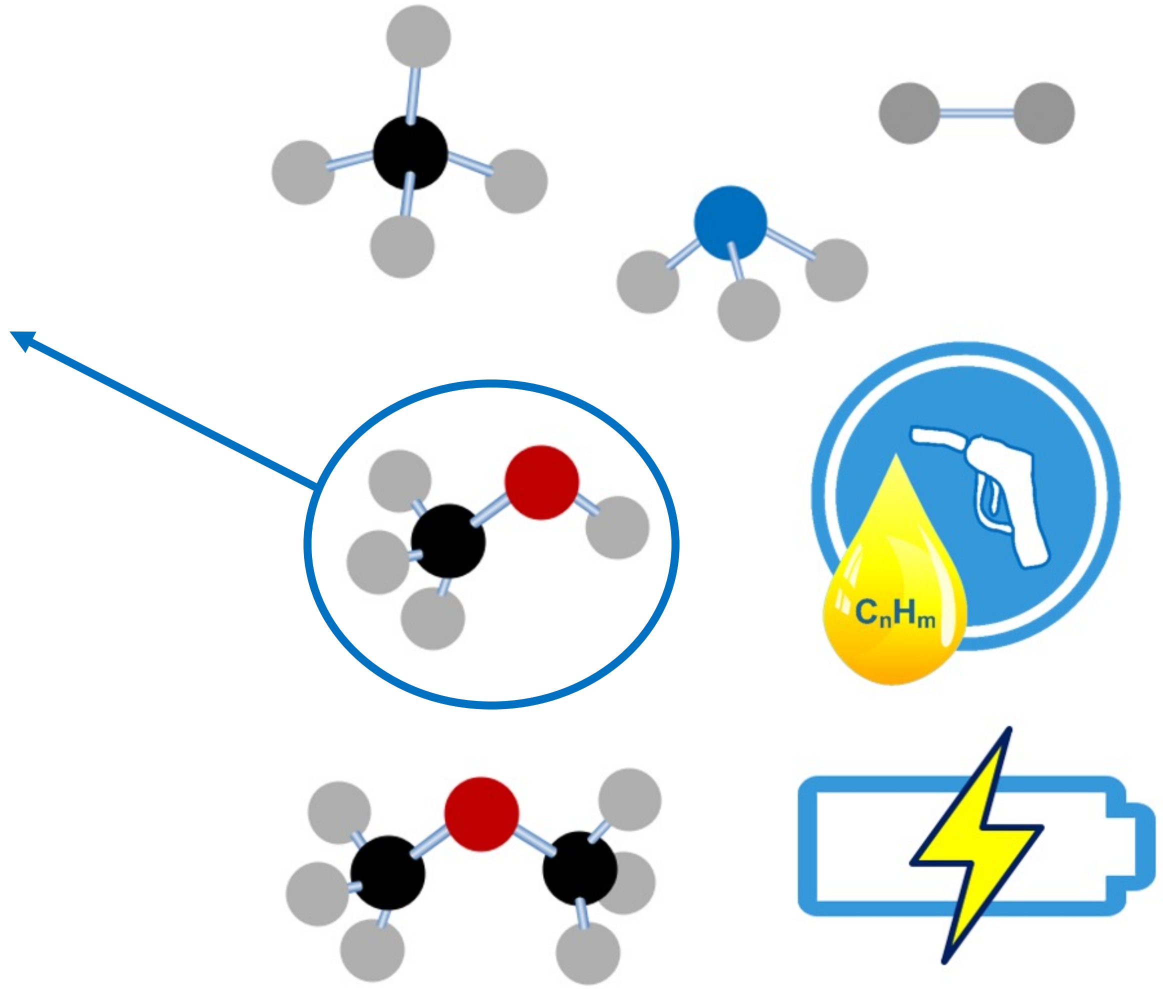
- Density comparable to other liquid hydrocarbons
- High heat of evaporation (charge formation & combustion)
- High autoignition temp. & high RON (combustion)
- High O_2 content and resulting low LHV (storage)
- Low viscosity (injection)
- Flammability limits and low flashpoint (safety)

Property	Unit	FUEL			
		Methanol	Ethanol	Gasoline	Diesel
Density @15°C	kg/m	**790**	790	740	835
LHV	MJ/kg	**20.1**	27	42.9	42.7
Oxygen content	%	**49.9**	34.7	0.0	0.0
Heat of evaporation	kJ/kg	**1170**	930	350	250
Viscosity (dynamic) @20°C	mPa	**0.57**	1.2	0.6	2.8
Autoignition temp.	K	**740**	700	470-740	520
Research Octane Number	-	**109**	109	98	c. 0
Lower flammability limit in air	vol.%	**6.7**	3.3	1.3	1.4
Upper flammability limit in air	vol.%	**36**	19	7.6	7.6
Flash point	°C	**11**	13	40	>55

Methanol among energy carriers

Methanol can be:

- **Fossil fuel** (from natural gas/coal)
- **Biofuel** (from sustainable biomass)
- **E-fuel** (from renewable H2 and CO_2/CO streams)

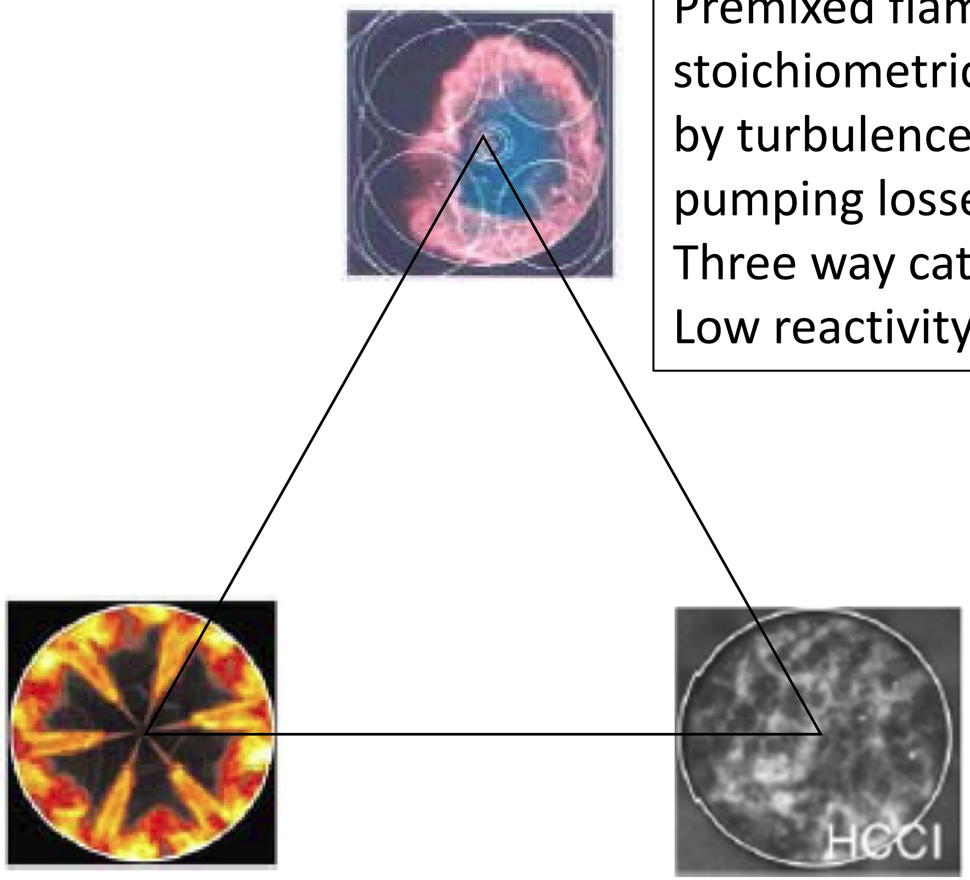


Methanol combustion modelling – engineering approach

Basic combustion regimes

Spark Ignited (SI)
Premixed flame propagation, stoichiometric or lean charge controlled by turbulence. Low efficiency, knock, pumping losses, large speed range. Three way catalyst and particulate filter. Low reactivity fuel preferred.

Compression Ignition (CI)
Diffusion combustion, lean charge, controlled by mixing, high efficiency, moderate speed range, spray physics in main role. High NOx and PM emissions, DPF and SCR, high reactivity fuel preferred.



Homogenous Charge Compression Ignition (HCCI)
Low temperature combustion, lean and/or diluted charge, controlled by combustion chemistry, highest efficiency, combustion control is challenging. Low emission levels due to low local temperatures and homogenous charge, easy premixing of fuel preferred.

