
Are Combustion Engines Entirely Bad?



- Electric
- Battery
- Renewable
- Carbon Free
- Zero-emission

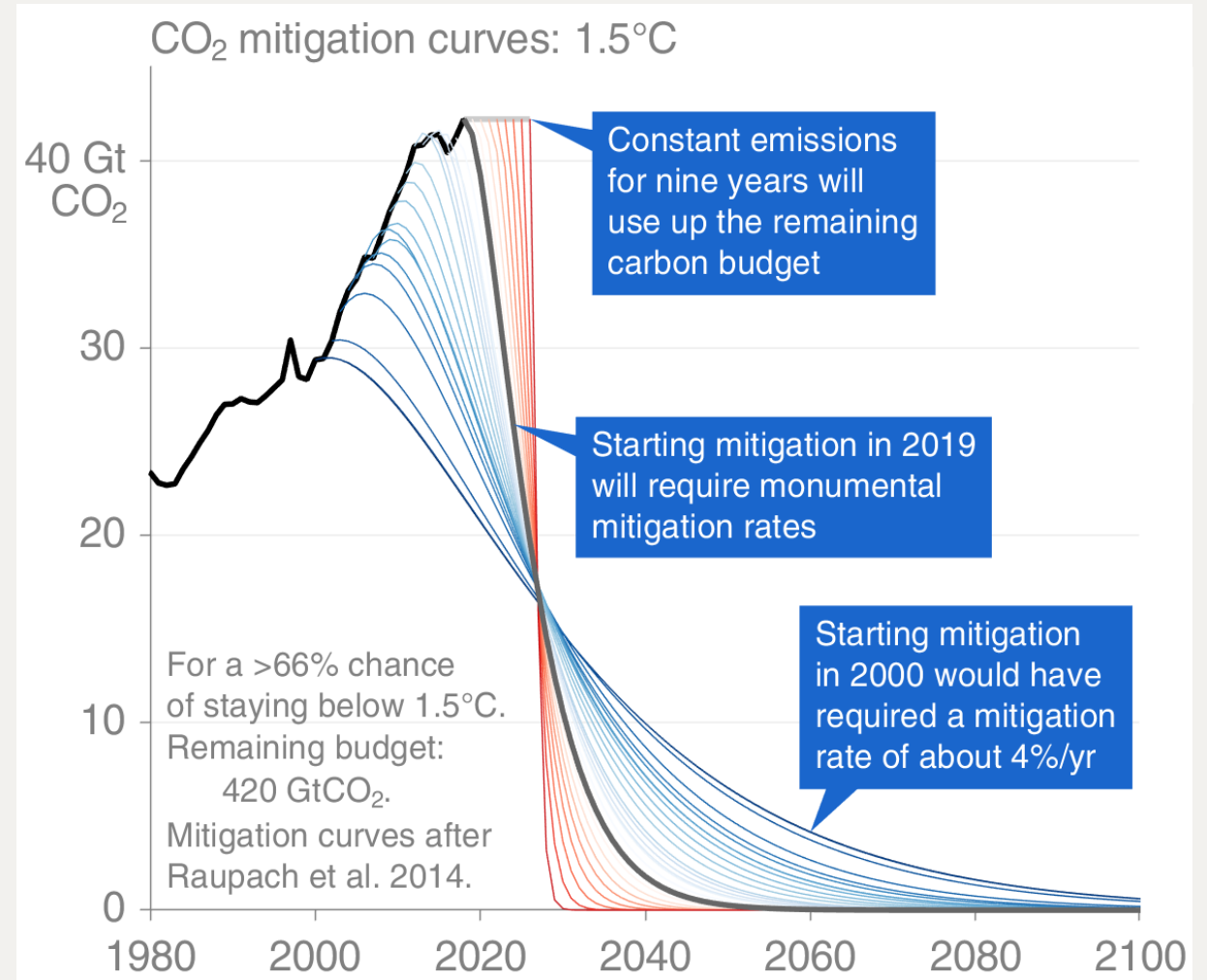


- Combustion
- Diesel
- Conventional
- Engine
- Fuel

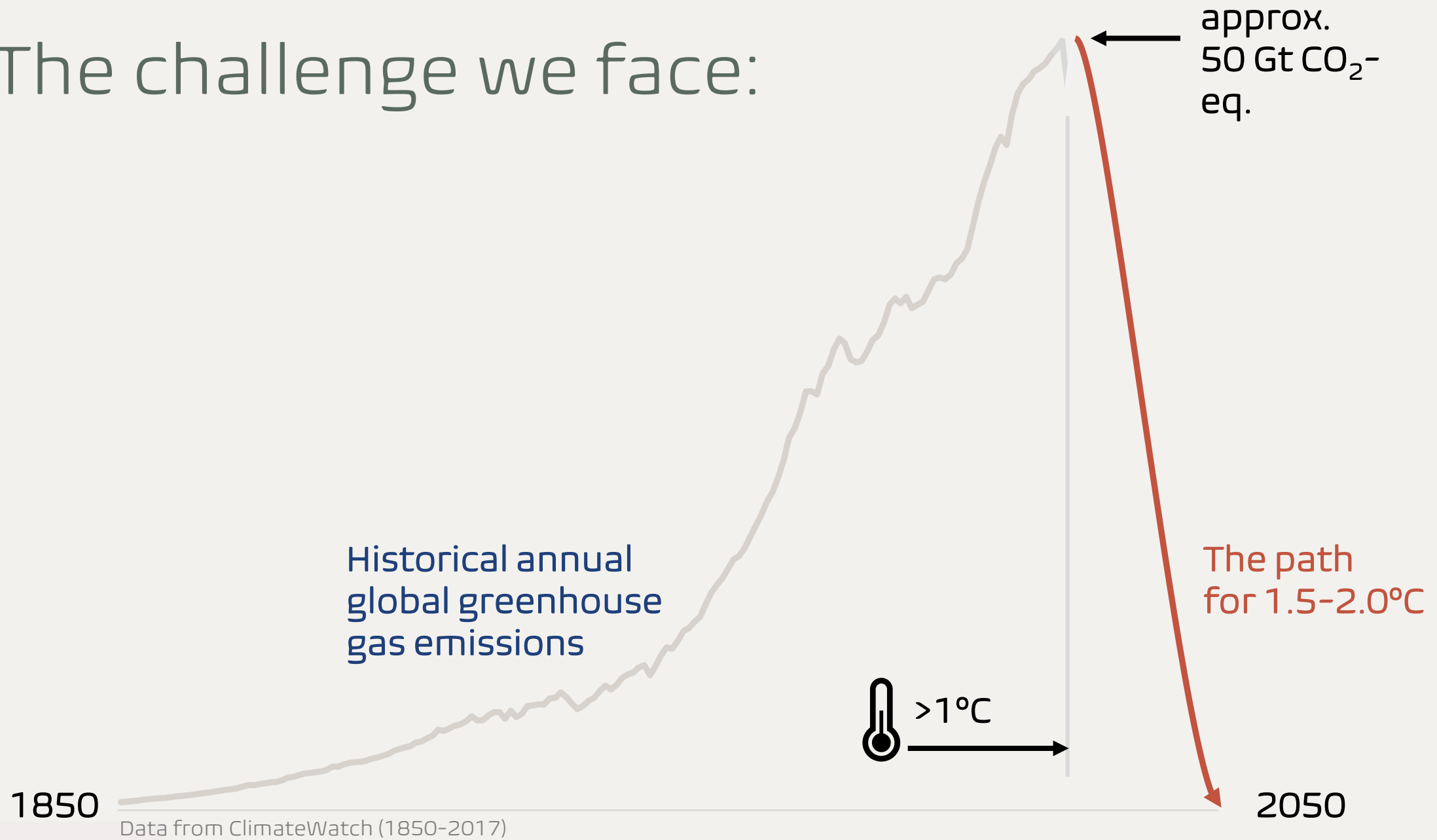


CO2 Budget

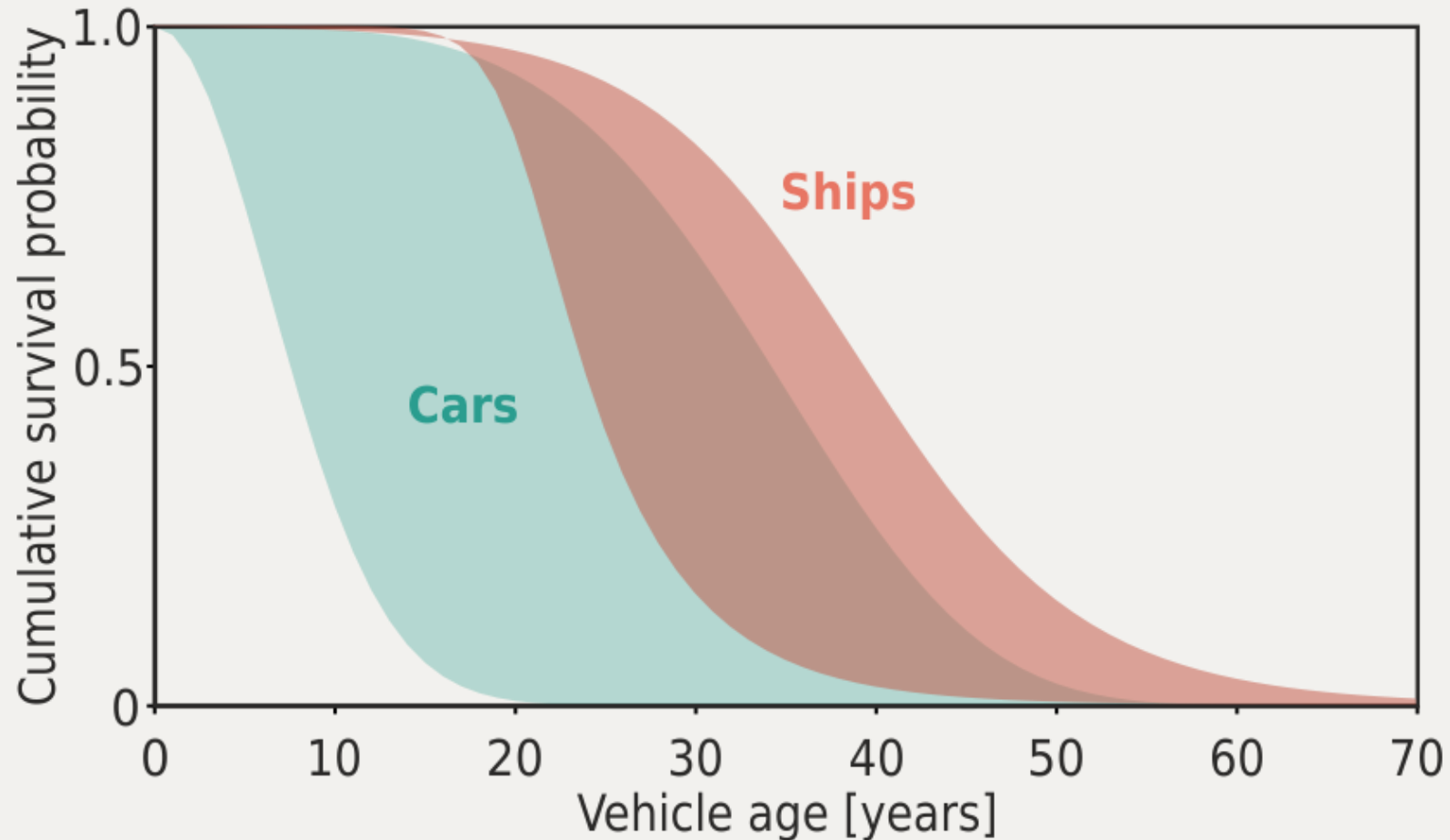
- After a certain amount of emitted CO₂, we cannot reverse the average temperature increase.
- Time is running out!



The challenge we face:



If we have 30 years, why is immediate action imperative?



Data for cars from Held et al. (2021): *European Transport Research Review*, vol. 13, art. 9

Data for ships from Held et al. (2021): *7th Internat. Symposium on Ship Operations, Management, & Economics*

Data for aircraft from Dray (2013): *Journal of Air Transport Management*, vol. 28, pp. 62-69

One Fast Solution

Global Lockdown

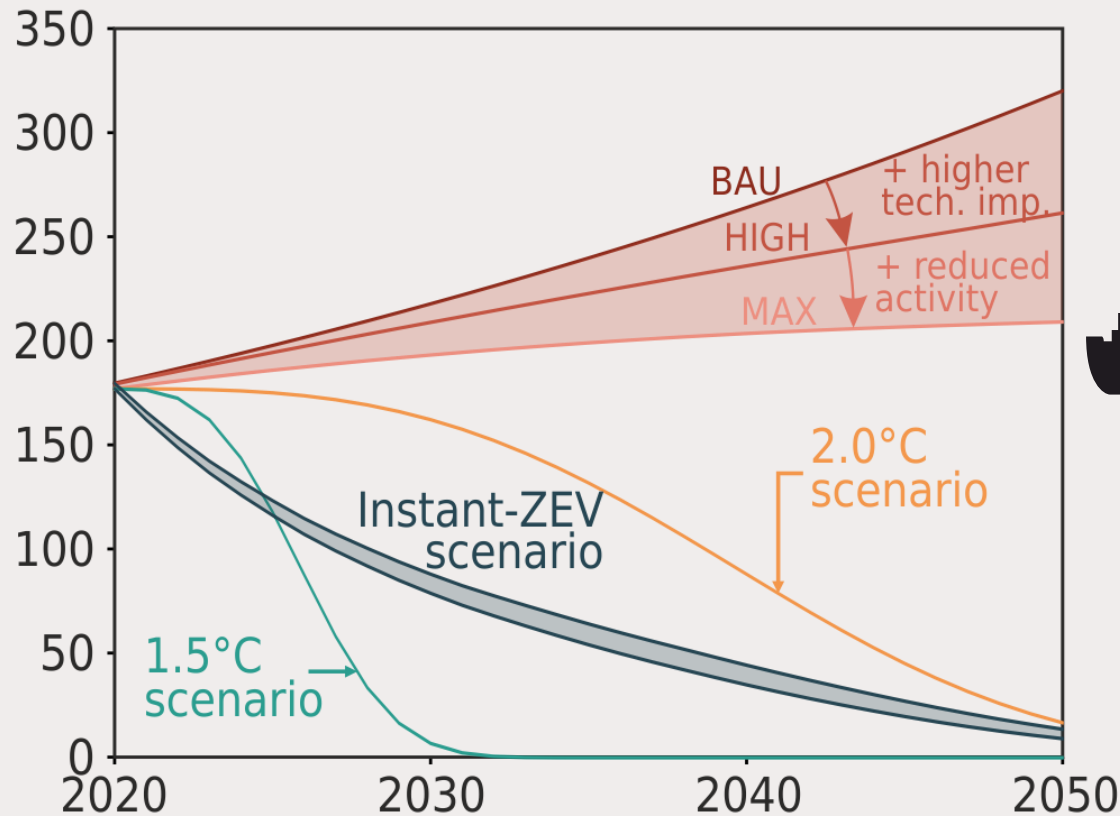


Parallel Parking Skills Level EVERGREEN

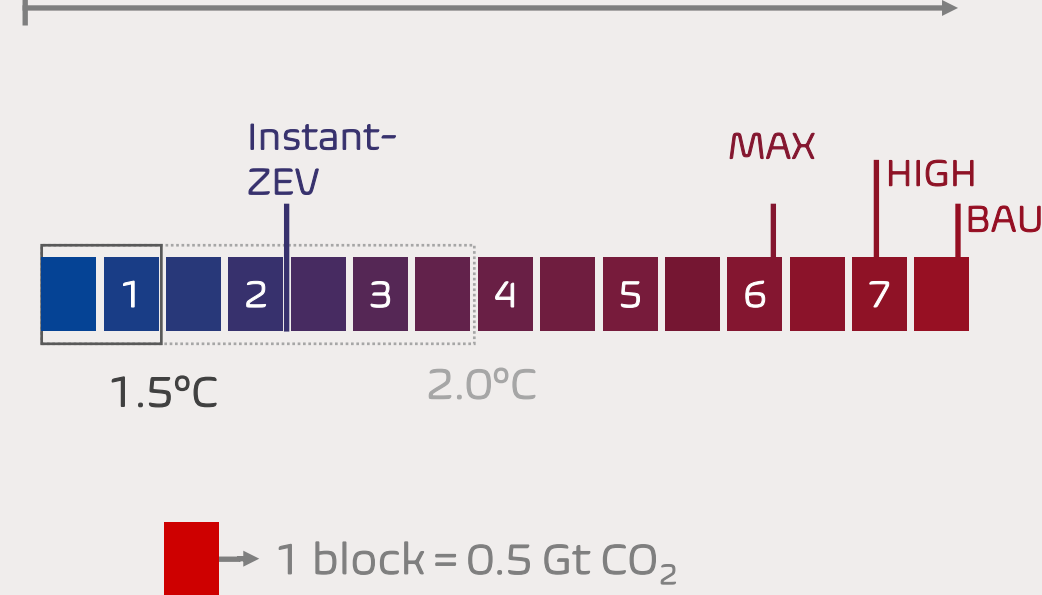


Emission trajectories for the European shipping sector...

CO₂ emission scenarios [Mt p.a.]