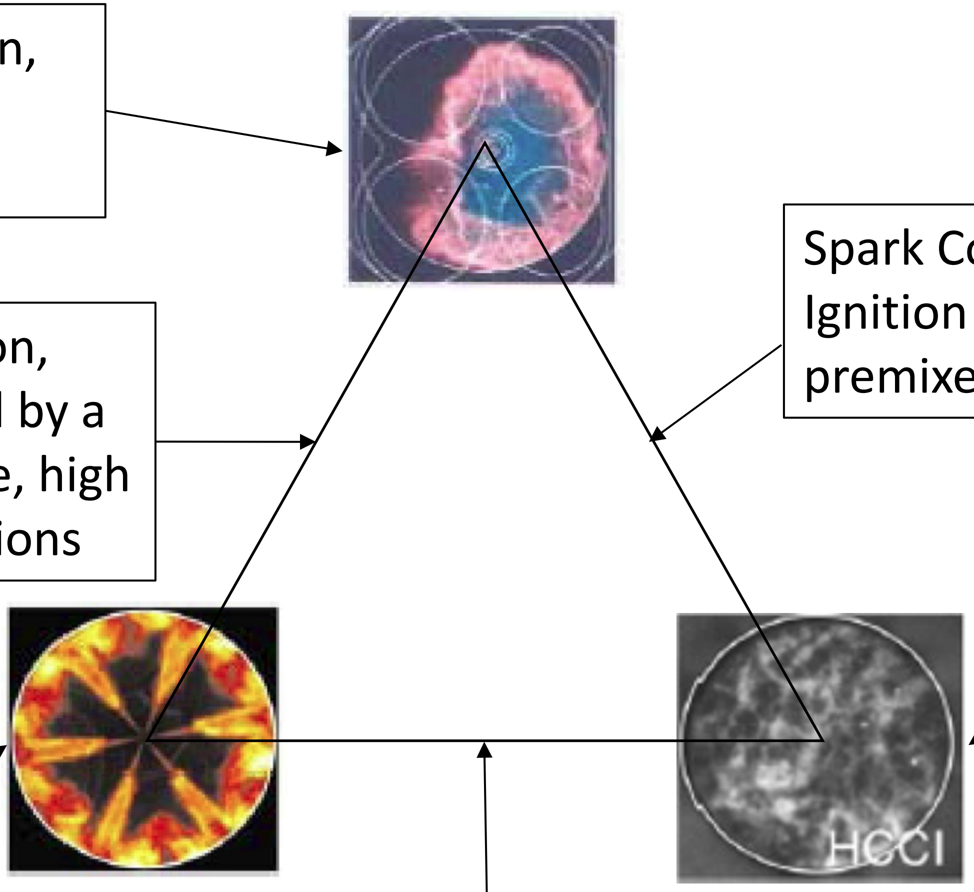
Reproduced from the slides of Gurpeet Singh DOE

Advanced combustion regimes

Spark ignited ultra lean burn, **Spark Gas (SG)** combustion with prechamber

Dual Fuel (DF) combustion, premixed flame is ignited by a ”diesel” pilot, lean charge, high efficiency, low NOx emssions

Low reactivity fuel compression ignition with a pilot fuel, **Gas diesel, (GD)**



Spark Controlled Compression Ignition (SpCCI), spark and premixed flame initializes HCCI

Reaction Controlled Compression Ignition (RCCI) with two different reactivity fuels for combustion control

Partially Premixed Compression Ignition (PPC, PCCI or PCI)

Methanol as a fuel for CI heavy duty and marine engines

Based on the physical and chemical properties of methanol, there are three main methodologies to use methanol in CI engine:

1. **Mixing controlled combustion:**
   Challenges due to low viscosity and low reactivity, requires a dedicated injector
   → a) CI methanol with improver
   b) CI with pilot fuel

2. **Premixed charge flame propagation:**
   Challenges are associated with premixed combustion and its high pressure rise rates, temperature drop due to high HoV
   → c) PFI with pilot
   d) Early DI with pilot

3. **HCCI type of combustion:**
   LTC type with high EGR, Reaction controlled with two fuels. Challenges with combustion control.
   → e) HCCI or PPC
   f) RCCI combustion

Methanol as a fuel for CI heavy duty and marine engines

Based on the physical and chemical properties of methanol, there are three main methodologies to use methanol in CI engine:

Our present focus

1 **Mixing controlled combustion:**
Challenges due to low viscosity and low reactivity, requires a dedicated injection system

a) CI methanol with improver
b) CI with pilot fuel ignition

2 **Premixed charge flame propagation:**
Challenges are associated with premixed combustion and its high pressure rise rates, temperature drop due to high HoV

c) PFI with pilot ignition
d) Early DI with pilot ignition
e) Spark ignited

3 **HCCI type of combustion:**
LTC type with high EGR, Reaction controlled with two fuels. Challenges with combustion control.

e) HCCI or PPC
f) RCCI combustion

Methanol - marine engine perspective

- Negligible PM, low NO_x and no SO_x compared with MGO
- Stena Line retrofit, AP Møller-Maersk 2021

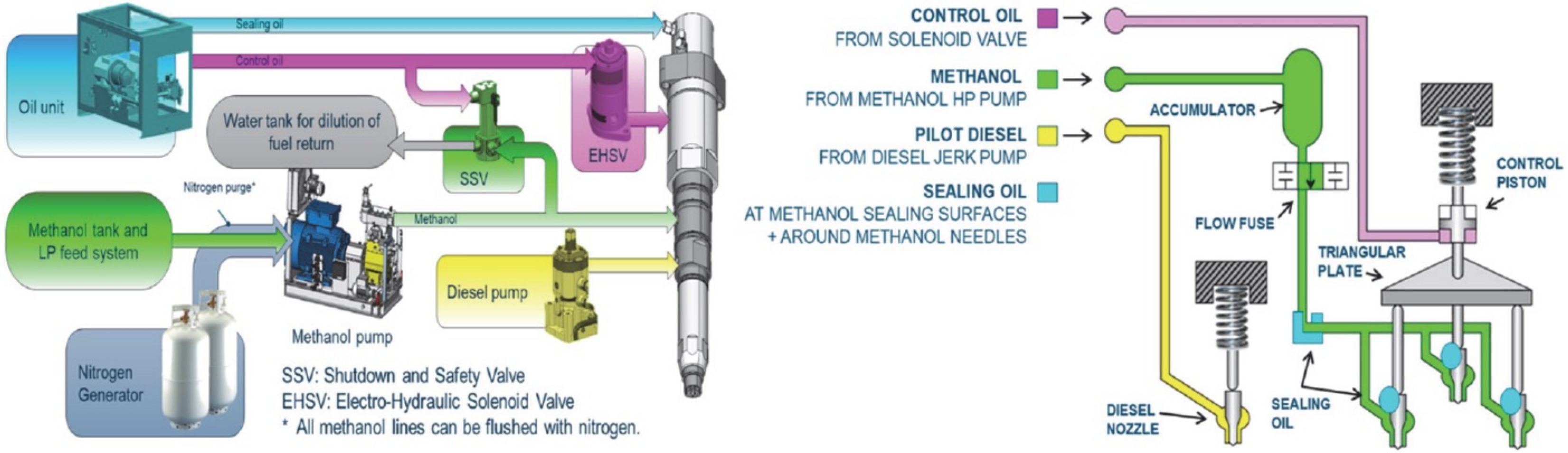


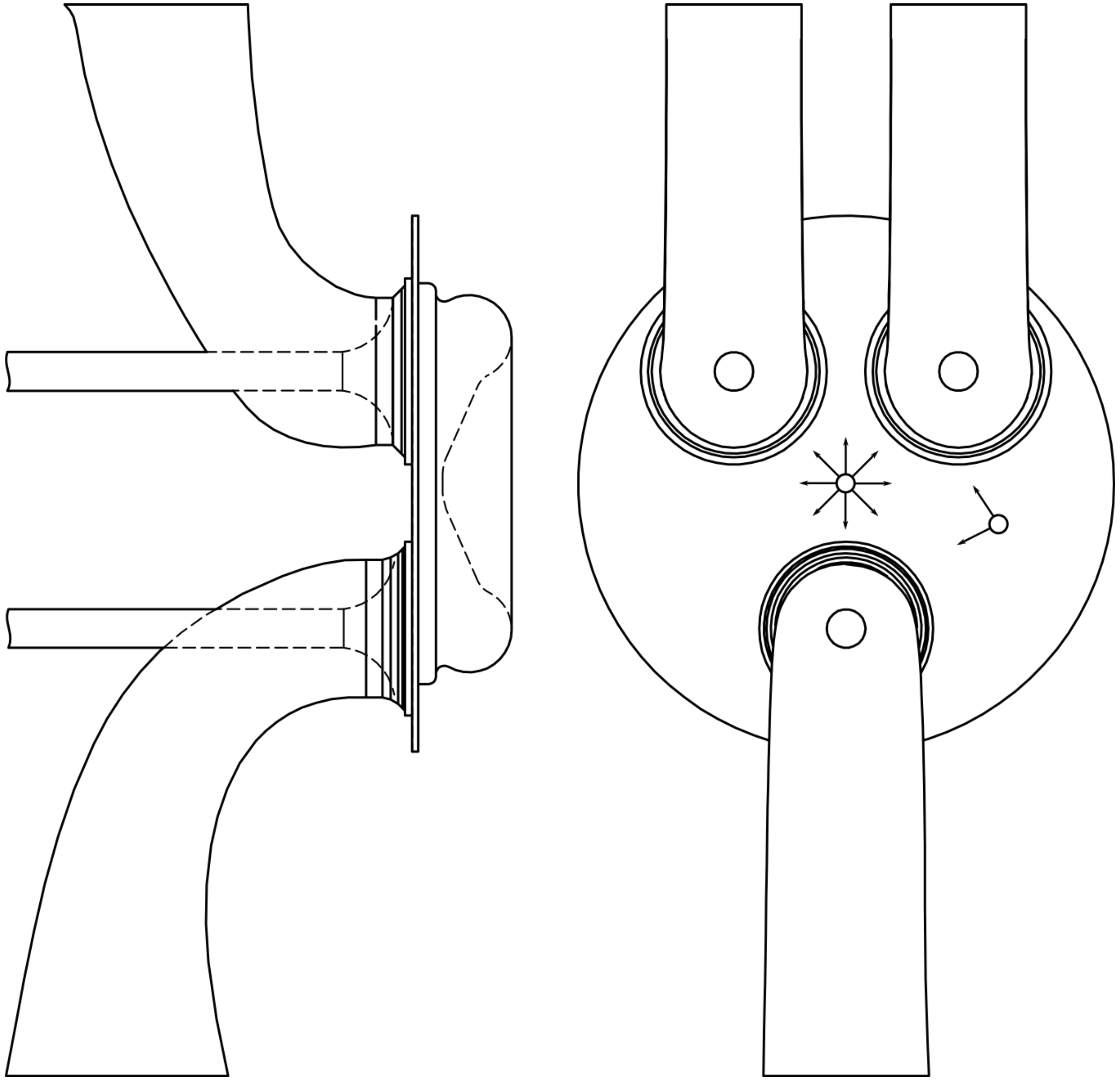
Figure 1: ZA40S methanol system layout and methanol injector working principle [1]

1. Delneri, D.: "Combustion System Optimization for Alternative Fuels", 17th Conference "The Working Process of the Internal Combustion Engine", Graz 2019
2. Stojcevski Toni, Jay Dave, Vincenzi Luca, "Operational experience of world's first methanol engine in a ferry installation", CIMAC congress Helsinki 2016, Paper 99

Methanol combustion modelling – engineering approach

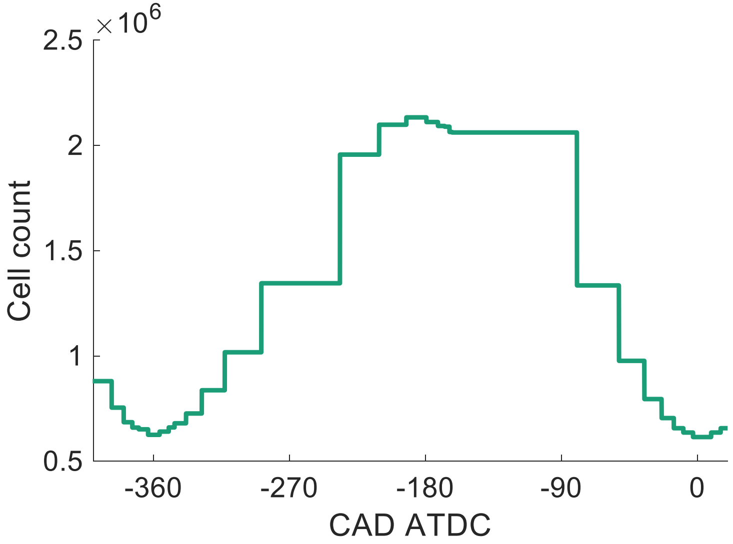
Flow and turbulence modelling

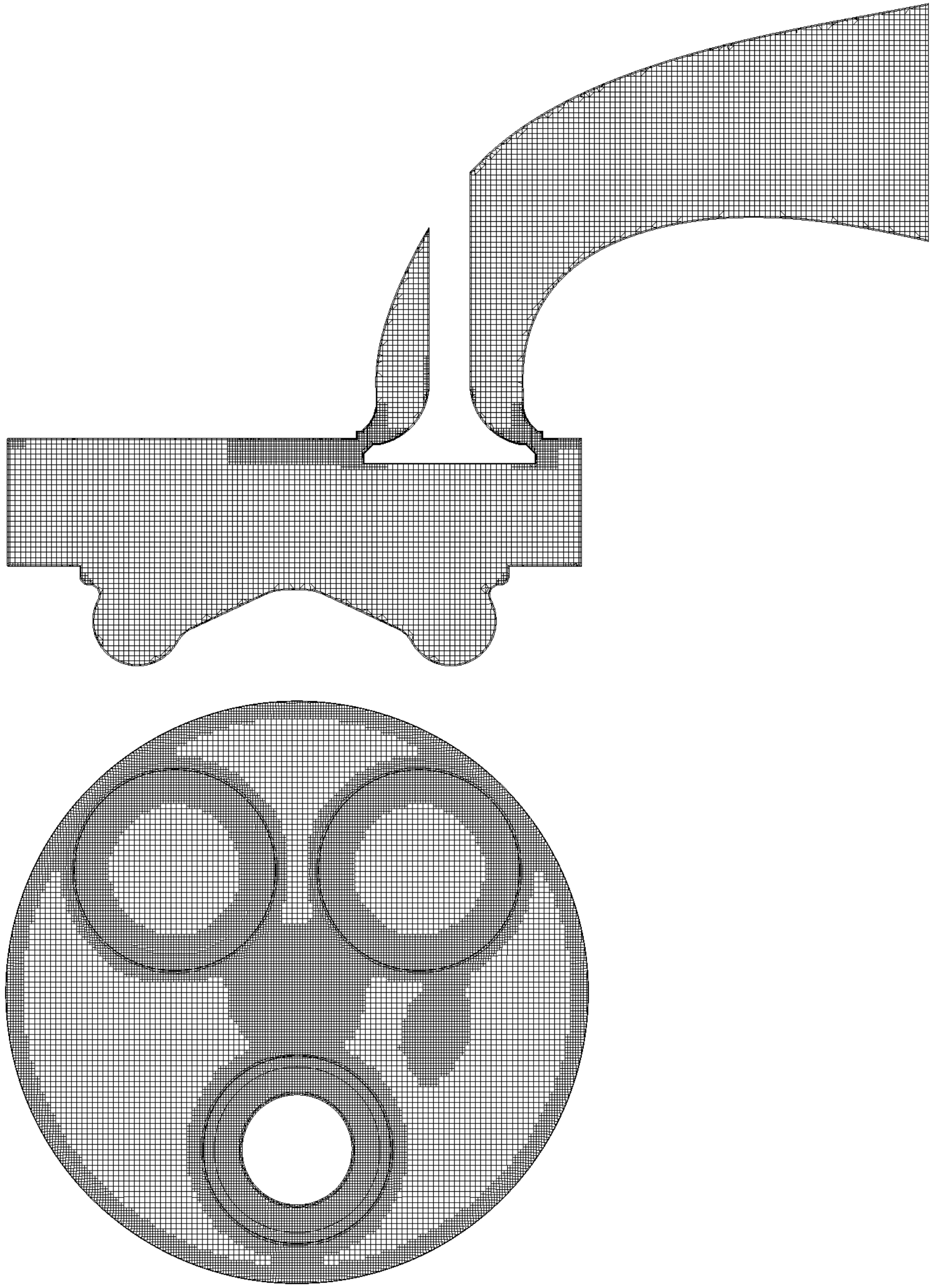
- **STARCCM+ InCylinder**
- **RANS turbulent approach, *k–ε* turbulence modeling**
- **Transport equations solved with so called Pressure-Implicit with Splitting of Operators (PISO) algorithm**
- **Second order upwind spatial discretization**



Flow and turbulence computational mesh

- Cells: 615 000 to 2 100 000
- Base cell size 1 mm
- Refinements





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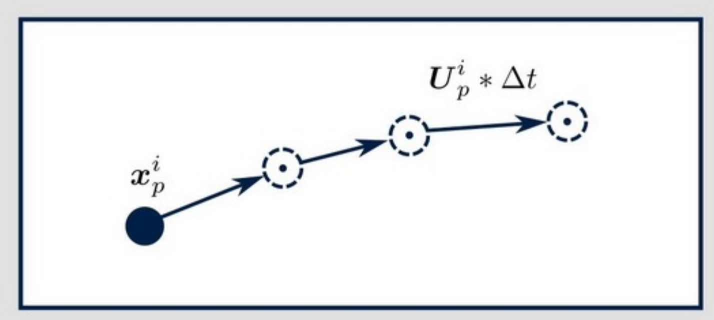
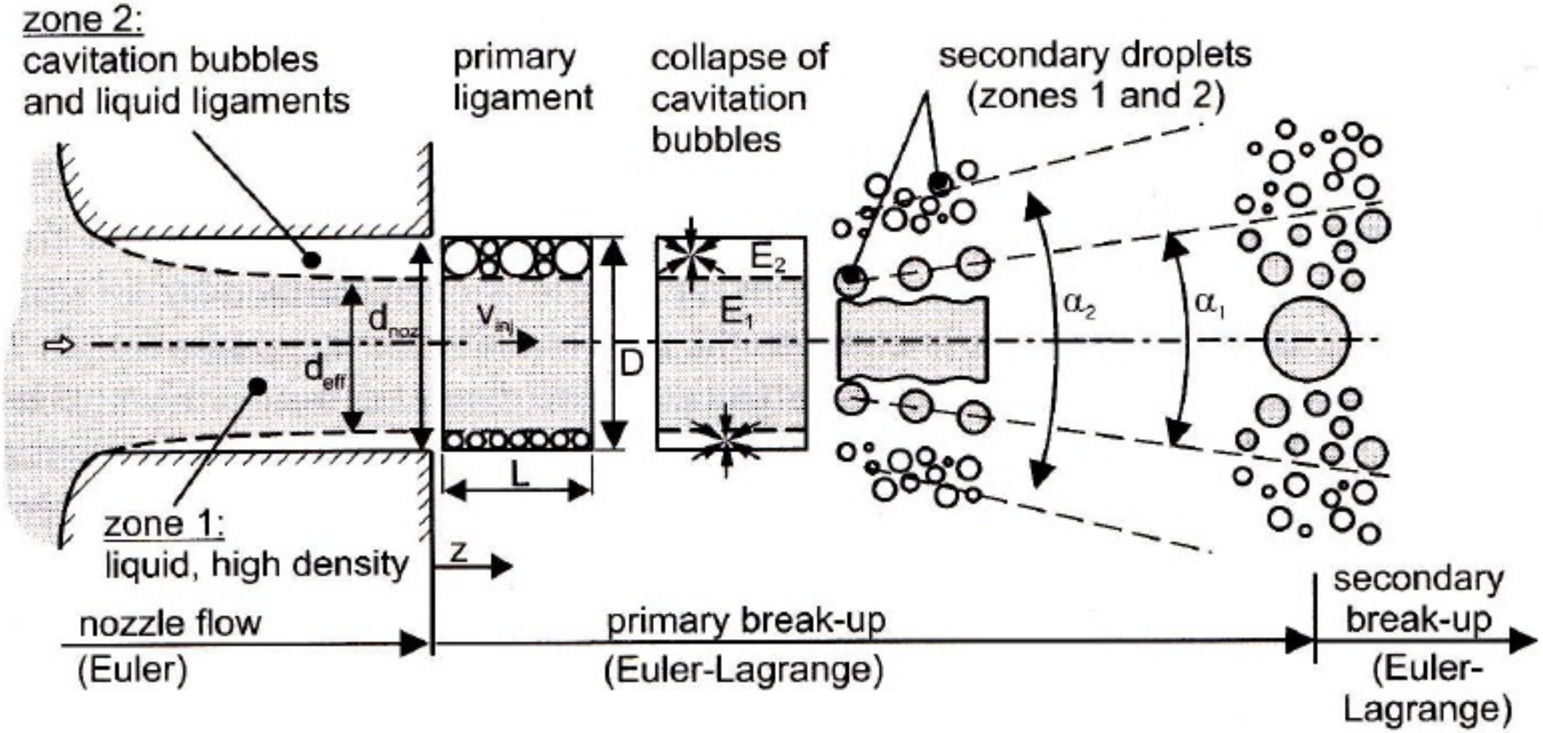
Lagrangian Particle Tracking



Droplet “parcels” are tracked (followed) in Lagrangian way, the coordination follows the parcels.