Cumulative emissions 2021-2050 in Gt CO₂



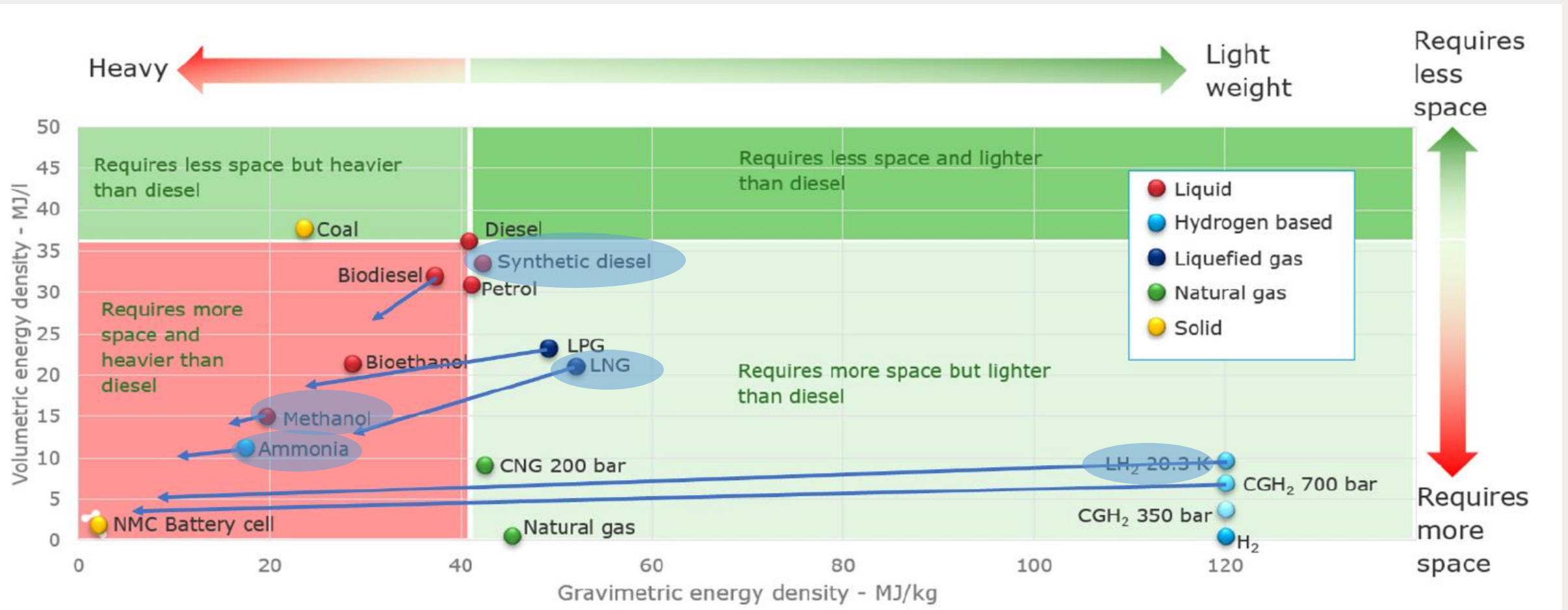
But immediate action could dramatically turn things around!

Used methodology for emission scenarios: Stolz & Held et al. (2021): *Applied Energy*, vol. 285: 116425

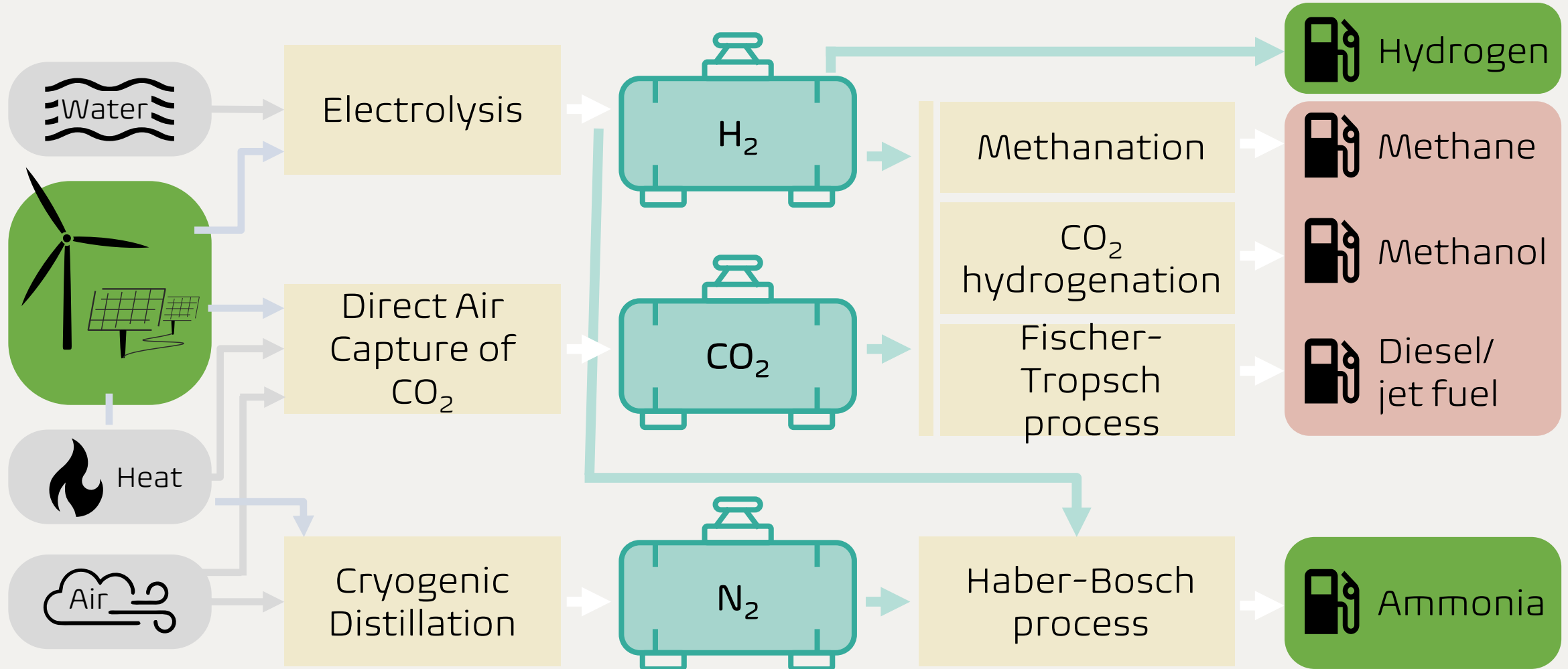
Maximillian Held!

Carbon Free or Carbon Neutral Fuels

Batteries are not feasible!



Production pathways for renewable fuels



Used methodology for emission scenarios: Stolz & Held et al. (2021): *Applied Energy*, vol. 285: 116425

The Challenge For the Shipping Industry Engine Manufacturers ?

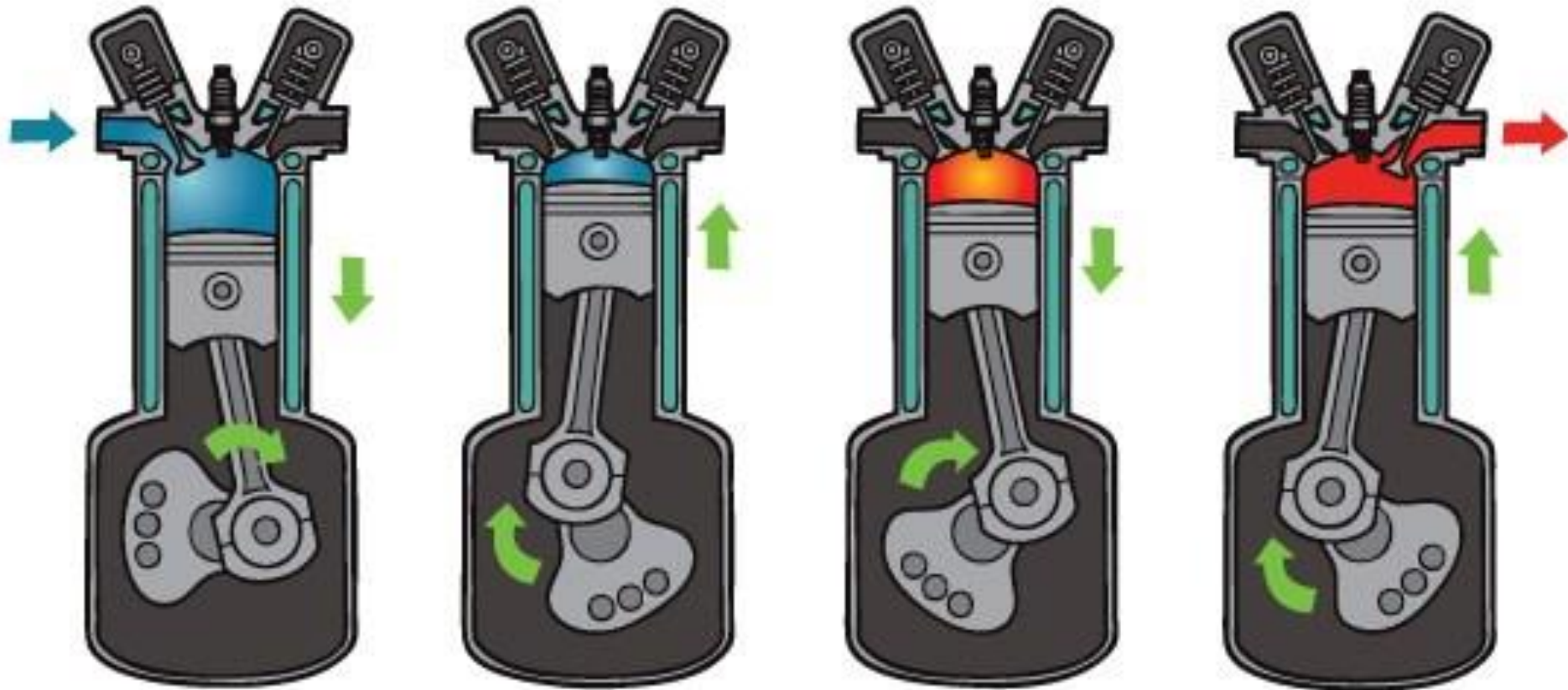
Not Enough Scientific Studies to
Incite Change!

Here is my proposed
solution:
A Dual Fuel Engine!

Fuel Flexible – Efficient – Low Capital Cost

Disclaimer: I did not invent it

FOUR STROKE CYCLE ENGINE



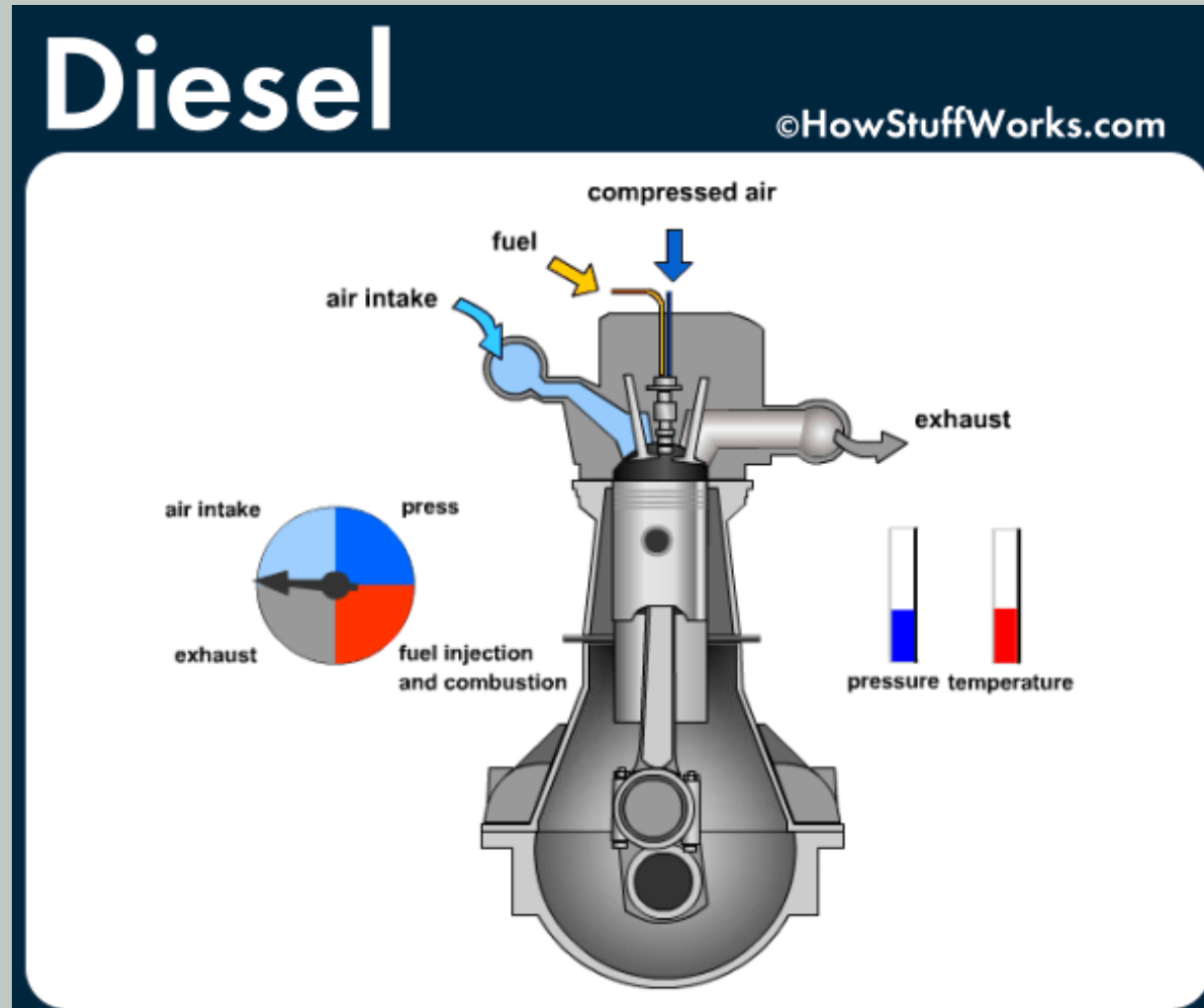
INTAKE

COMPRESSION

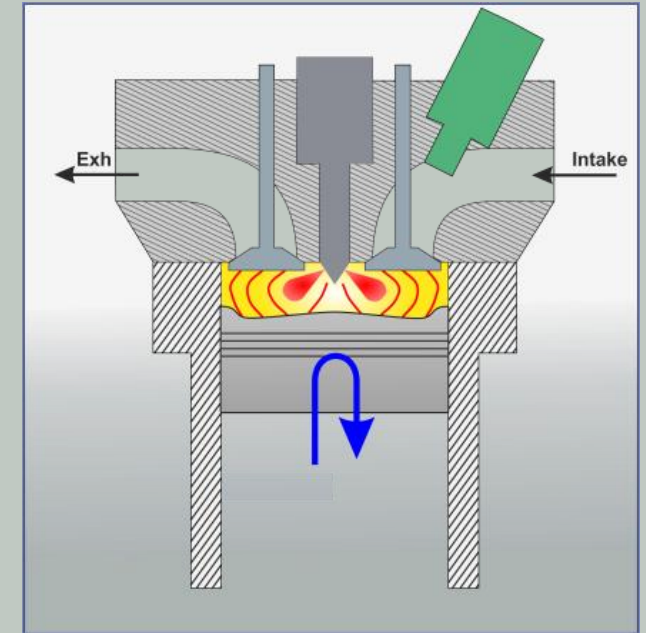
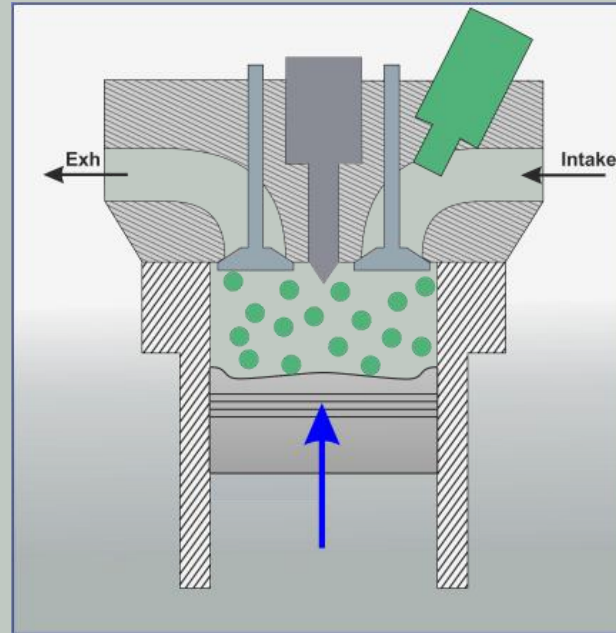
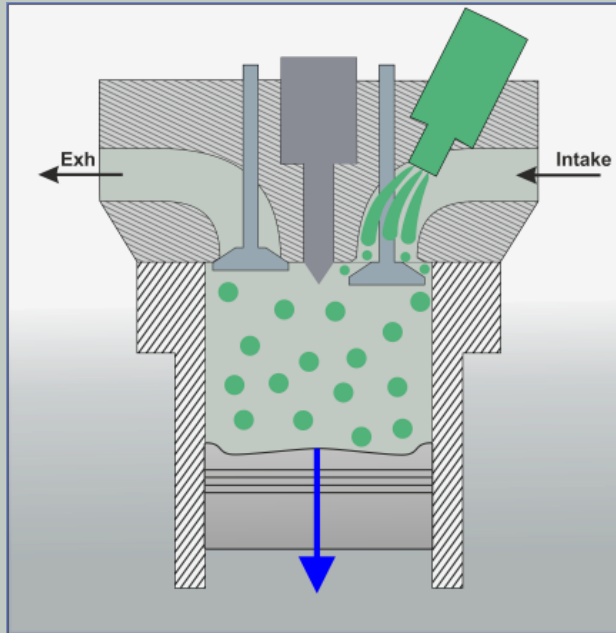
COMBUSTION

EXHAUST

Compression Ignited (CI) Engines

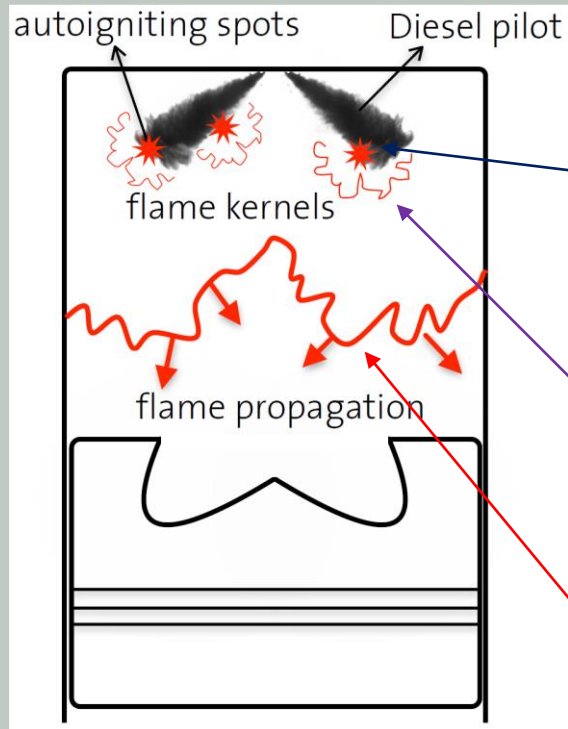


Dual Fuel Engine



Fuel Flexible – Efficient – Low Capital Cost

Dual Fuel Engine



Auto-igniting Diesel/fuel spray
Atomization and secondary break-up
Evaporation and fuel-air mixing
Auto-ignition
Non-premixed flame

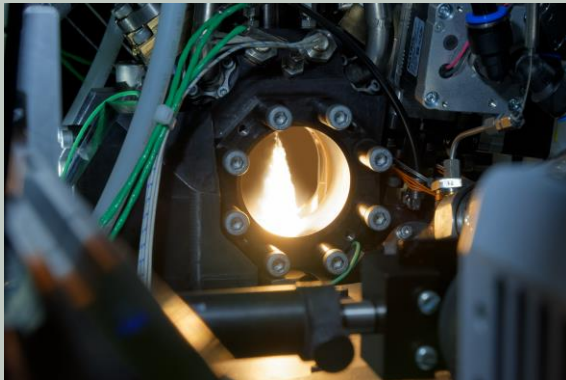
Regime transition
Premixed charge forced ignition
Flame kernel(s) growth

Turbulent premixed flame
Turbulent flame propagation
Extinction?
Flame-wall interaction!

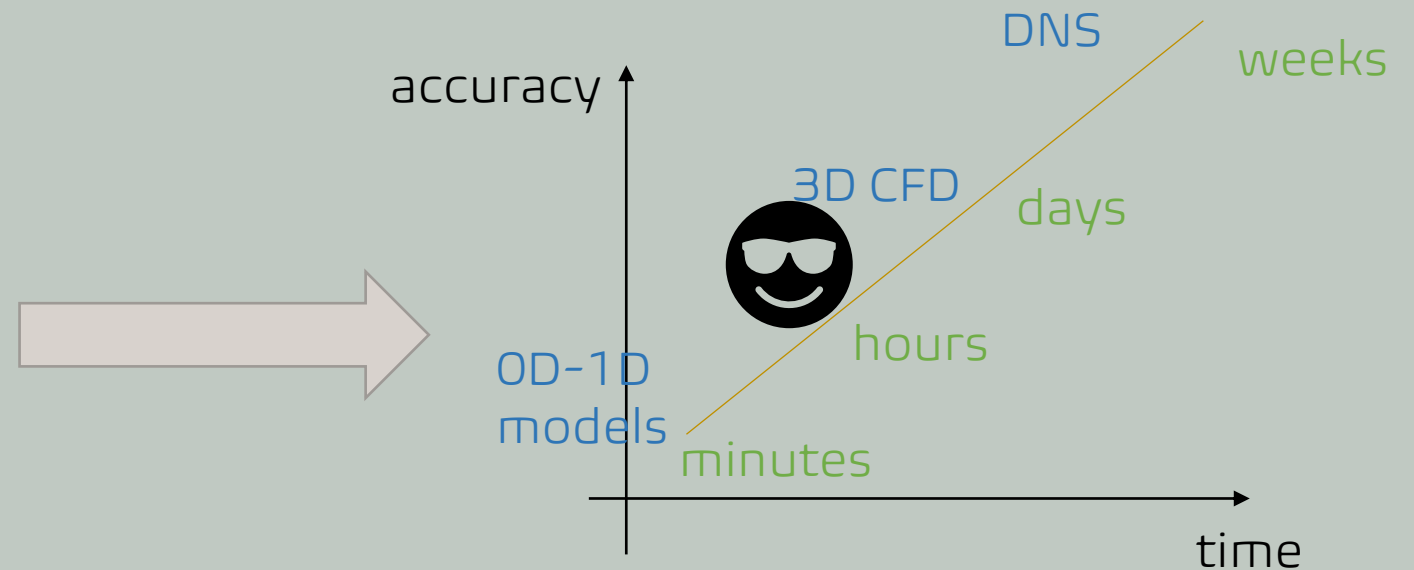
Dual Fuel engines are
gaining market share but
not well understood!

We need to provide tools to help manufacturers design better engines

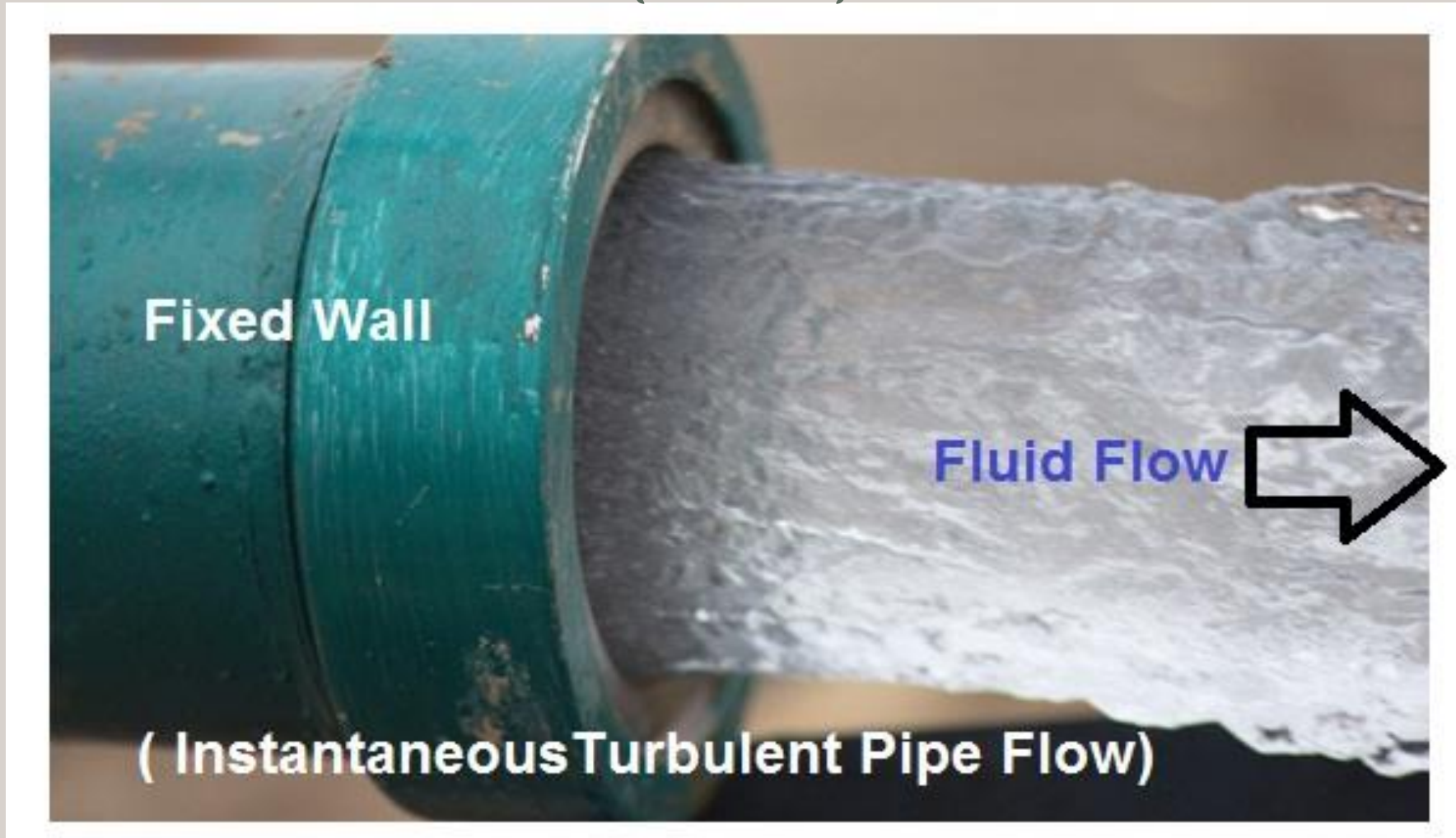
- Experiments
 - Expensive
 - Burns fuel (>10,000tons/year!!)→ emissions!
 - time consuming
 - Cannot “see” everything



- Simulation
 - Accuracy vs. speed



Computational Fluid Dynamics (CFD)

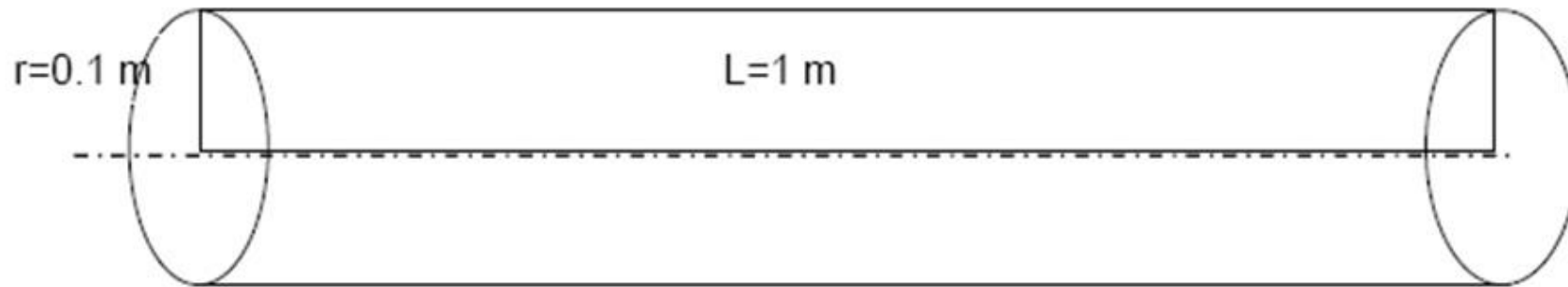


Basics of CFD Modeling for Beginners - CFD Flow Engineering

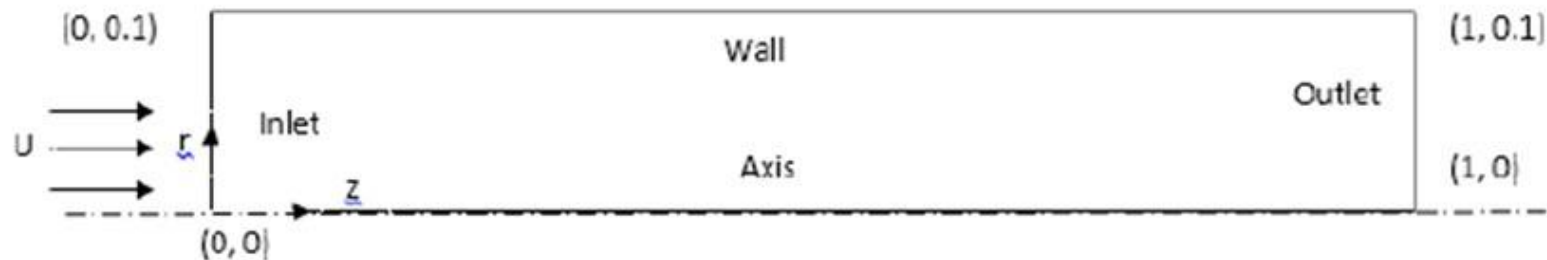
Jiyuan Tu Guan Heng Yeoh Chaoqun Liu, *Computational Fluid Dynamics: A Practical Approach*, Butterworth-Heinemann, Elsevier Publication, 2018

Henk Kaarle Versteeg, Weeratunge Malalasekera, *An Introduction to Computational Fluid Dynamics: The Finite Volume Method*, Pearson Education Limited, 2007

Problem Geometry



(a) Pipe Geometry



Grid Generation

$N_y=20$, $N_x=200$



Governing equations

Mass

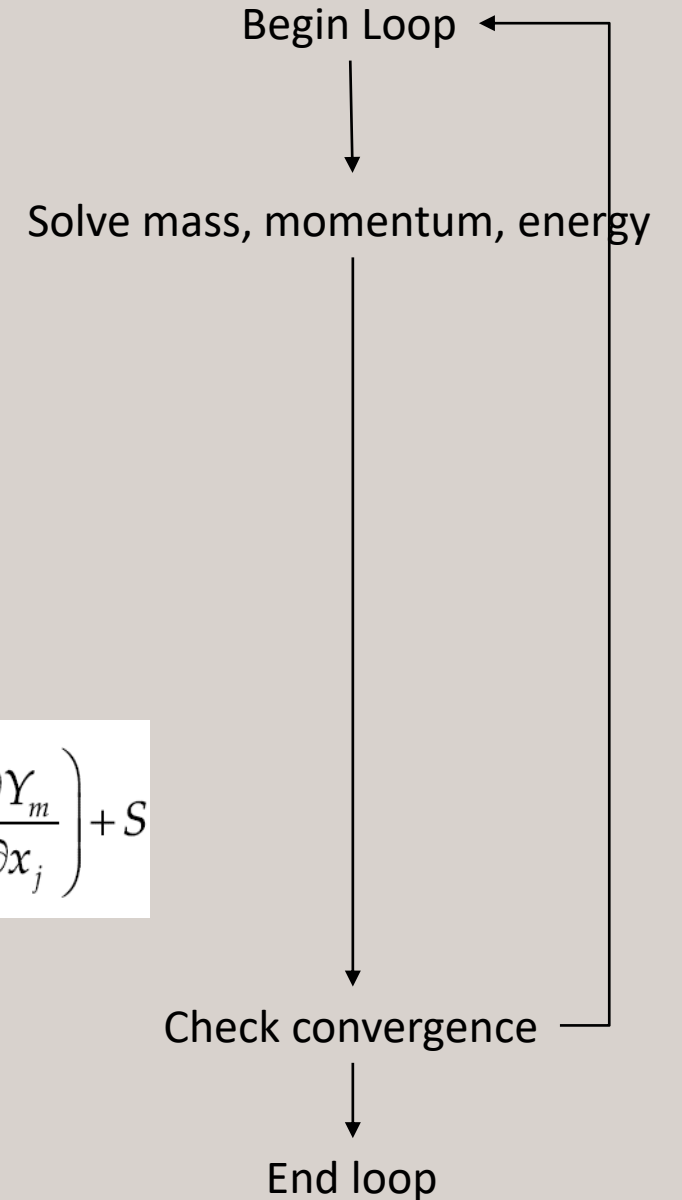
$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = S$$

Momentum

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + S_i$$

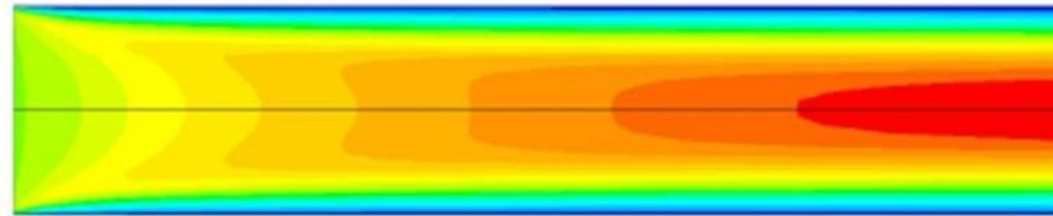
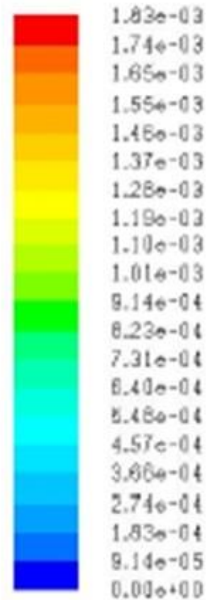
Energy

$$\frac{\partial \rho e}{\partial t} + \frac{\partial u_j \rho e}{\partial x_j} = -P \frac{\partial u_j}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left(K \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\rho D \sum_m h_m \frac{\partial Y_m}{\partial x_j} \right) + S$$