Droplets are thus not part of the Eulerian fluid domain, but they do interact with the fluid via momentum, energy and mass transfer.



G.Stiesch: Modeling Engine Spray and Combustion Processes, Springer 2003

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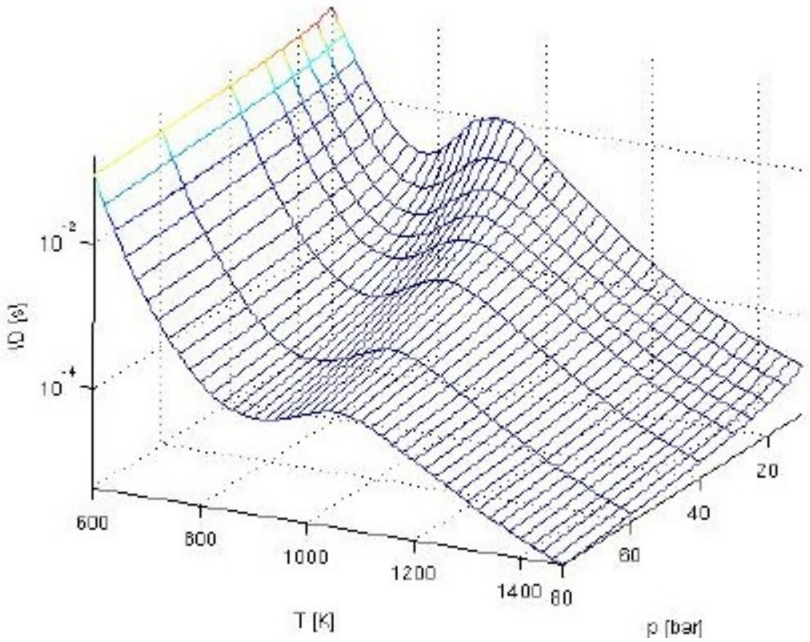
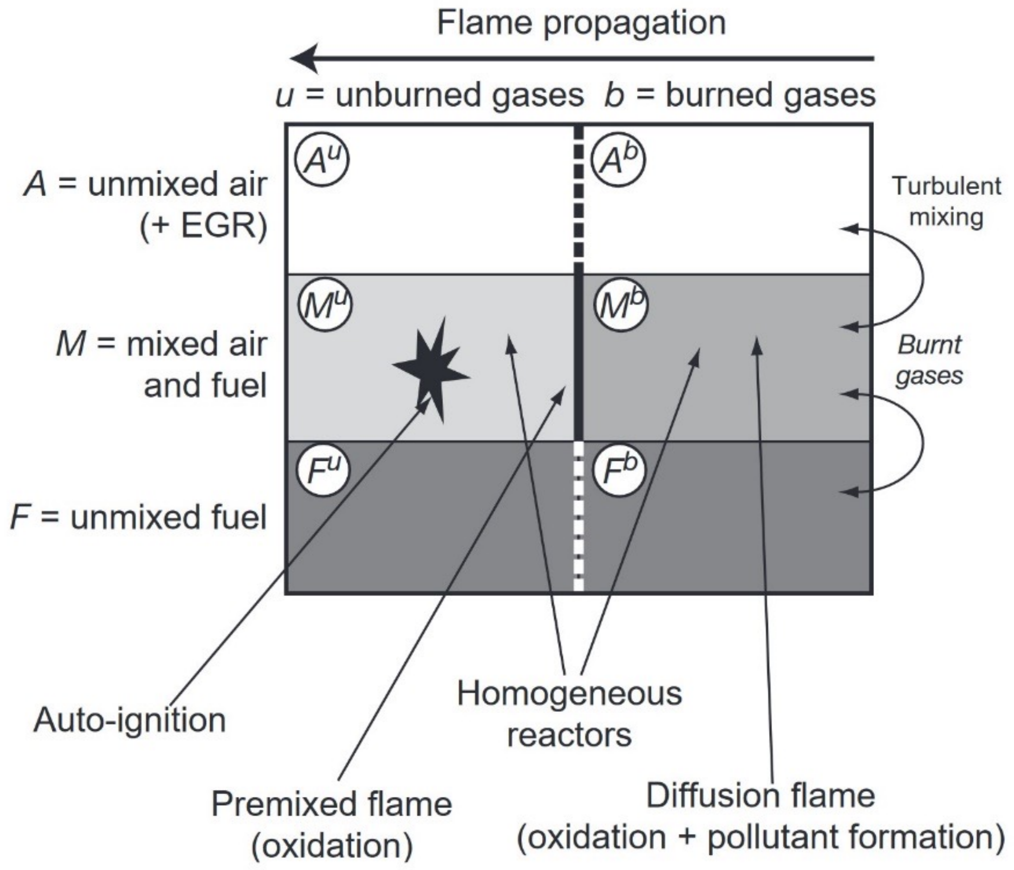
Ignition and Combustion

Pre-calculated ignition table (TKI model) based on chemical kinetics from Reduced PoliMi mechanism, by Frassoldati et al. (2015)



Example of TKI tabulation by Reinhard Tatschl and Peter Priesching AVL List GmbH

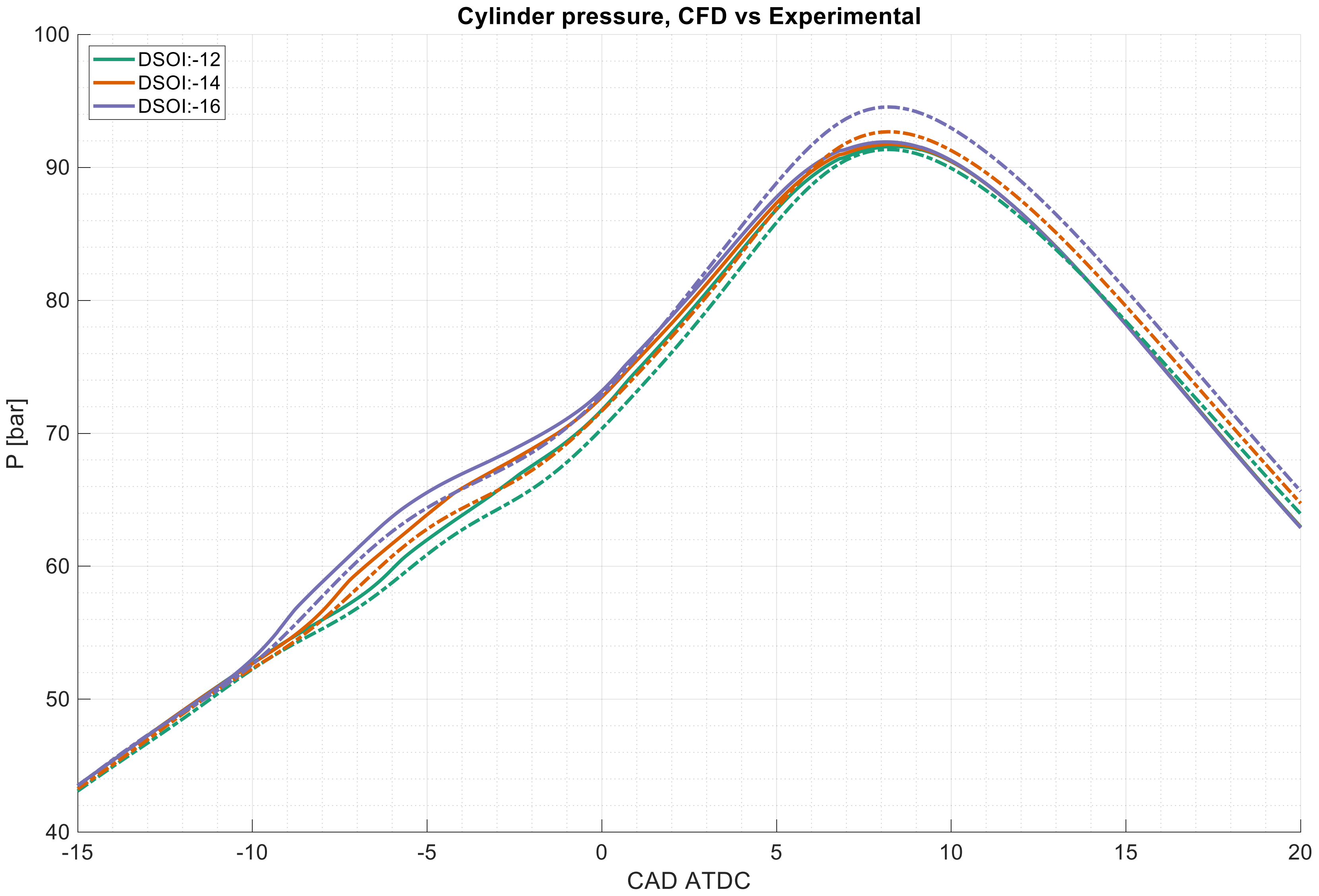


Extended coherent flame modelling (ECFM-3Z), visualization from Colin and Benkenida (2004)

Methanol combustion modelling – engineering approach

In-cylinder pressure

Accurate pressure and piston position measurement via crank angle encoder is the key to good combustion analysis