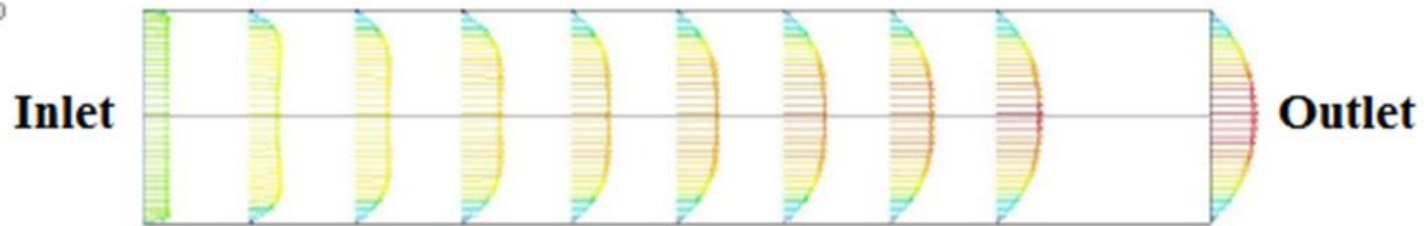


Results and Analysis

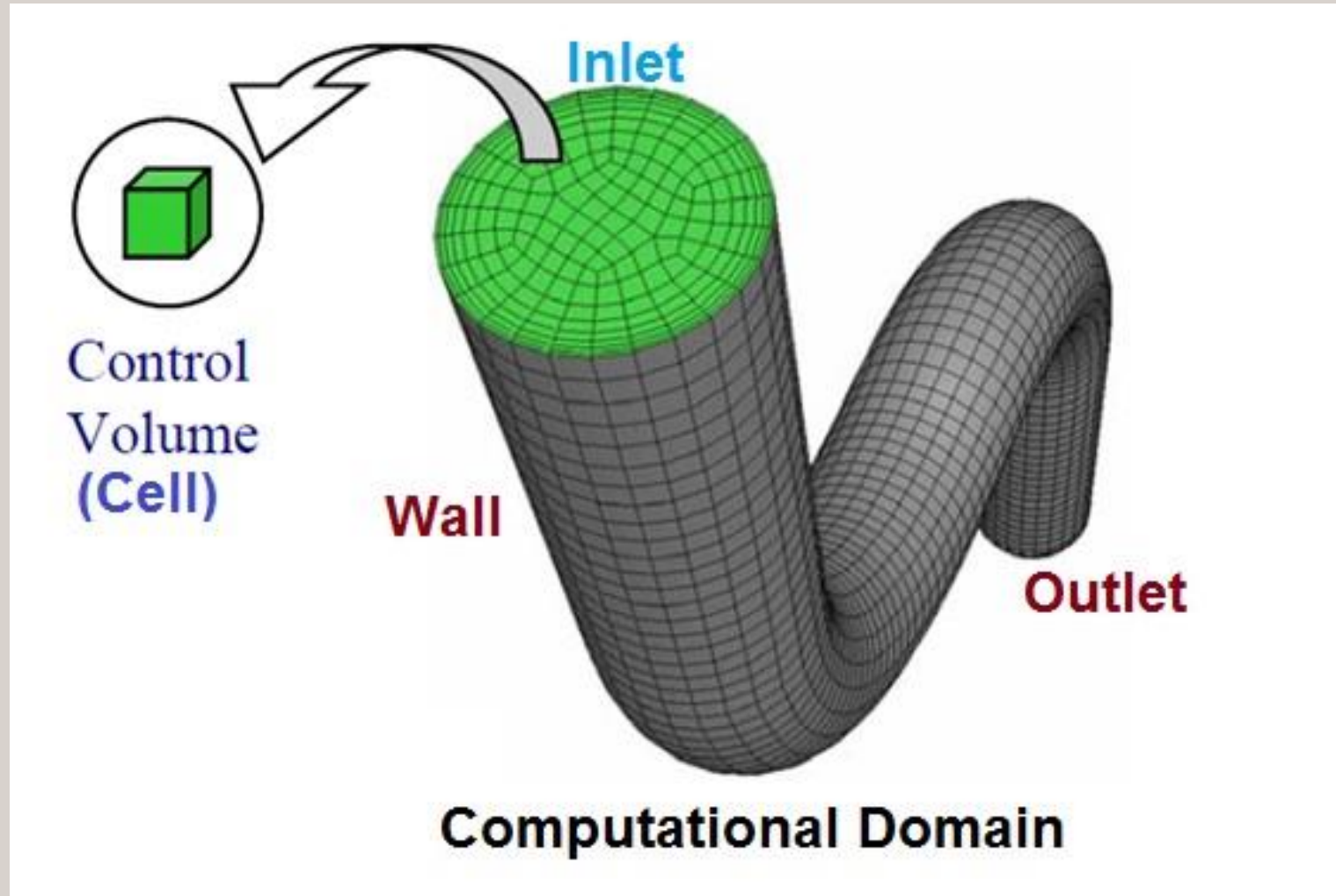
Velocity Distribution:



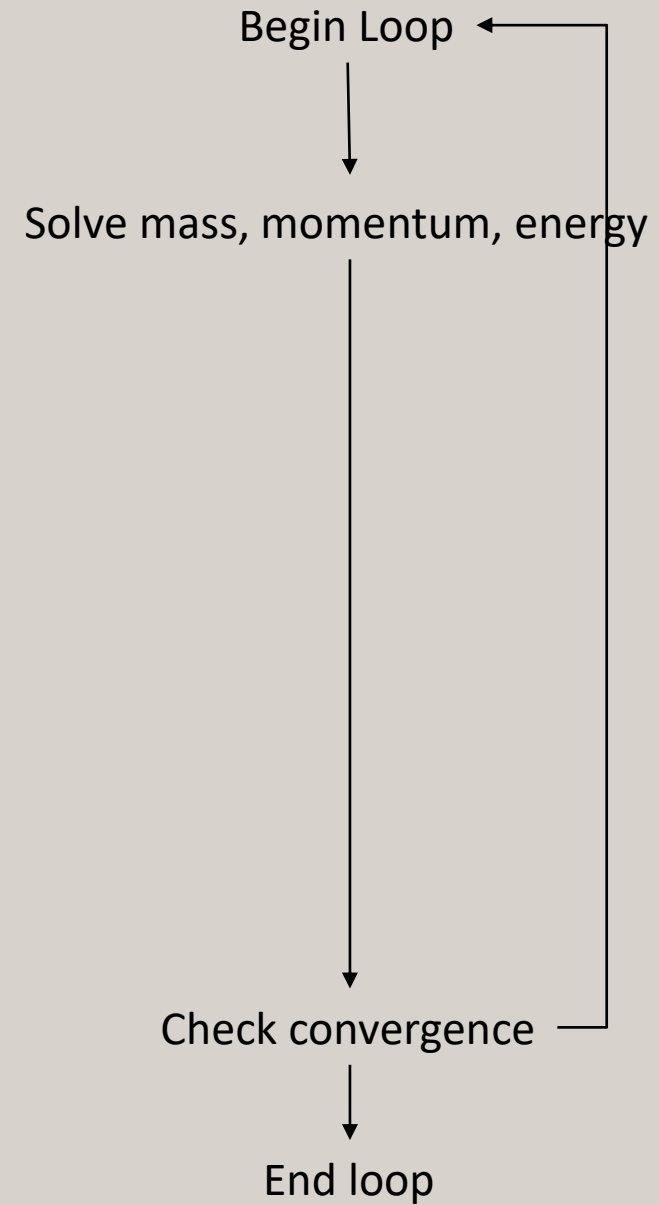
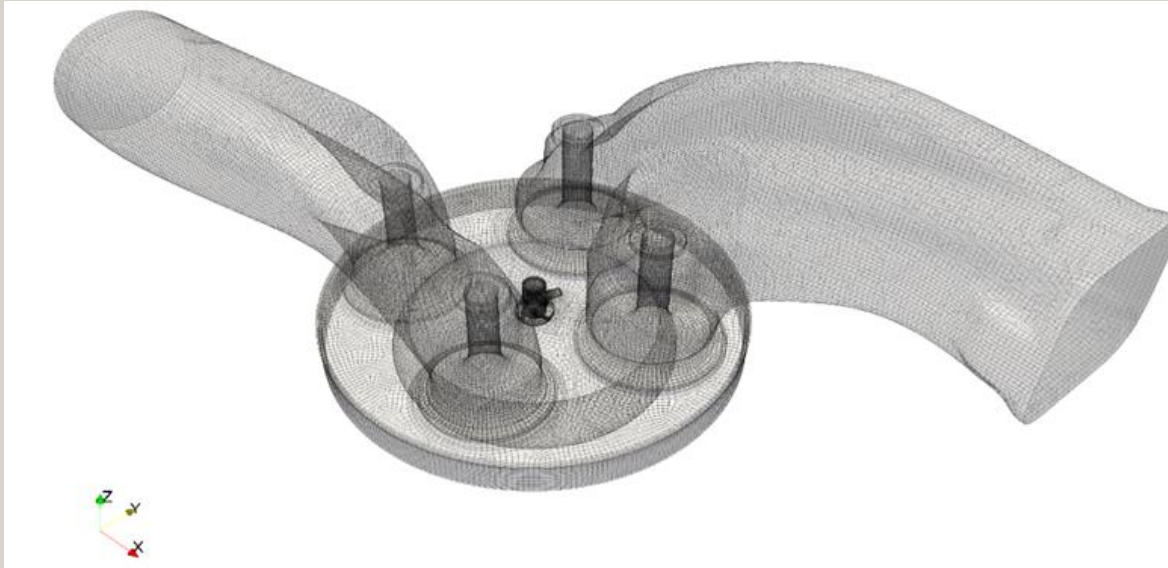
Velocity Vector



3-D Grid



CFD Solver Flow



And with Combustion...



Mass

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = S$$

Momentum

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + S_i$$

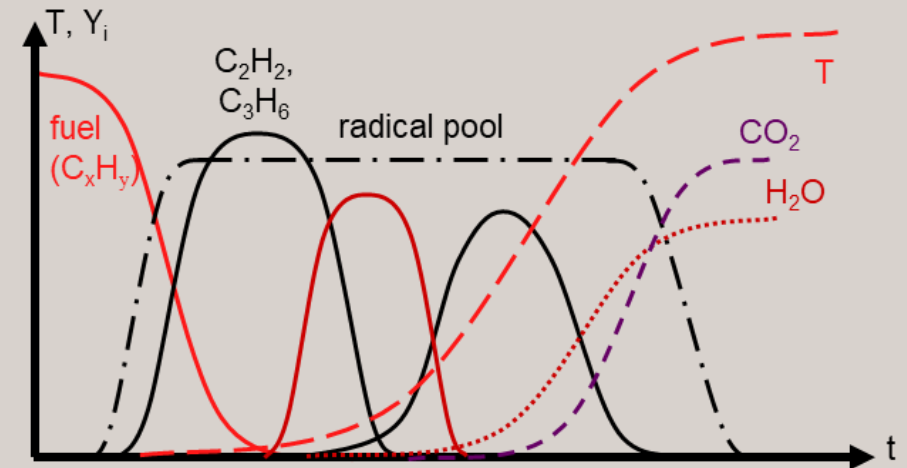
Energy

$$\frac{\partial \rho e}{\partial t} + \frac{\partial u_j \rho e}{\partial x_j} = -P \frac{\partial u_j}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left(K \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\rho D \sum_m h_m \frac{\partial Y_m}{\partial x_j} \right) + S$$

Species

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_m u_j}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial Y_m}{\partial x_j} \right) + S_m$$

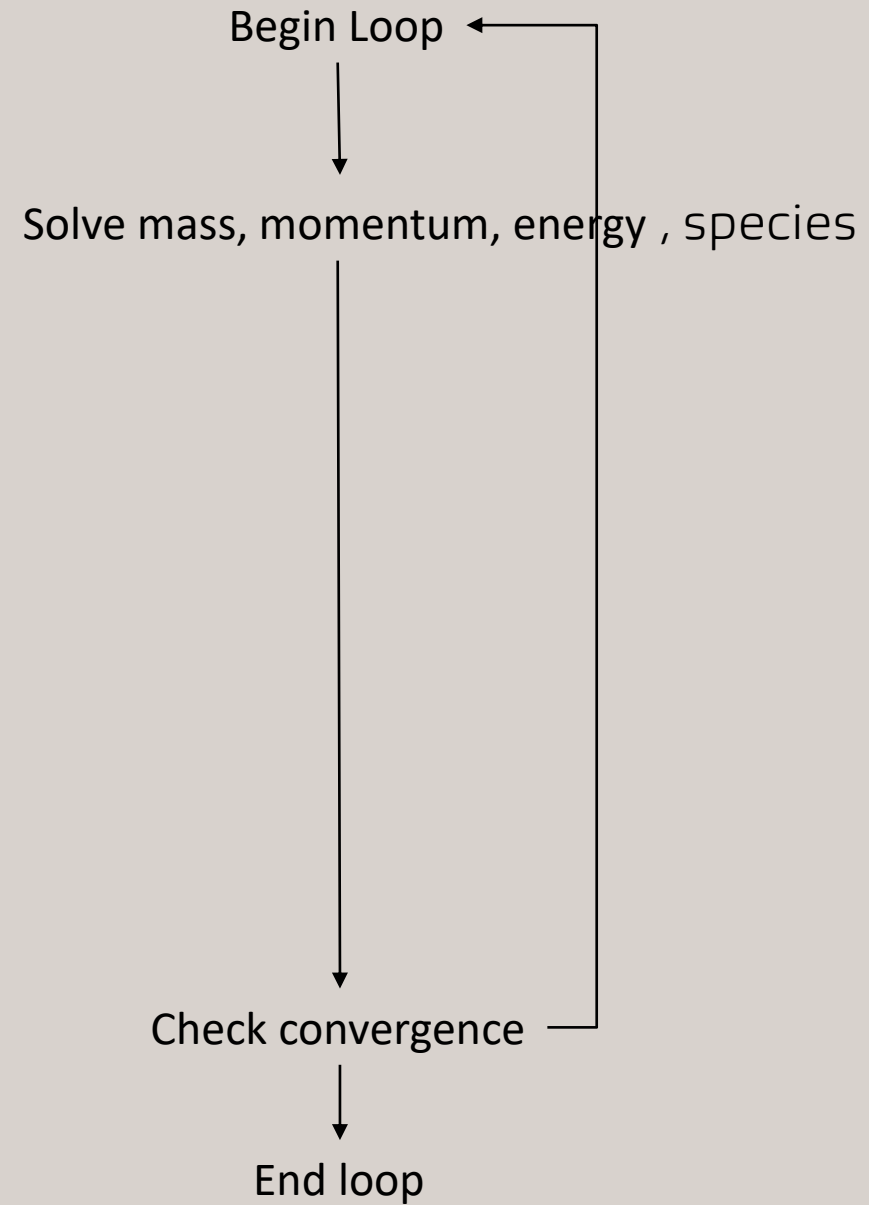
Species: chemical molecules (e.g. O₂, CO₂)



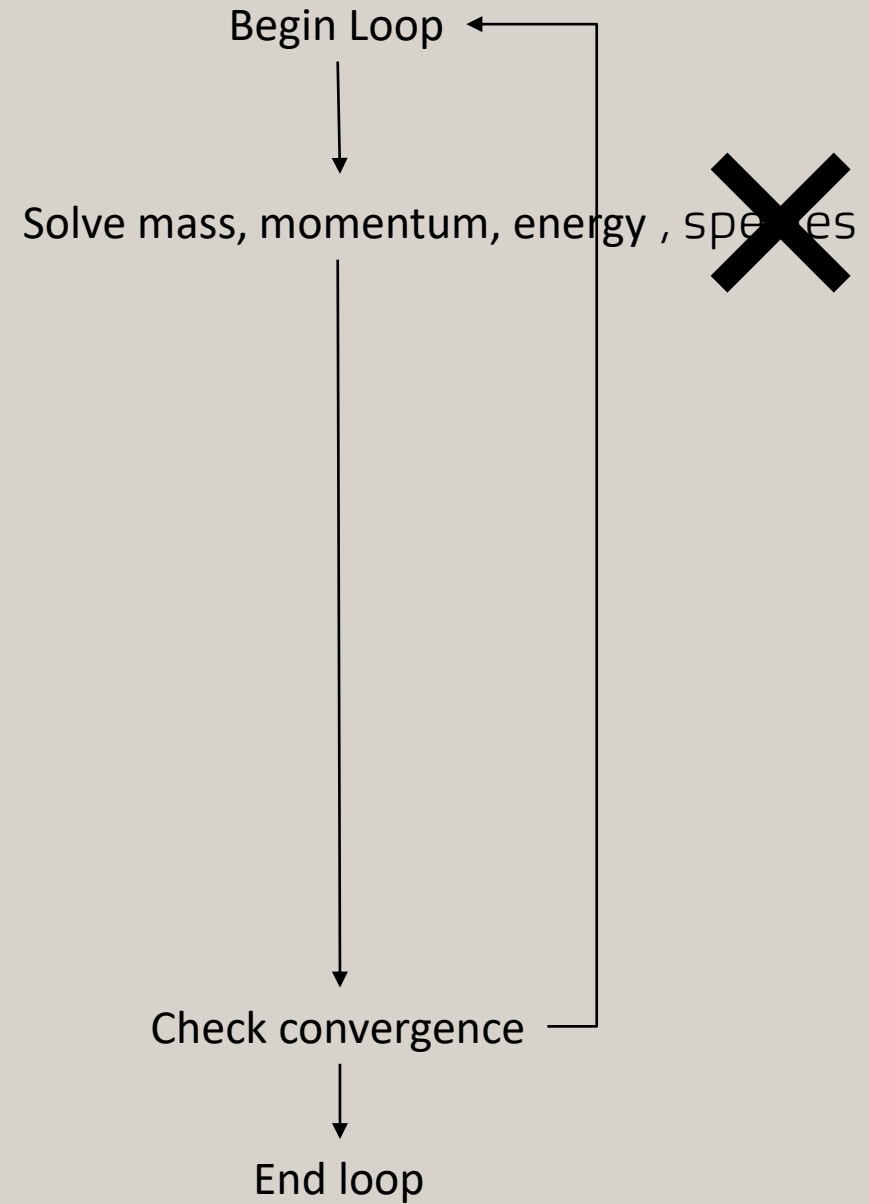
Dual Fuel Model

- Reduces computation time by not solving the chemical species equations
- Still chemically accurate
- Accounts for both non-premixed and premixed combustion modes

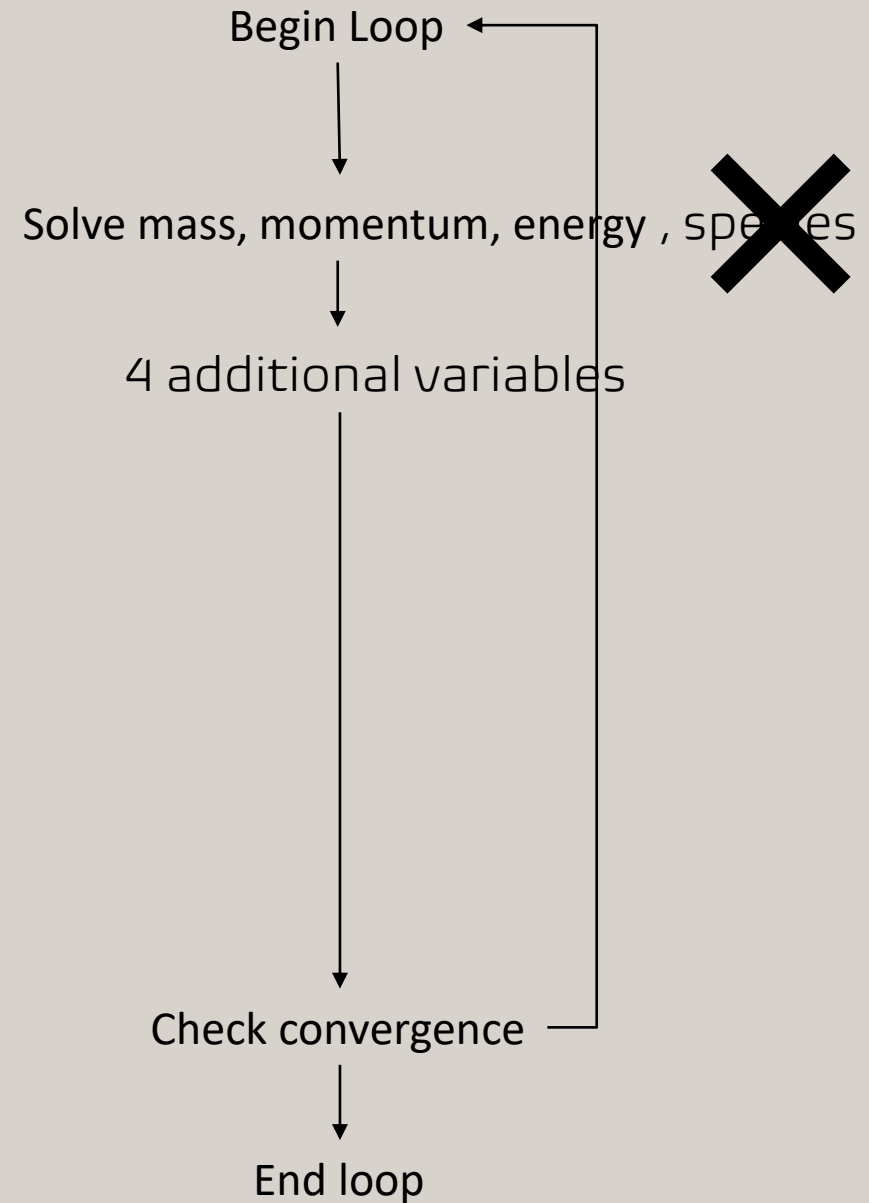
Dual Fuel Model



Dual Fuel Model

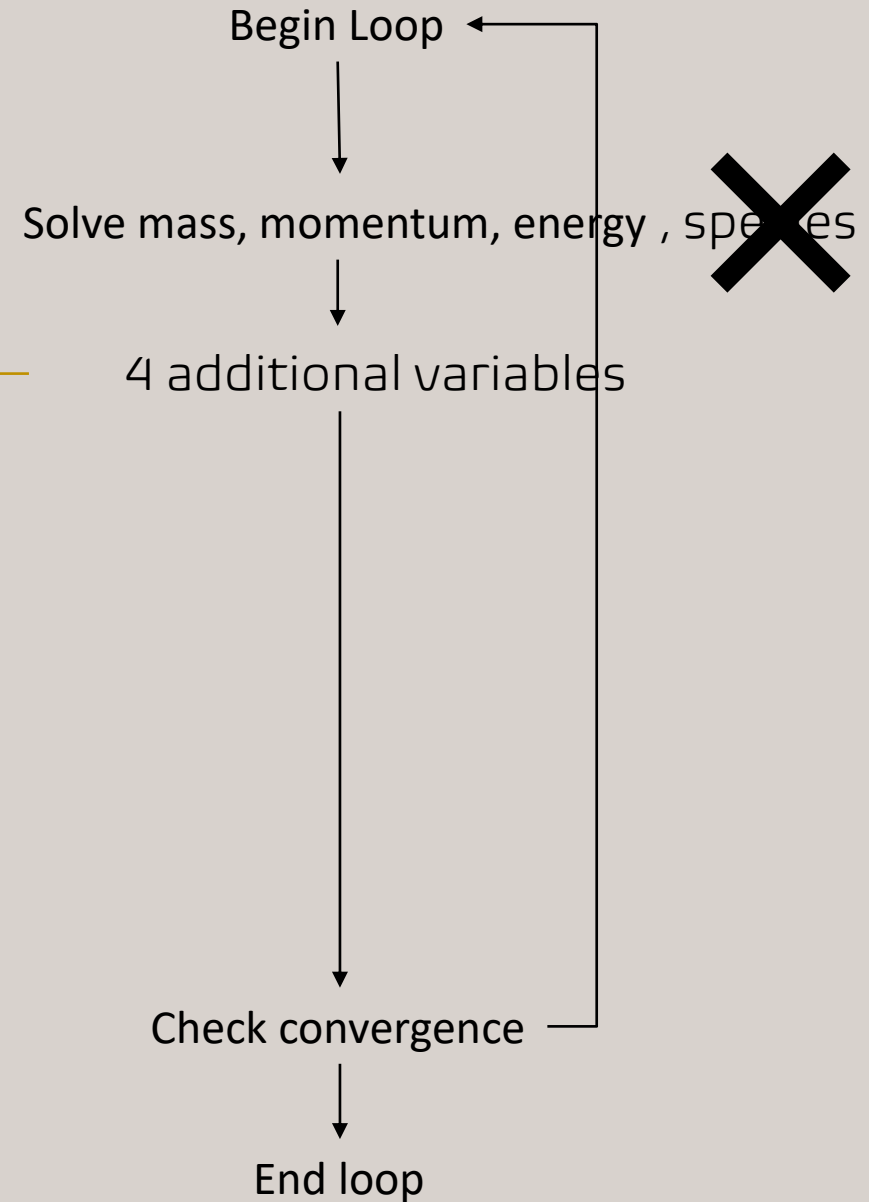


Dual Fuel Model



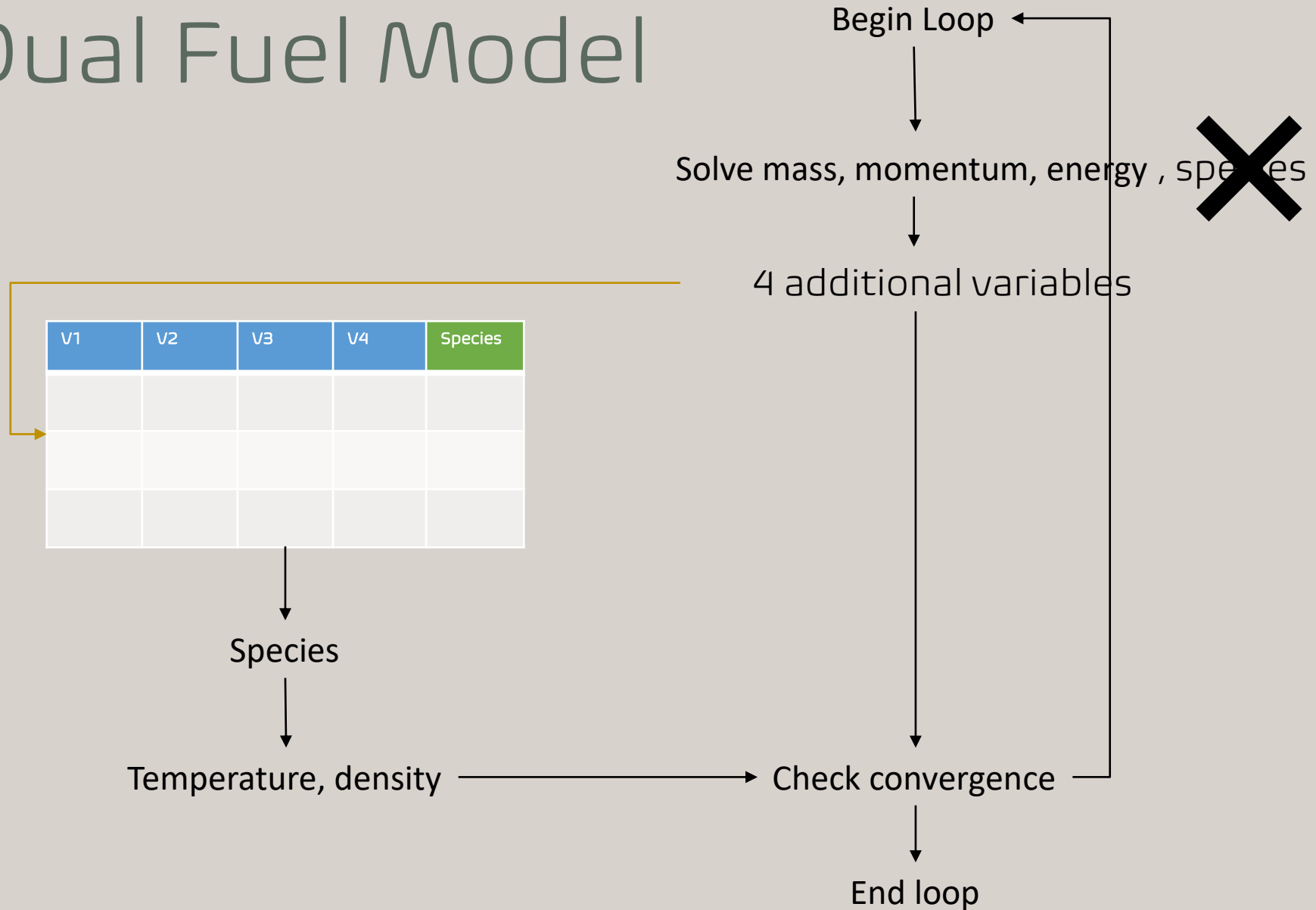
Dual Fuel Model

V1	V2	V3	V4	Species



Dual Fuel Model

2 Tables:
Premixed and
Non-Premixed



Dual Fuel Model

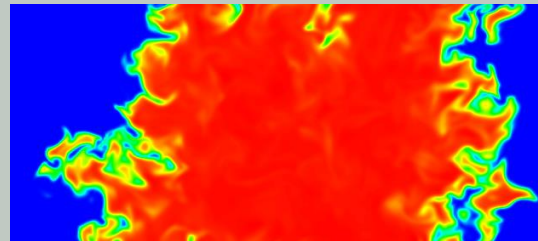
- Reduces computation time by not solving the chemical species equations
 - Only 4 additional equations
- Still chemically accurate as complex chemical mechanisms could be used in the tabulation step
- Accounts for both non-premixed and premixed combustion modes
 - 1 table for each combustion mode

Model Validation

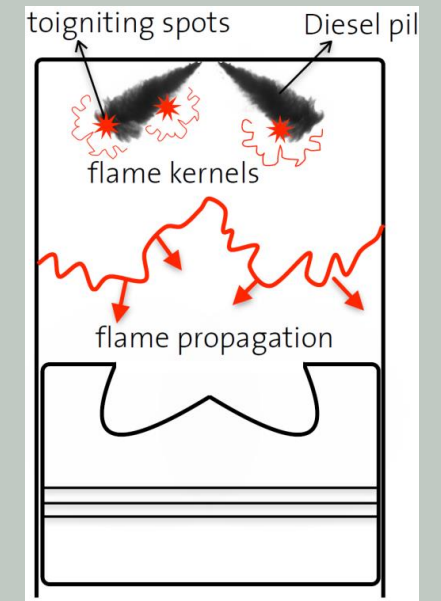
Non Premixed



Premixed

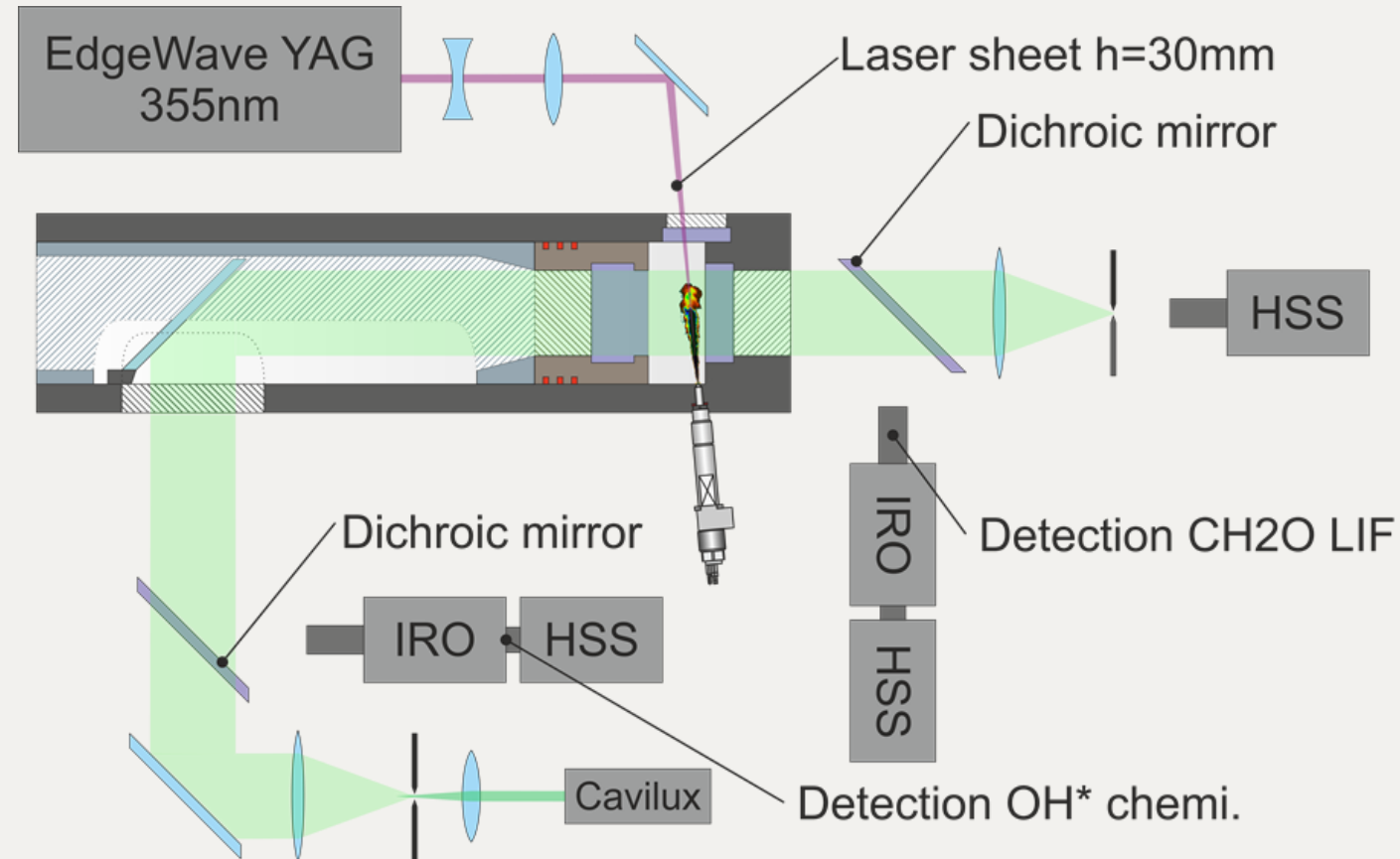


Dual Fuel



Ignition Validation

Rapid compression-expansion machine (RCEM)



Srna, Aleš, et al. "Effect of methane on pilot-fuel auto-ignition in dual-fuel engines." *Proceedings of the Combustion Institute* 37.4 (2019): 4741-4749.