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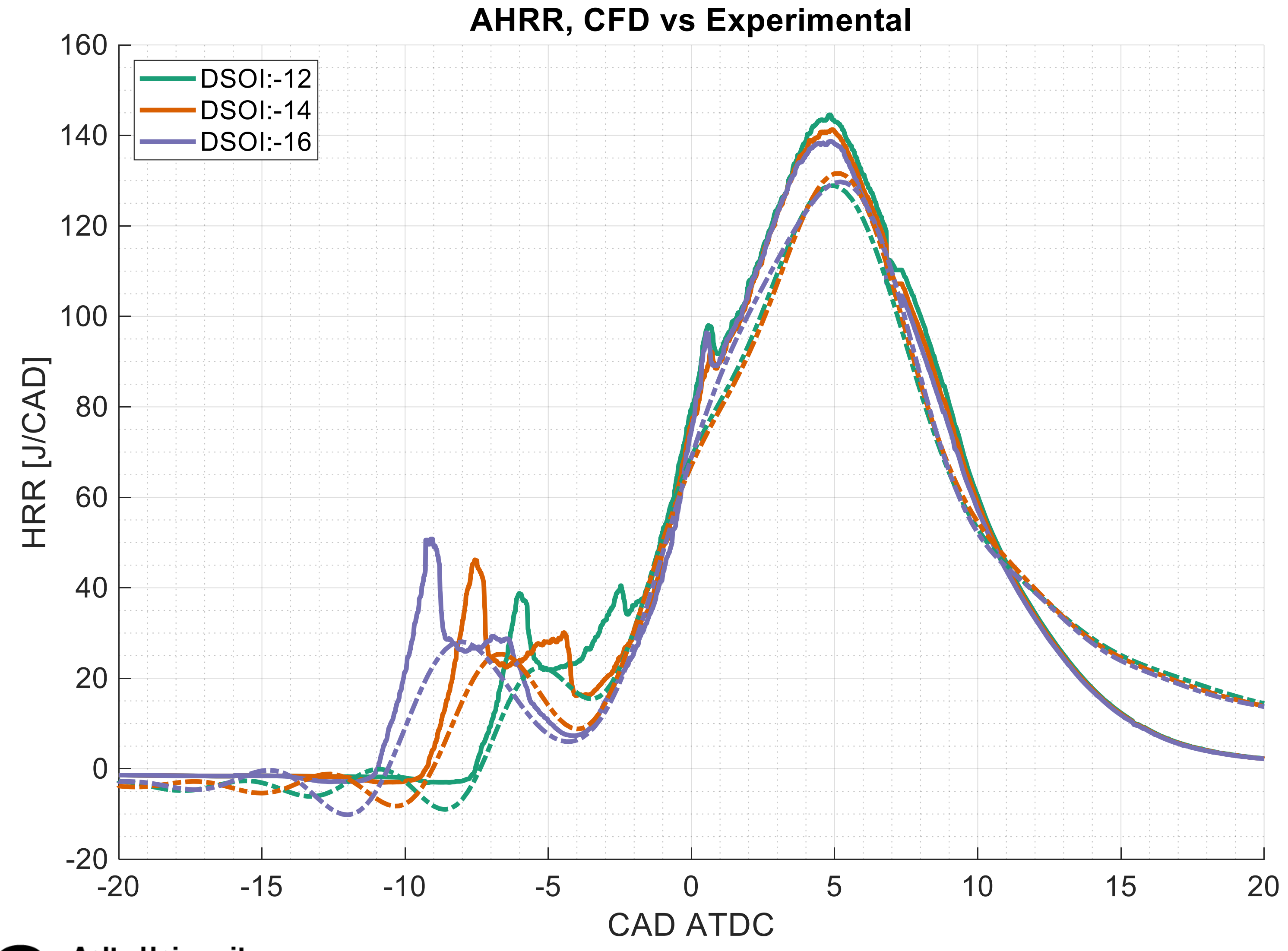
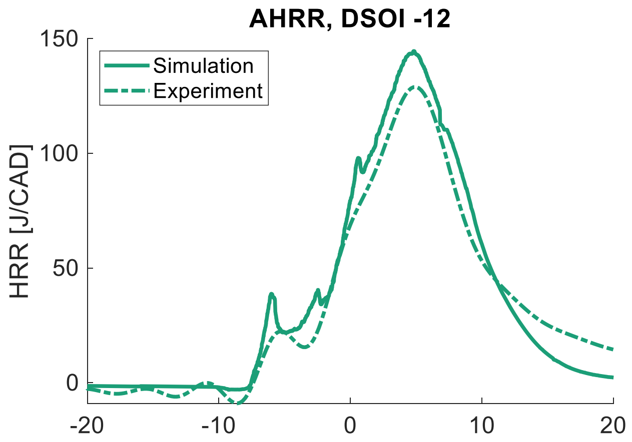
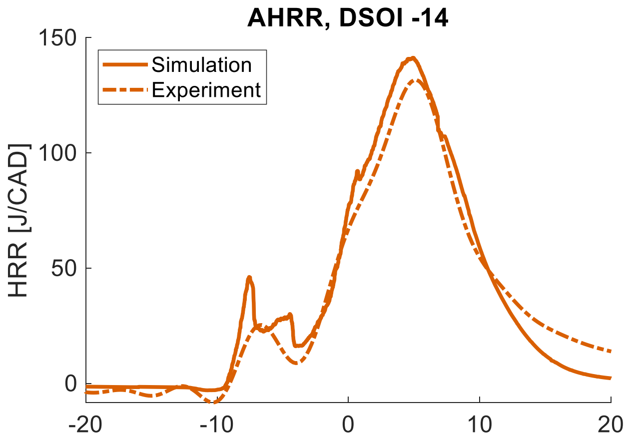
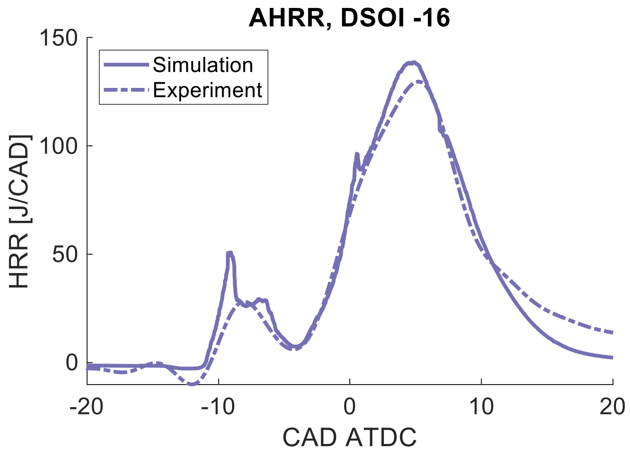
Heat Release









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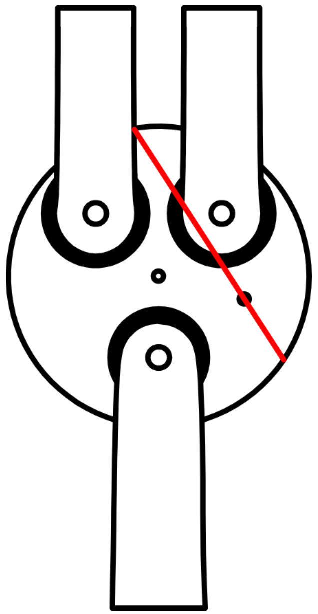
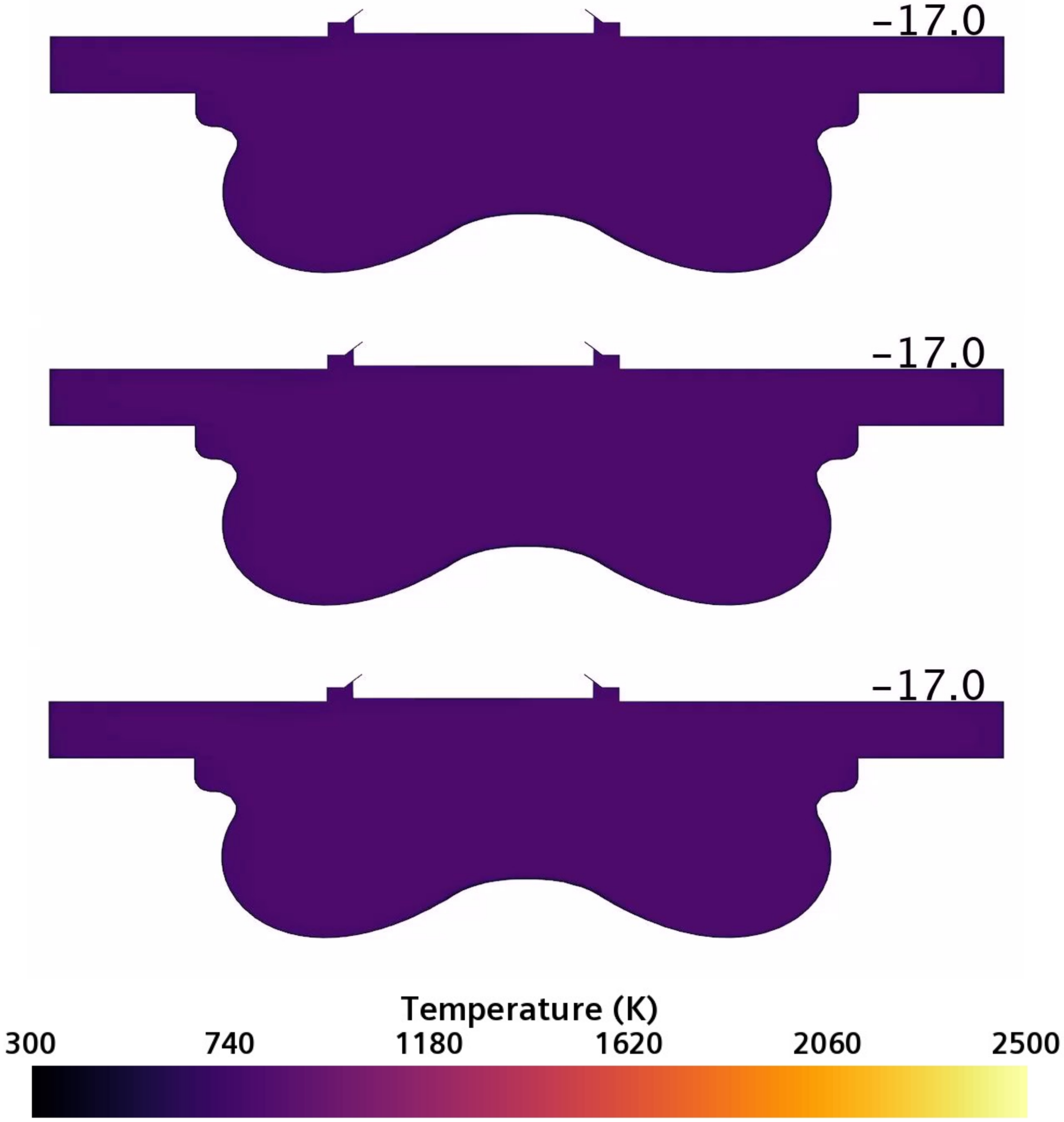
Pilot Temperature