Srna, Aleš, et al. "Experimental investigation of pilot-fuel combustion in dual-fuel engines, Part 2: Understanding the underlying mechanisms by means of optical diagnostics." *Fuel* 255 (2019): 115766.

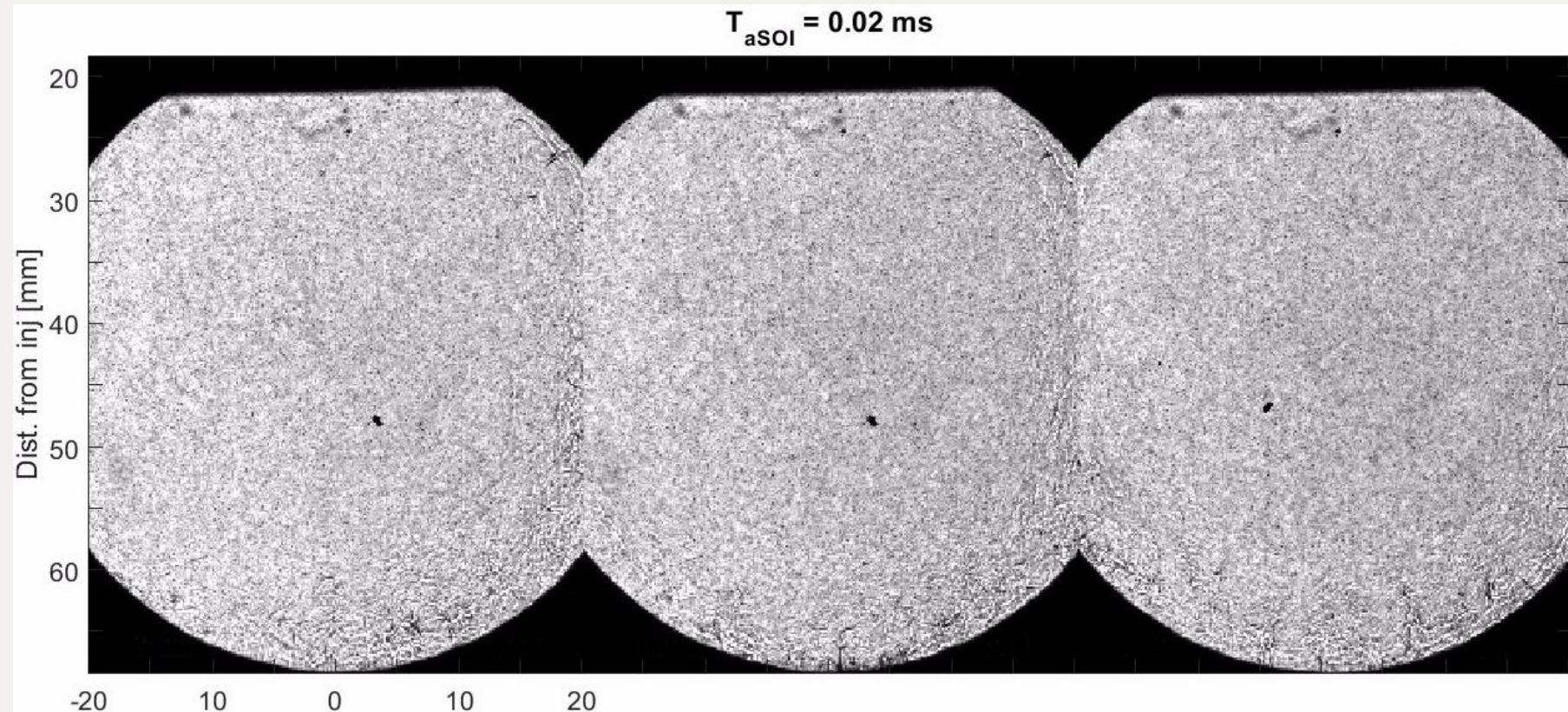
Dual-fuel combustion: optical diagnostics

Conditions: $T_{\text{SOI}} = 810\text{K}$, pilot: 600bar ET = 400 μs

Only Diesel ($\lambda_{\text{CH}_4} = \infty$)

$\lambda_{\text{CH}_4} = 3.0$

$\lambda_{\text{CH}_4} = 1.5$

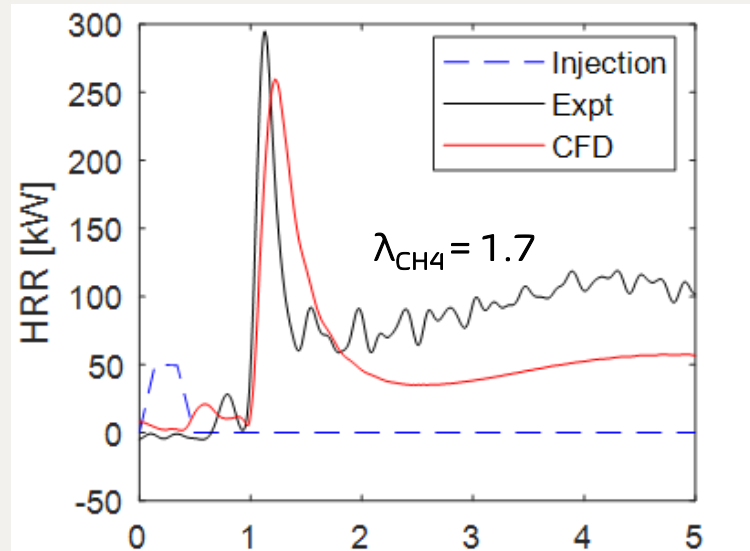
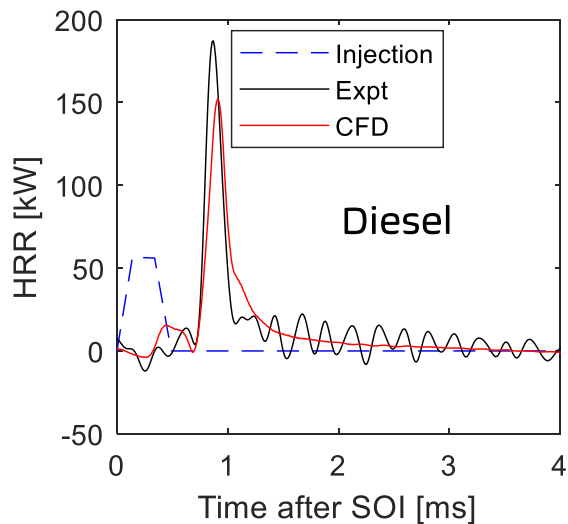


Srna, Aleš, et al. "Effect of methane on pilot-fuel auto-ignition in dual-fuel engines." *Proceedings of the Combustion Institute* 37.4 (2019): 4741-4749.

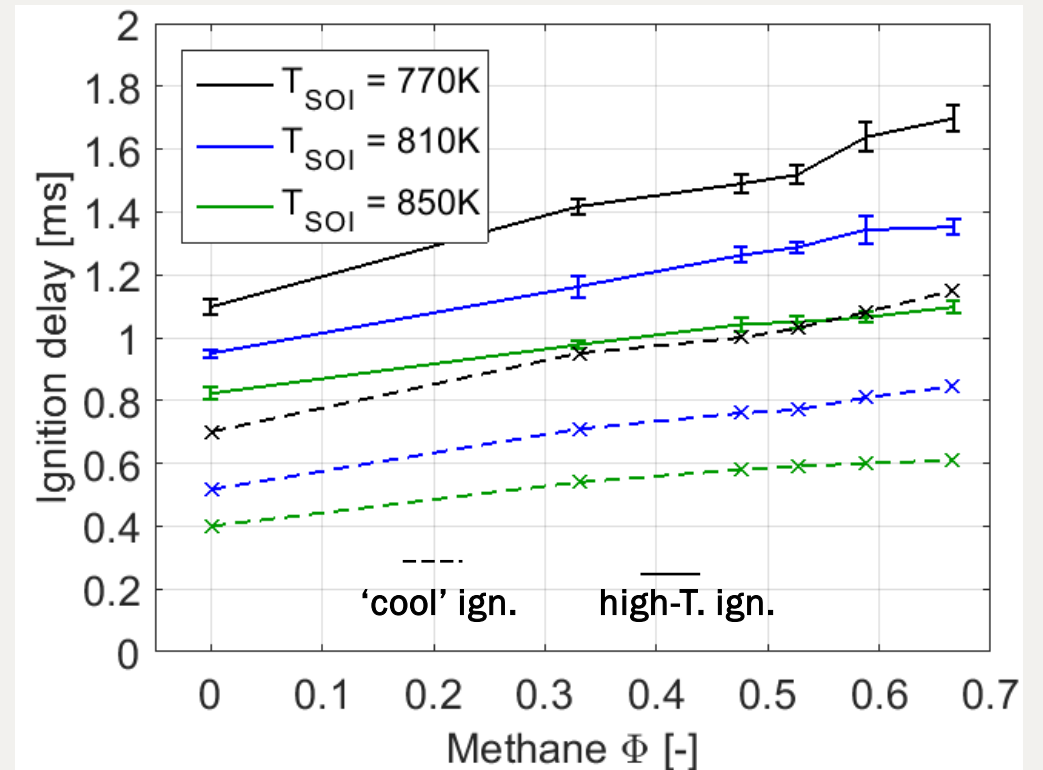
Srna, Aleš, et al. "Experimental investigation of pilot-fuel combustion in dual-fuel engines, Part 2: Understanding the underlying mechanisms by means of optical diagnostics." *Fuel* 255 (2019): 115766.

CH₄ influence on the ignition delay

- CH₄ chemically influences ignition
- Ignition modelling has to capture this behavior



Ignition delay



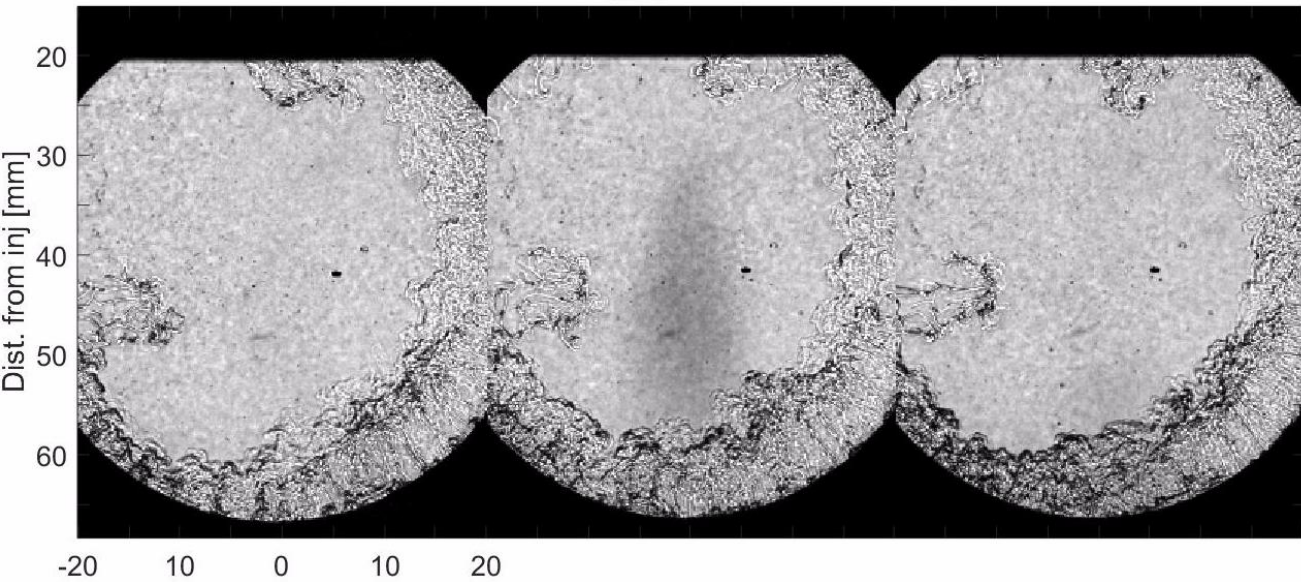
Higher-T Diesel Combustion

$\lambda_{CH_4} = \text{Inf}$

$\lambda_{CH_4} = 3.0$

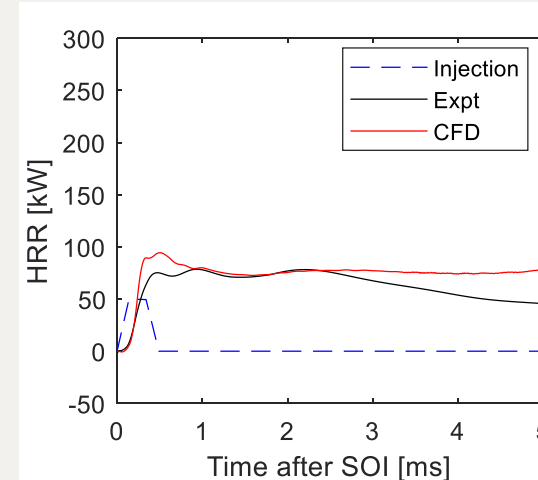
$\lambda_{CH_4} = 2.1$

$T_{aSOI} = 0.02 \text{ ms}$

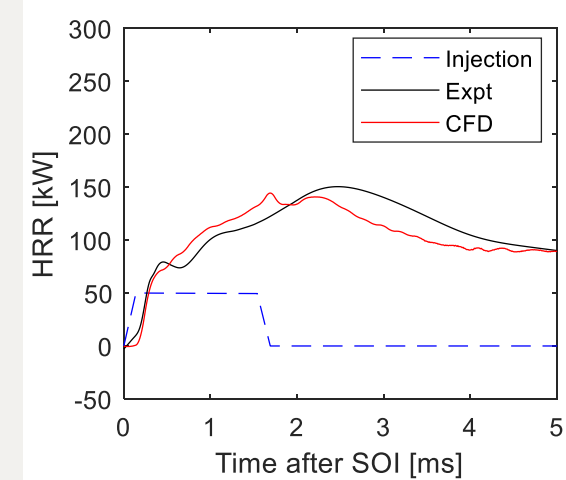


Characteristic difference from gas-engine condition cases:

- Very short (negligible) ignition delay
- Methane has no influence on ignition delay



Short injection (0.7 ms)



Long injection (1.7 ms)

Srna, Aleš, et al. "Effect of methane on pilot-fuel auto-ignition in dual-fuel engines." *Proceedings of the Combustion Institute* 37.4 (2019): 4741-4749.

Srna, Aleš, et al. "Experimental investigation of pilot-fuel combustion in dual-fuel engines, Part 2: Understanding the underlying mechanisms by means of optical diagnostics." *Fuel* 255 (2019): 115766.

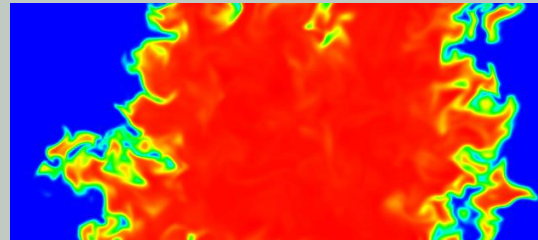
Seddik, Omar, et al. *Flamelet generated manifolds applied to Dual-Fuel combustion of lean methane/air mixtures at engine relevant conditions ignited by n dodecane micro pilot sprays*. No. 2019-01-1163. SAE Technical Paper, 2019.

Model Validation

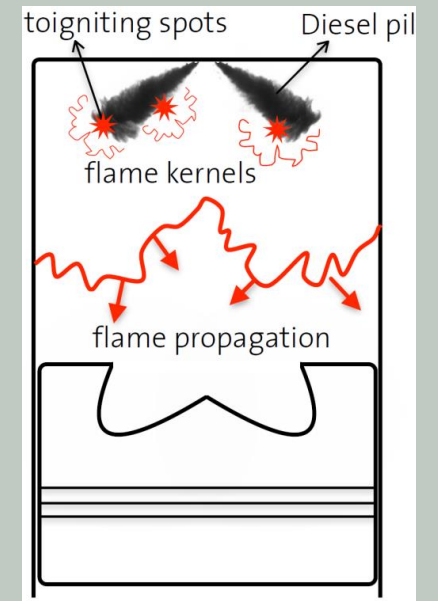
Non Premixed 



Premixed

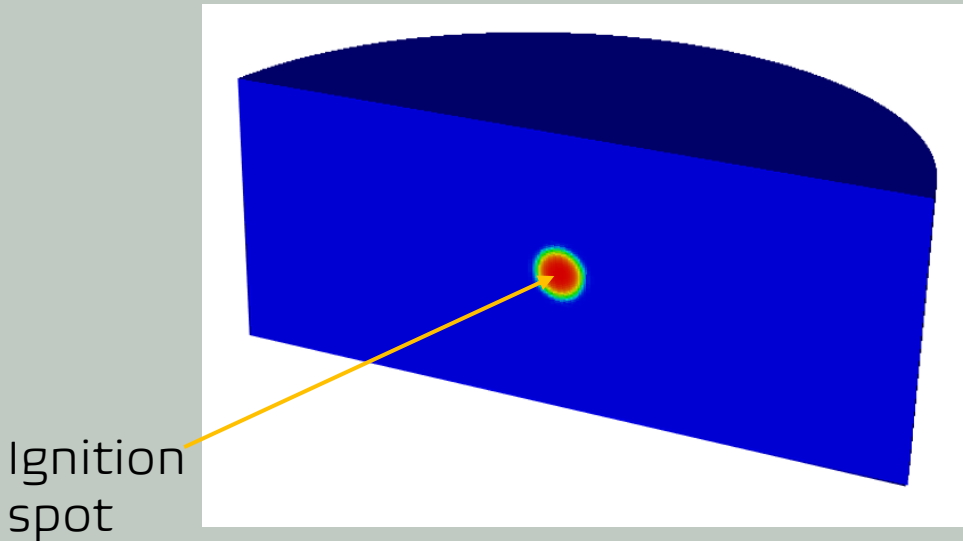


Dual Fuel

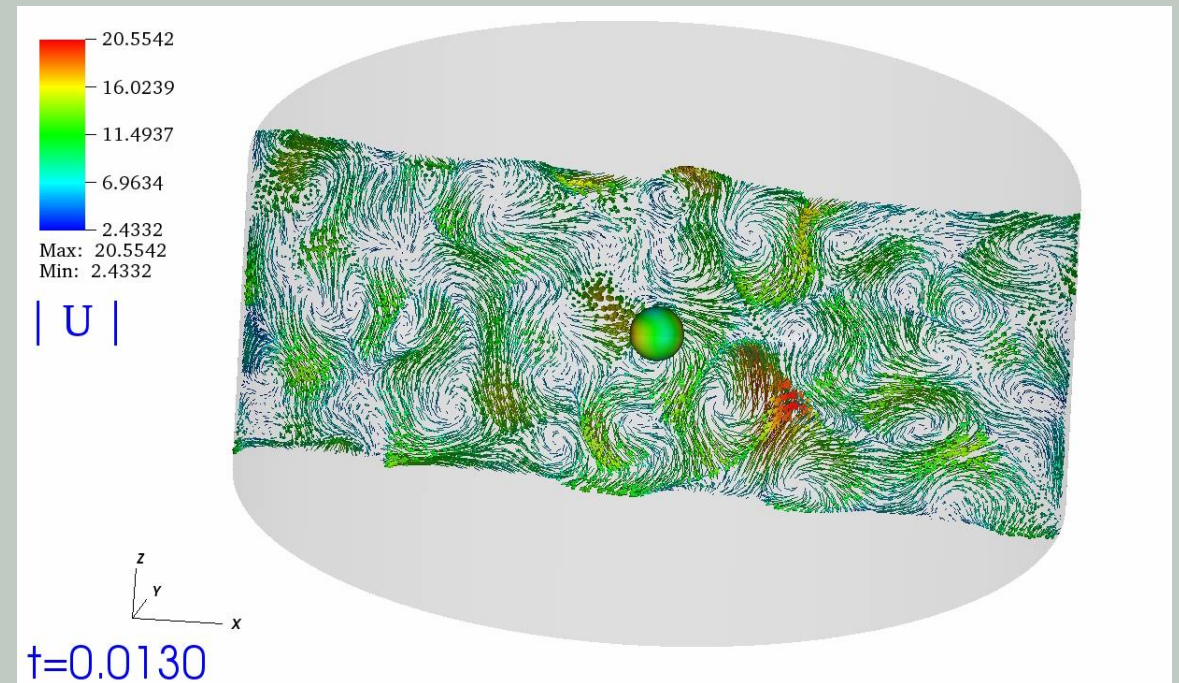


Flame Propagation Validation

Direct Numerical Simulation of Syngas Premixed Flame



S_L^0	1.38m/s
d_L^0	1.14mm
p^0	1bar
T_{wall}	550K
T_u	822K
Fuel	Syngas (H ₂ & CO)



Jafarholi, Frouzakis et al., LAV/ETHZ

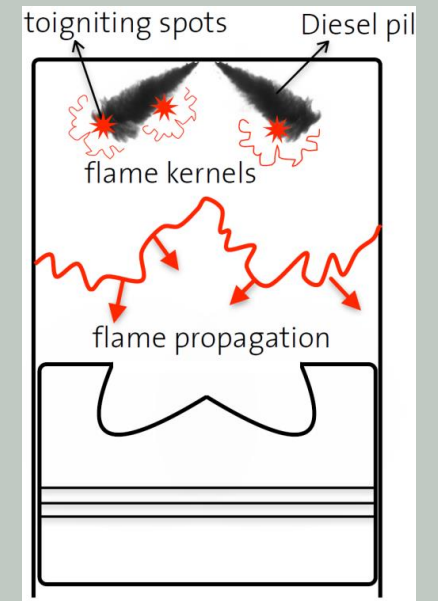
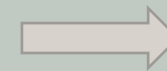
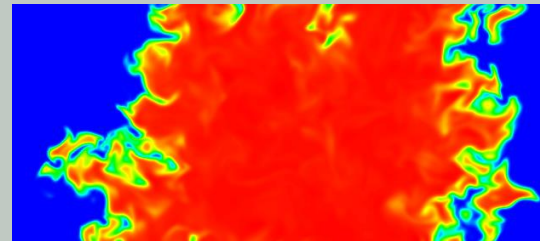
Millions of CPU hours!!

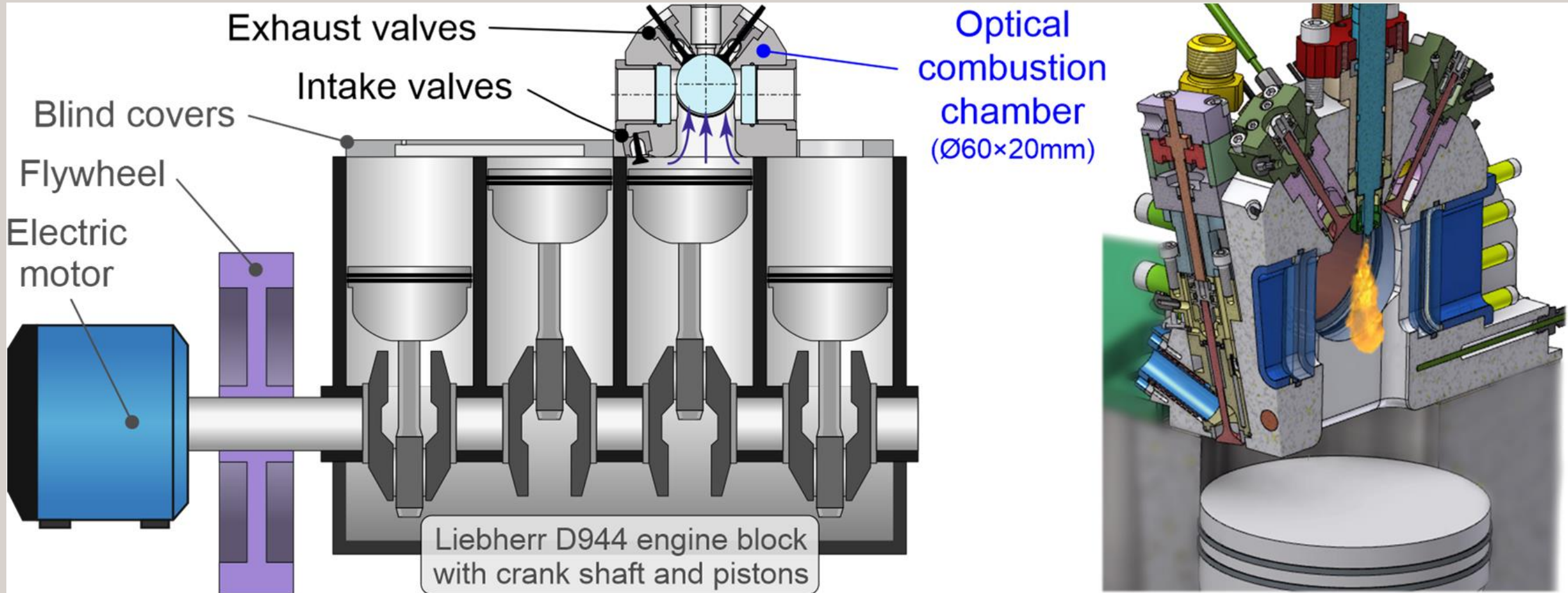
Model Validation

Non Premixed 

Premixed 

Dual Fuel

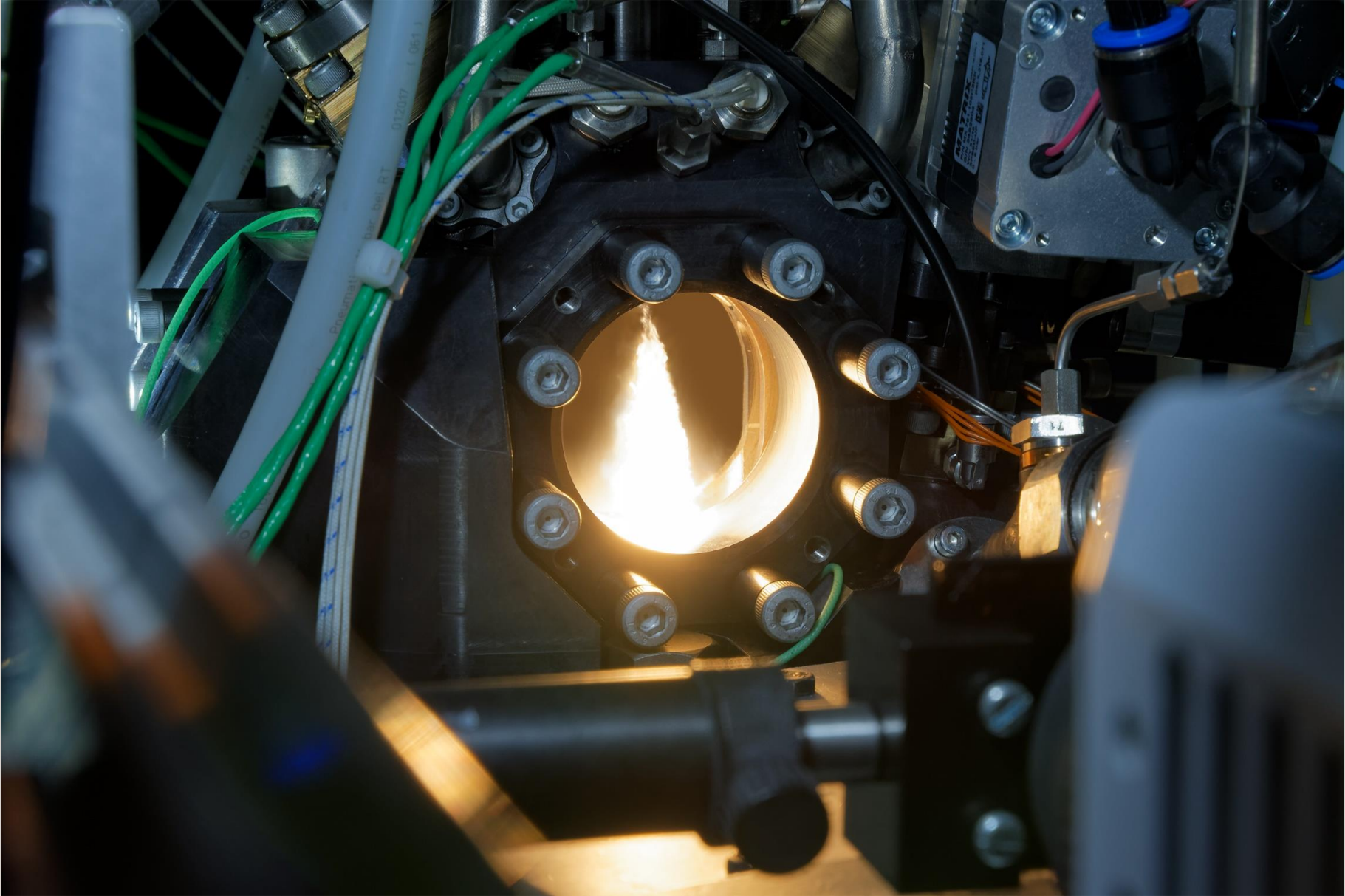




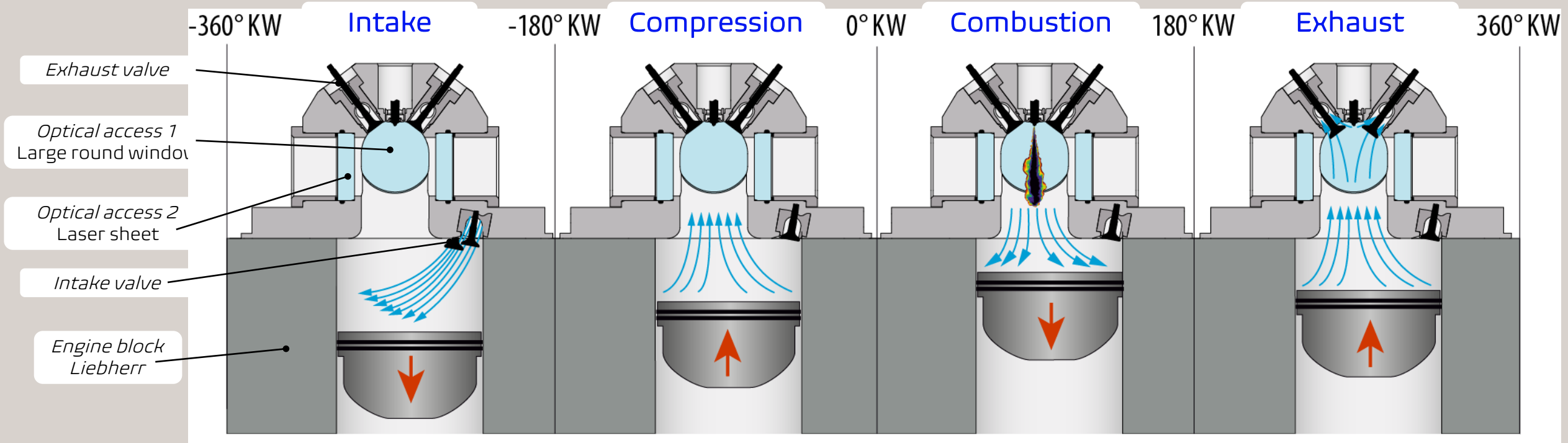
Characterization of dual-fuel combustion processes