Top to Bottom

- DSOI –16
- DSOI –14
- DSOI –12

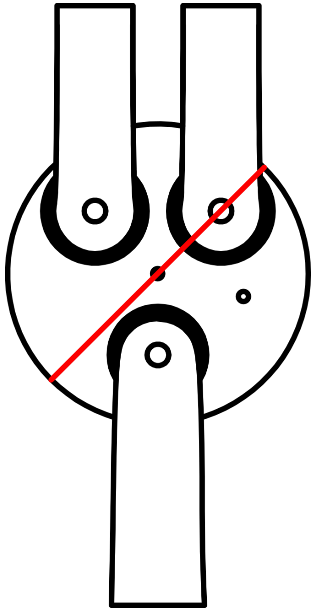


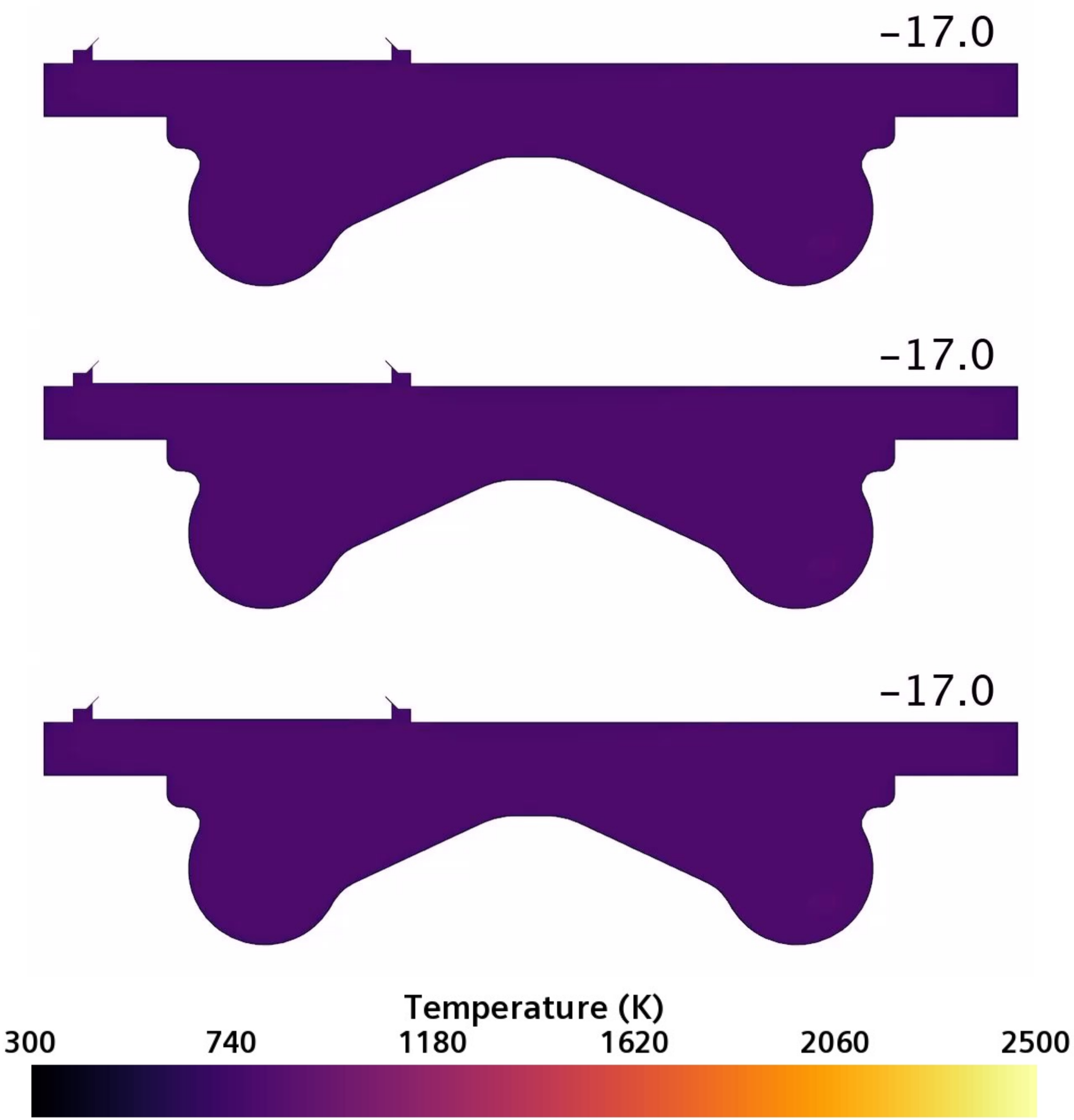


Methanol Temperature

Top to Bottom

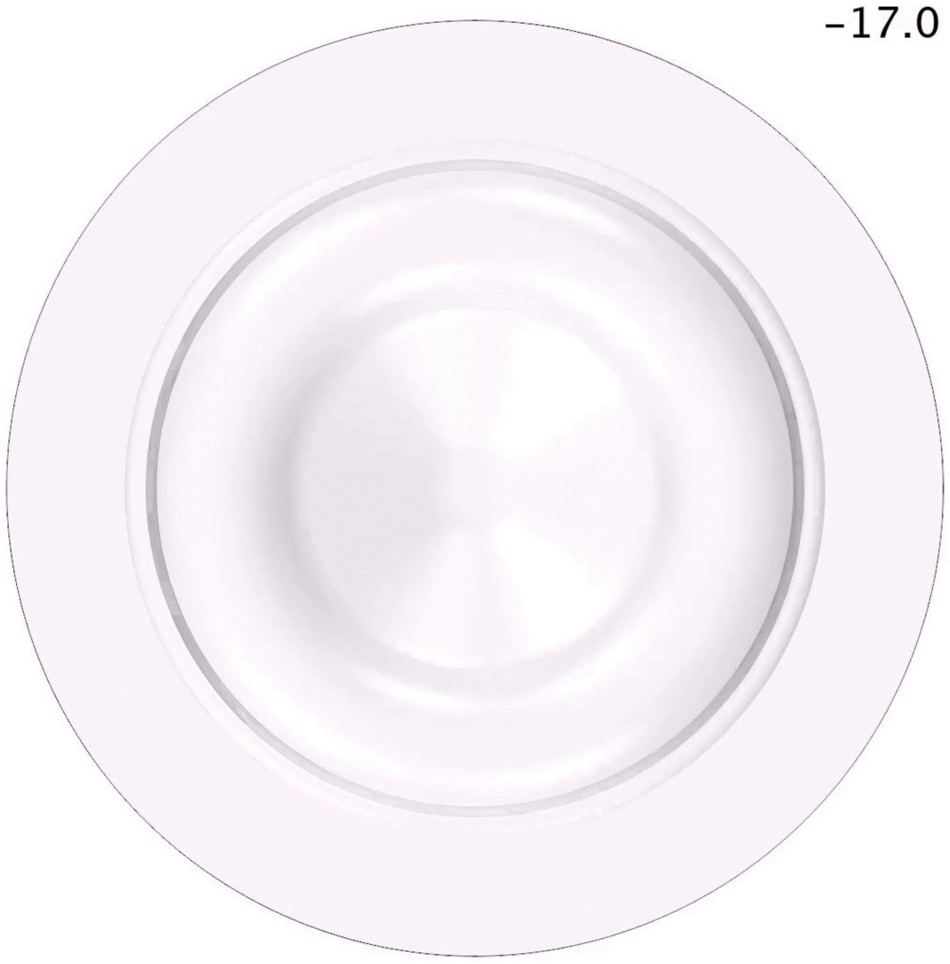
- DSOI −16
- DSOI −14
- DSOI −12





Fuel Spray

Diesel droplets
Diesel λ = 1 isosurface
Methanol droplets
Methanol λ = 1 isosurface



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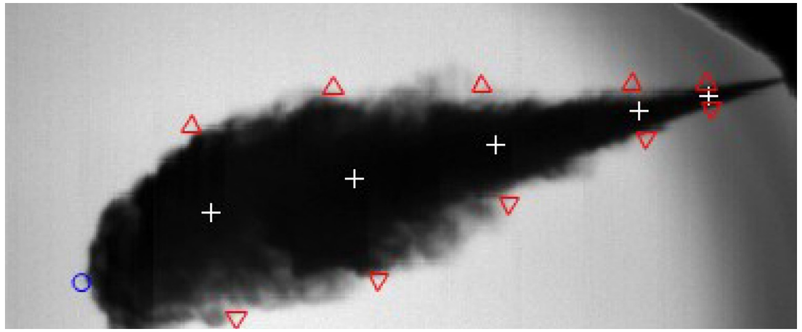
Sub-models used in the simulation