D. Humair, P. Cartier, P. Süess, S. Wüthrich, K. Herrmann, C. Barro, B. Schneider, C. Schürch, K. Boulouchos

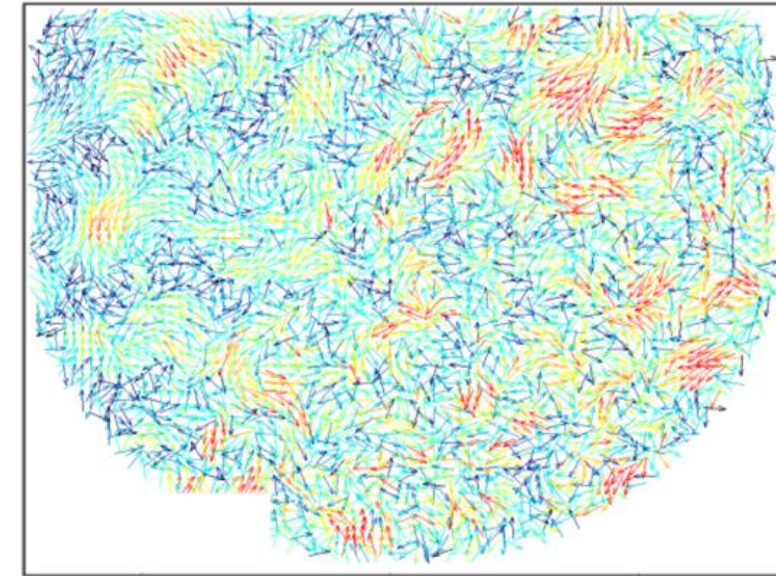
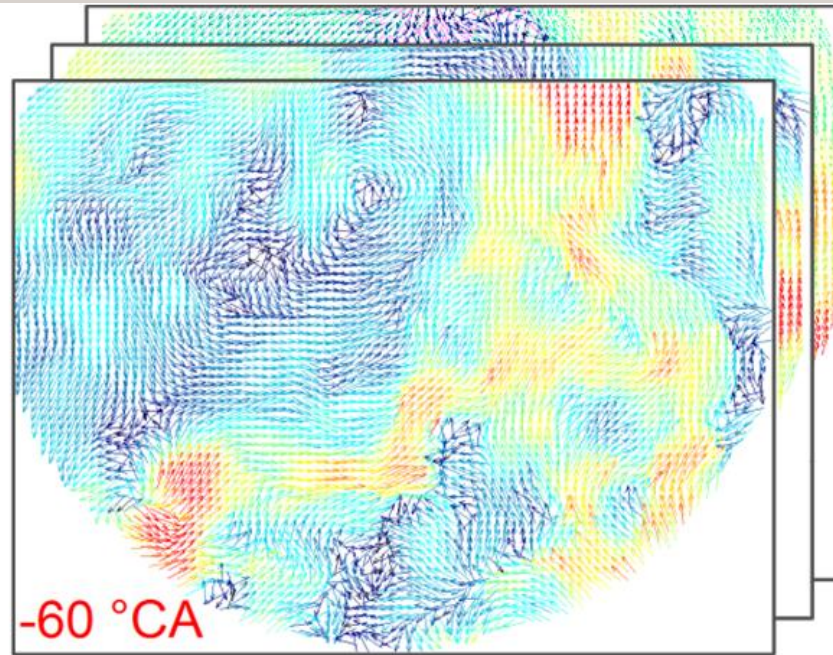
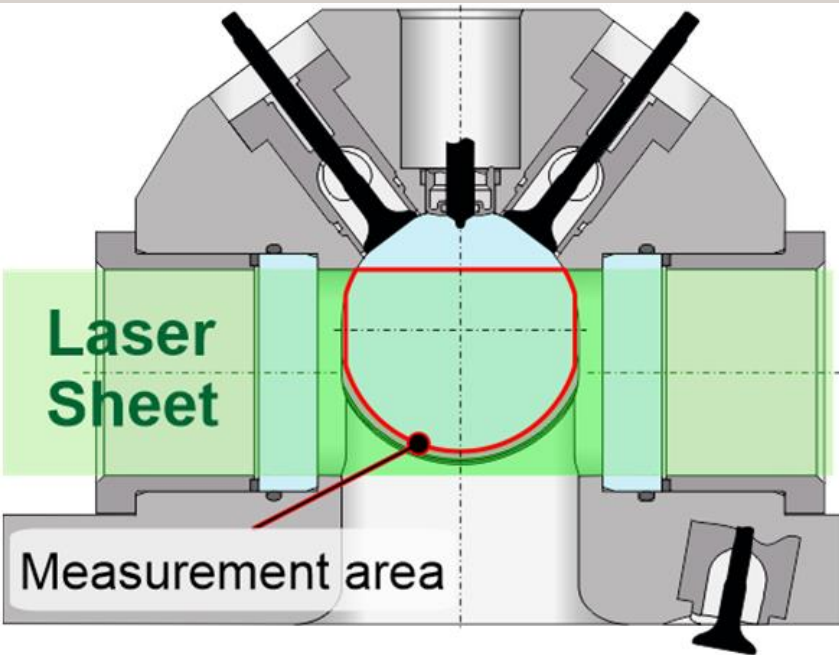
Optical Access?



Test Rig Working Principle



Schneider, B.; Schürch, C.; Boulouchos, K.; Herzig, S.; Hangartner, M.; Humair, D.; Wüthrich, S.; Gossweiler, C.; Herrmann, K. The Flex-OeCoS—a Novel Optically Accessible Test Rig for the Investigation of Advanced Combustion Processes under Engine-Like Conditions. *Energies* **2020**, *13*, 1794. <https://doi.org/10.3390/en13071794>

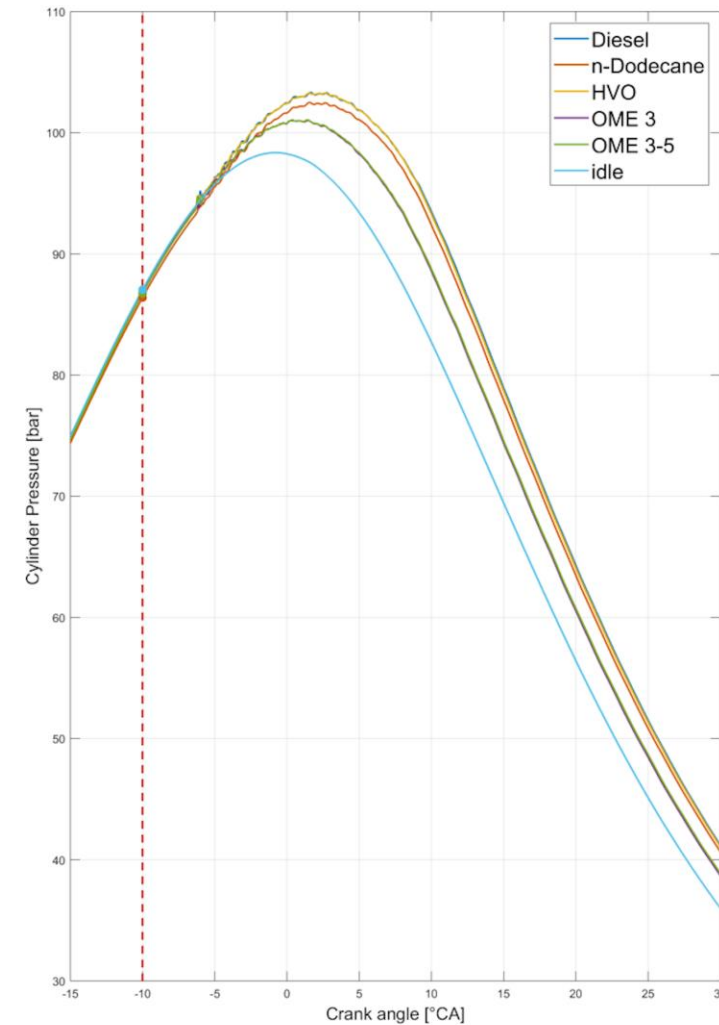
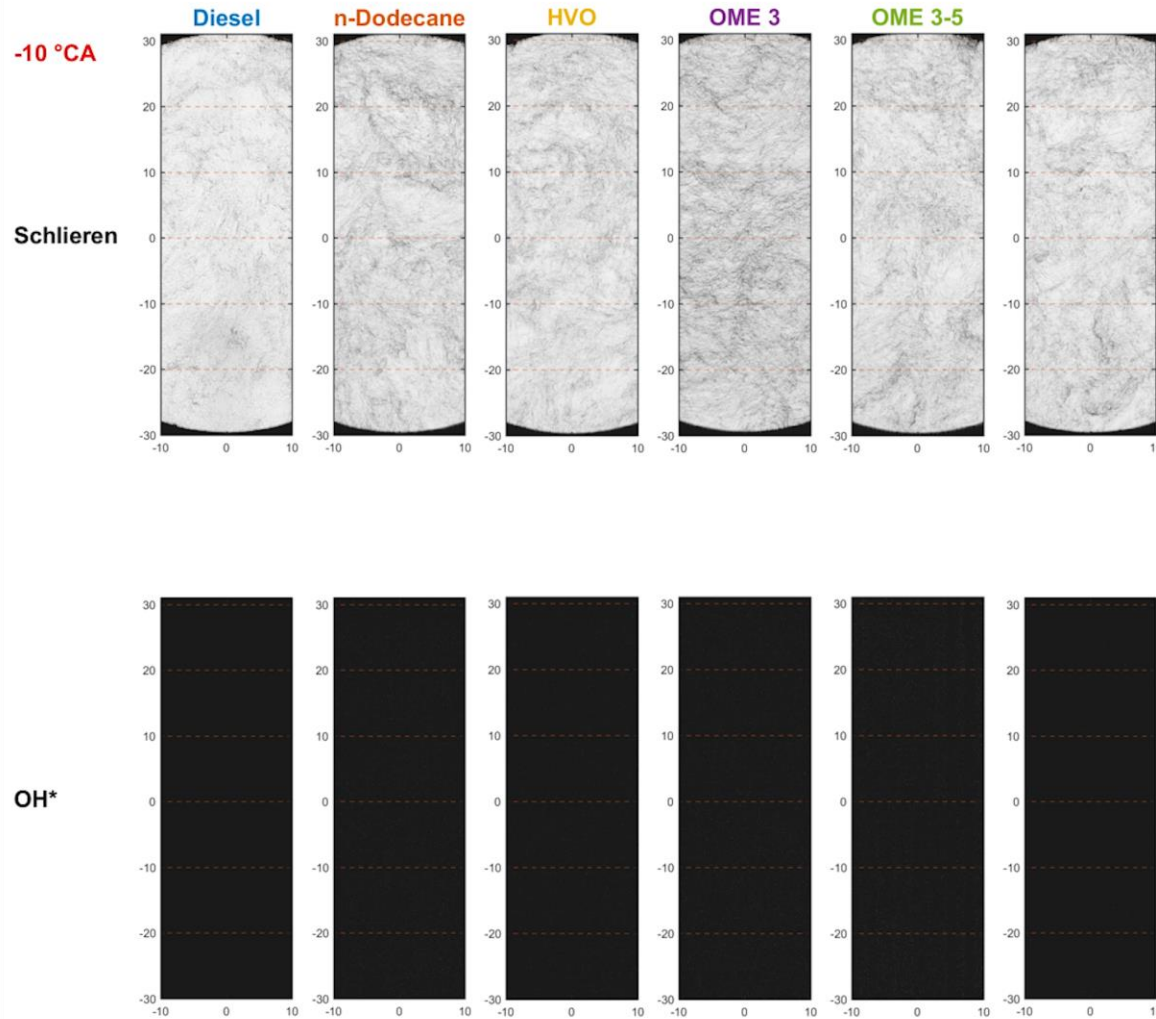


Characterization of dual-fuel combustion processes

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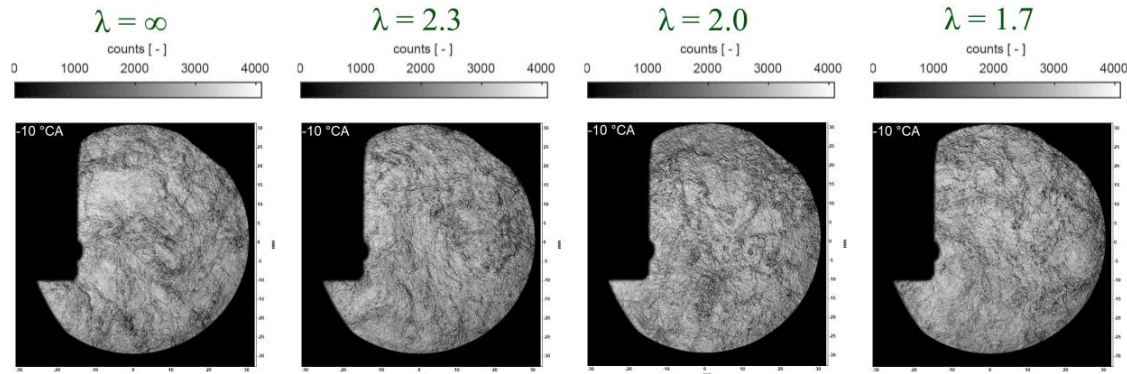
Schneider, B.; Schürch, C.; Boulouchos, K.; Herzig, S.; Hangartner, M.; Humair, D.; Wüthrich, S.; Gossweiler, C.; Herrmann, K. The Flex-OeCoS—a Novel Optically Accessible Test Rig for the Investigation of Advanced Combustion Processes under Engine-Like Conditions. *Energies* **2020**, *13*, 1794. <https://doi.org/10.3390/en13071794>

Fuel Variation

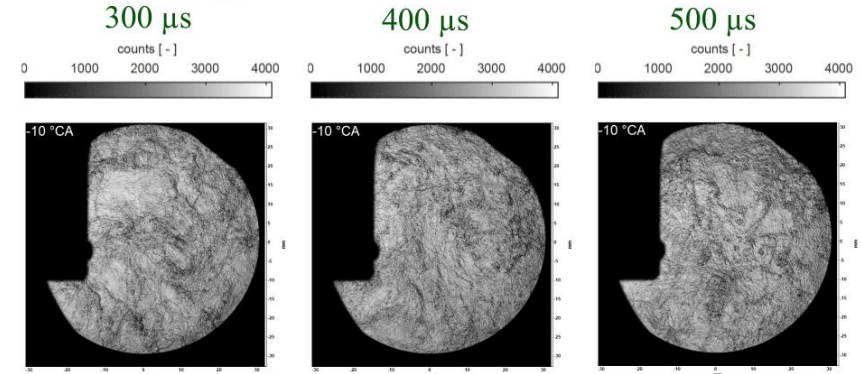


Schneider, B.; Schürch, C.; Boulouchos, K.; Herzig, S.; Hangartner, M.; Humair, D.; Wüthrich, S.; Gossweiler, C.; Herrmann, K. The Flex-OeCoS—a Novel Optically Accessible Test Rig for the Investigation of Advanced Combustion Processes under Engine-Like Conditions. *Energies* **2020**, *13*, 1794. <https://doi.org/10.3390/en13071794>

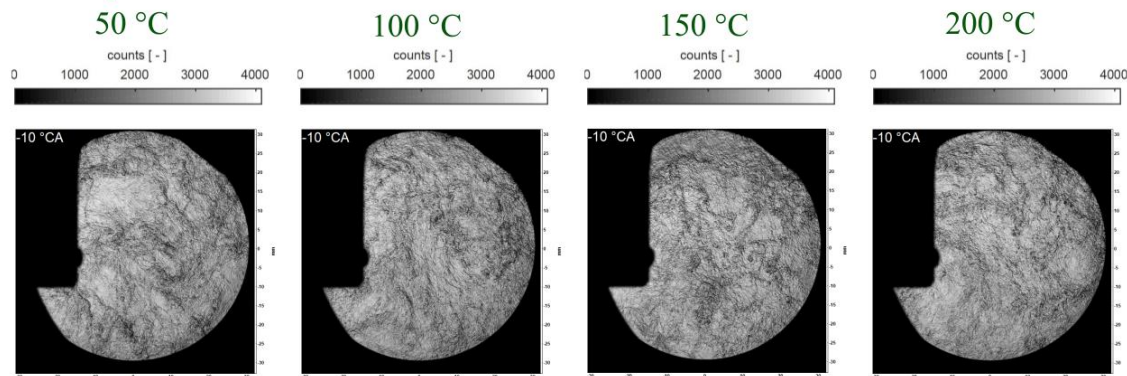
Lambda Variation



Energizing Time Variation



Temperature Variation



Schneider, B.; Schürch, C.; Boulouchos, K.; Herzig, S.; Hangartner, M.; Humair, D.; Wüthrich, S.; Gossweiler, C.; Herrmann, K. The Flex-OeCoS—a Novel Optically Accessible Test Rig for the Investigation of Advanced Combustion Processes under Engine-Like Conditions. *Energies* **2020**, *13*, 1794. <https://doi.org/10.3390/en13071794>

Stay Tuned For More CFD
Results!

Summary

We must act NOW

~50 Gtons CO2 in 30 years

Combustion Engines are not that bad

Fossil fuel is

The shipping industry's future is still unclear

Communication between academia and industry is crucial

Dual Fuel engines could be the solution

They are already gaining popularity

A good dual fuel CFD model will already mitigate thousands of tons of CO2

Industry still relies heavily on experimental R&D testing

We as academic researchers must play our role in the energy challenge

Develop fast and reliable tools to help engine manufacturers

References

- Energy Systems
 - Held et al. (2021): *European Transport Research Review*, vol. 13, art. 9
 - Held et al. (2021): *7th Internat. Symposium on Ship Operations, Management, & Economics*
 - Stolz & Held et al. (2021): *Applied Energy*, vol. 285: 116425
- Experimental investigations
 - Schneider, B.; Schürch, C.; Boulouchos, K.; Herzig, S.; Hangartner, M.; Humair, D.; Wüthrich, S.; Gossweiler, C.; Herrmann, K. The Flex-OeCoS—a Novel Optically Accessible Test Rig for the Investigation of Advanced Combustion Processes under Engine-Like Conditions. *Energies* 2020, *13*, 1794.
<https://doi.org/10.3390/en13071794>
 - Characterization of dual-fuel combustion processes: D. Humair, P. Cartier, P. Süess, S. Wüthrich, K. Herrmann, C. Barro, B. Schneider, C. Schürch, K. Boulouchos
 - Srna, Aleš, et al. "Effect of methane on pilot-fuel auto-ignition in dual-fuel engines." *Proceedings of the Combustion Institute* 37.4 (2019): 4741–4749.
 - Srna, Aleš, et al. "Experimental investigation of pilot-fuel combustion in dual-fuel engines, Part 2: Understanding the underlying mechanisms by means of optical diagnostics." *Fuel* 255 (2019): 115766.
- Simulations
 - Seddik, Omar, et al. *Flamelet generated manifolds applied to Dual-Fuel combustion of lean methane/air mixtures at engine relevant conditions ignited by n dodecane micro pilot sprays*. No. 2019-01-1163. SAE Technical Paper, 2019.