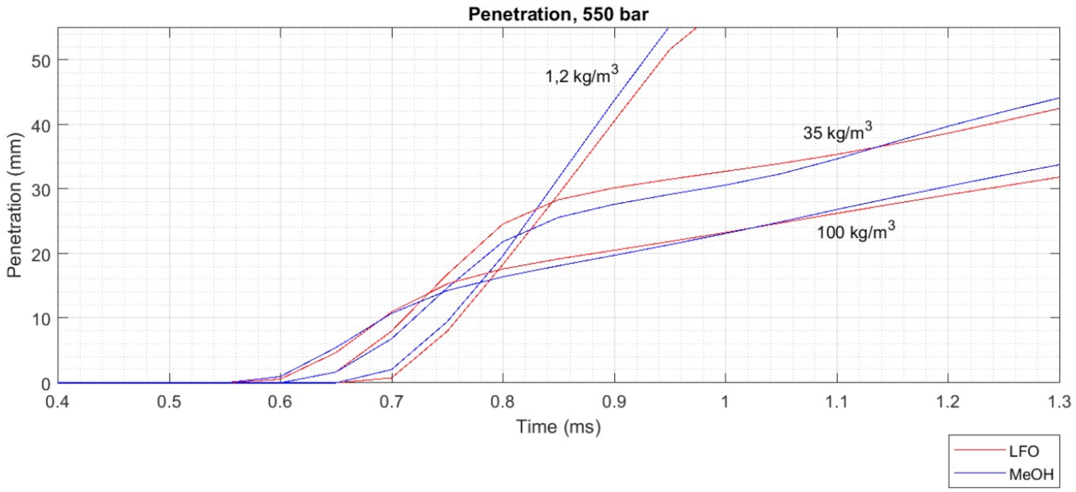
- Solution Interpolation and Remeshing
- PISO Unsteady
- Two-Layer All y+ Wall Treatment
- Wall Distance
- Realizable K-Epsilon Two-Layer
- K-Epsilon Turbulence
- Reynolds-Averaged Navier-Stokes
- Ideal Gas
- Cell Quality Remediation
- Multi-Component Gas

- Lagrangian Multiphase
- Huh Atomization
- Reitz-Diwakar Breakup
- Two-Way Coupling
- Droplet Evaporation
- Bai-Gosman Wall Impingement
- Turbulent Dispersion
- Constant Density
- Drag Force
- Species
- Multi-Component Liquid
- Spherical Particles
- Pressure Gradient Force

- ECFM TKI Auto-Ignition
- Auto-Ignition
- Conditional Enthalpy
- Flame Surface Density Transport
- ECFM-3Z Post Flame Scheme
- ECFM-3Z
- In-Cylinder Combustion
- Reacting
- Adaptive Time-Step

Spray studies: chamber experiments



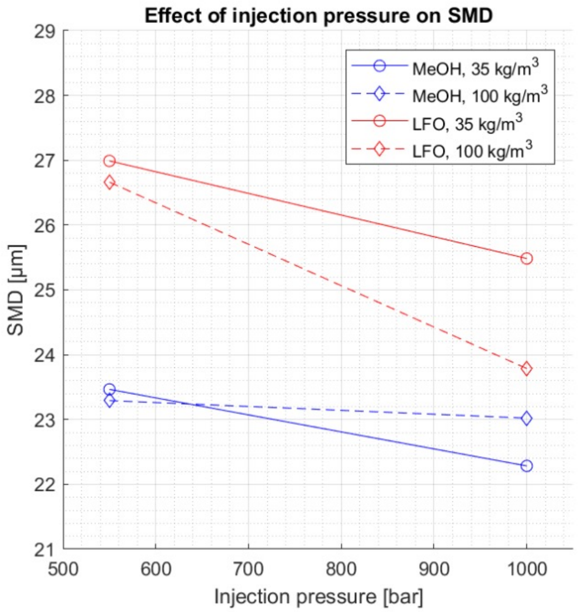


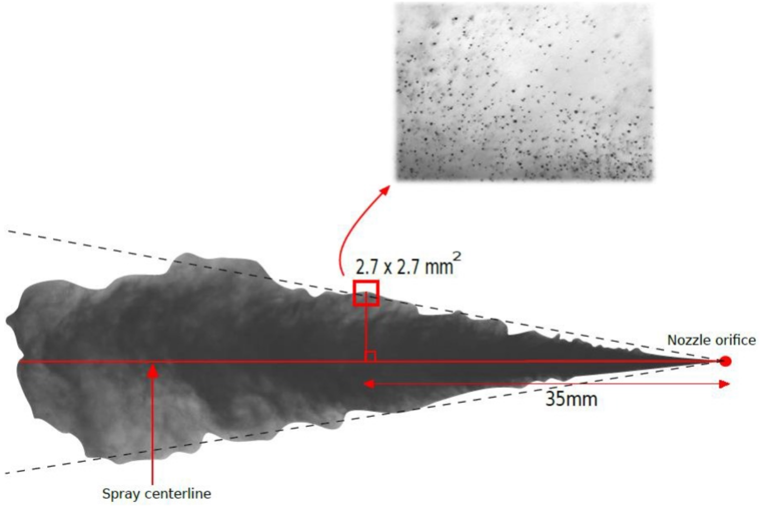
Room temperature non-evaporative measurements

- **Gas density 1 – 100 kg/m3**
- **Injection pressure 500 -1000 bar**

Conclusions:

- **Relatively similar spray penetration and opening angle compared to LFO**
- **Methanol has smaller droplet sizes**





A. Ainsalo, R. Sallinen, O. Kaario, and M. Larmi, Optical investigation of spray characteristics for light fuel oil, kerosene, hexane, methanol, and propane, **Atomization and Sprays, Vol. 29 (6), 2019**

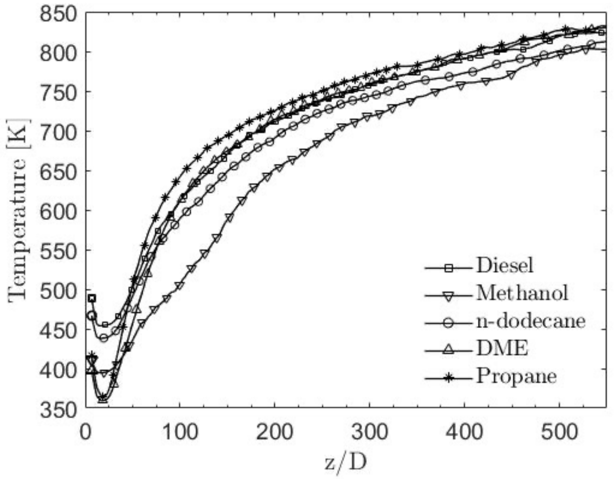
Spray studies: simulations

Large-eddy simulation (LES)

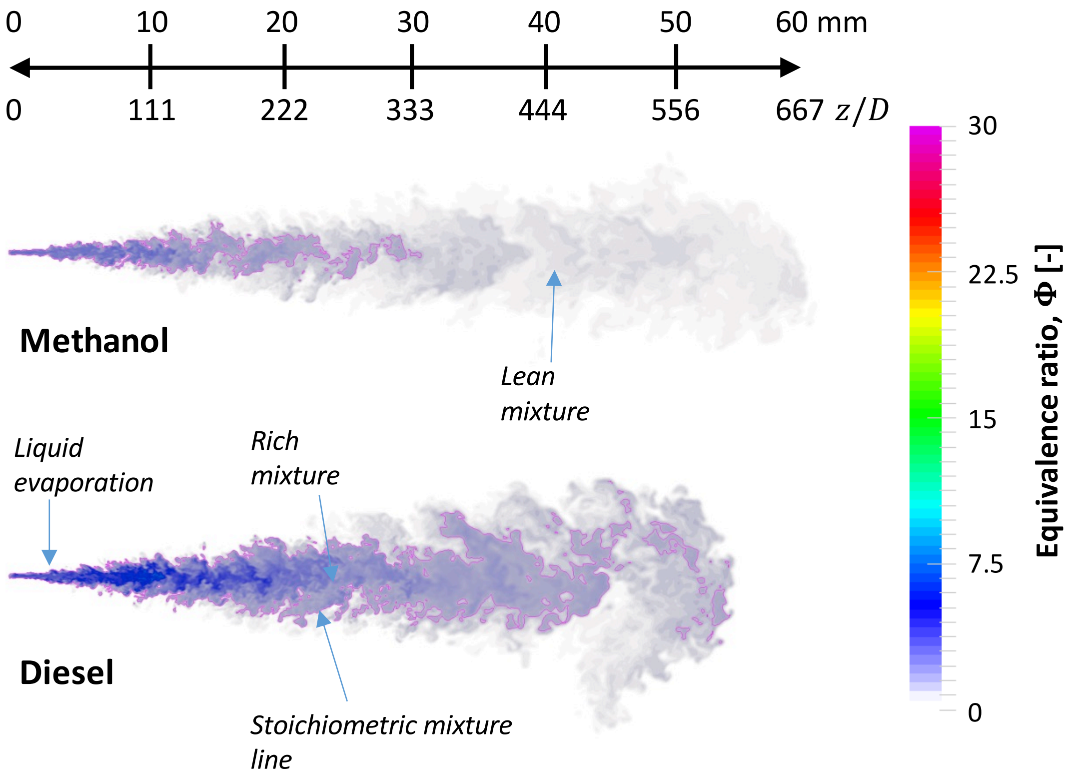
- Non-reacting cases simulated to **understand the fuel spray mixing and evaporation**
- Validation for the Engine Combustion Network (ECN) Spray A for Diesel (n-dodecane)

Conclusions

- Lower temperature within the spray due to high latent heat of methanol
- Spray penetration in accordance to experiments, i.e. no big differences between the fuels



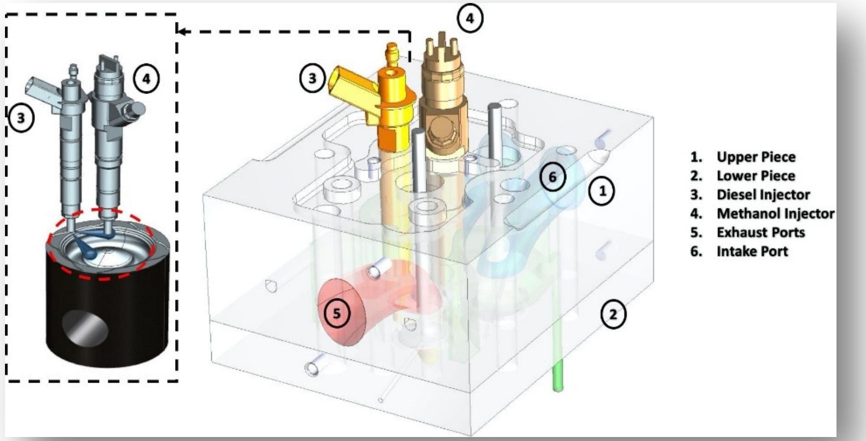
Spray centerline temperature showing 50 -100K lower temperature for methanol

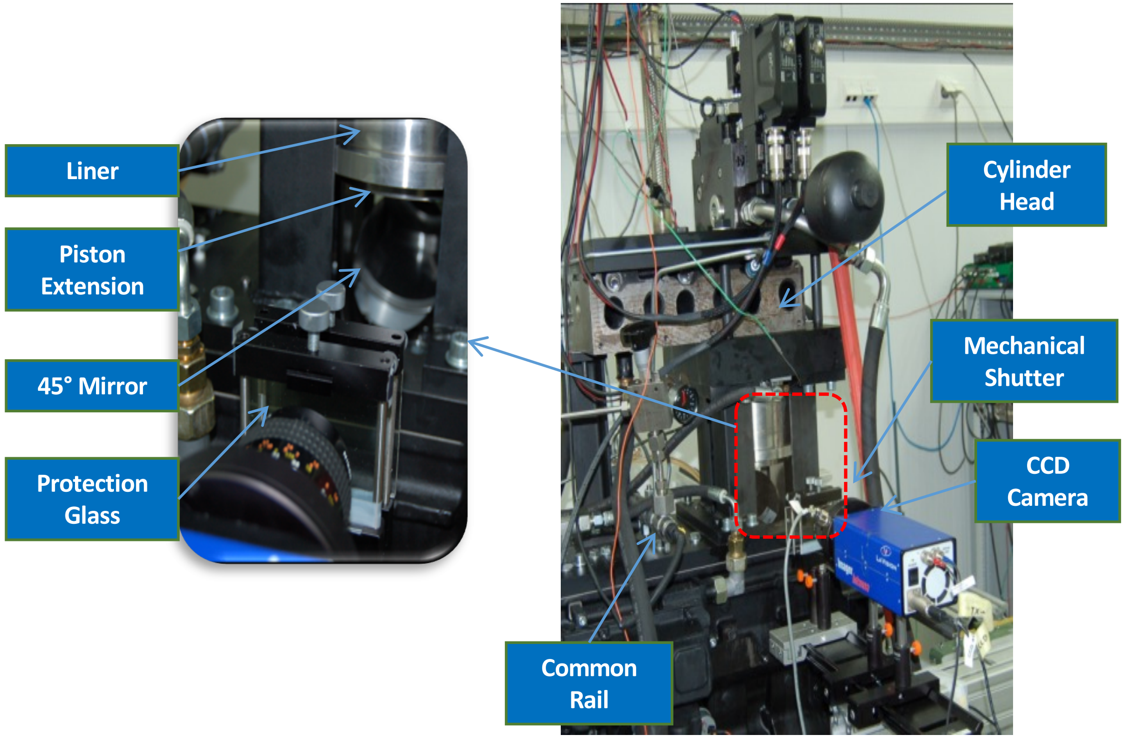


O. Kaario, V. Vuorinen, H. Kahila, H. Im, and M. Larmi, The effect of fuel on high velocity evaporating fuel sprays: Large-Eddy Simulation of Spray A with various fuels, **Int. Journal of Engine Research, Vol. 21(1), 2020**

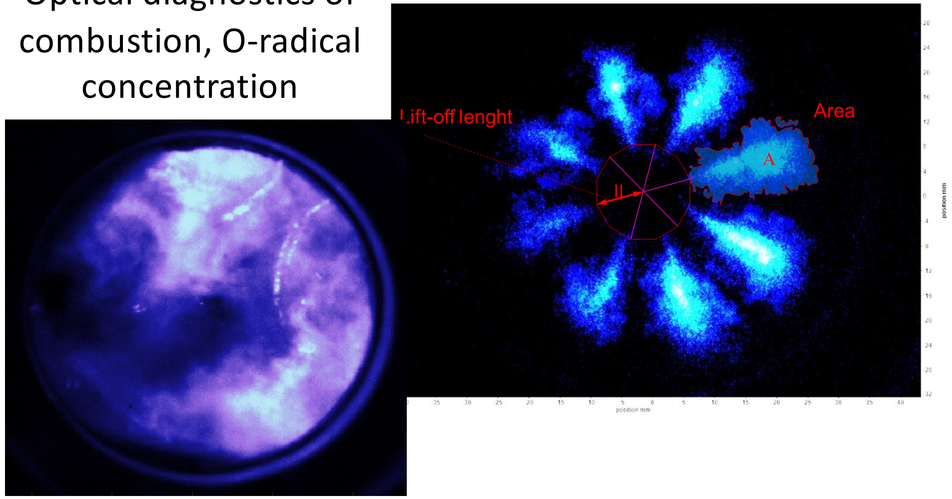
Methanol-to-Power

High efficiency CI combustion possible with new dual fuel technologies





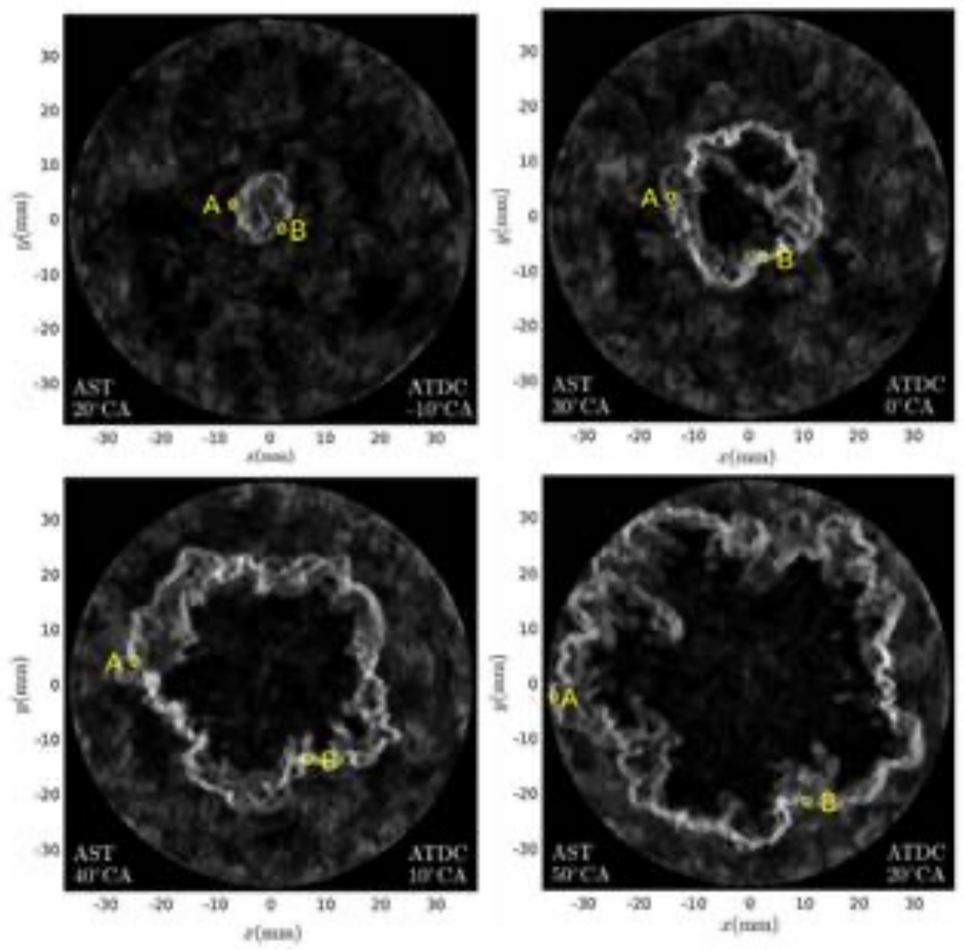
Optical diagnostics of combustion, O-radical concentration



Dong, Y., Kaario, O., Hassan, G., Ranta, O., Larmi, M. and Johansson, B., 2020. **High-pressure direct injection of methanol and pilot diesel: A non-premixed dual-fuel engine concept**. *Fuel*, 277, p.117932, DOI: https://doi.org/10.1016/j.fuel.2020.117932

Methanol-to-Power

SI premixed turbulent flame propagation combustion could still be a feasible option



Ghaderi Masouleh, Mahdi: "Numerical modeling of ignition and flame propagation in gas engines ", Aalto University 2019

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Concluding remarks

1. High energy conversion efficiencies, minimal local emissions, together with easy storage, make methanol an interesting future energy carrier option, especially for maritime transport
2. (**XtP**): MeOH dual-fuel combustion concepts has been successfully demonstrated, both experimentally and numerically
3. Developments in production and combustion technologies can bring further improvement in overall environmental performance of MeOH as a transport fuel

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