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Challenges in Simulation of Ammonia Diesel Combustion for Dual-fuel Heavy-duty Engines

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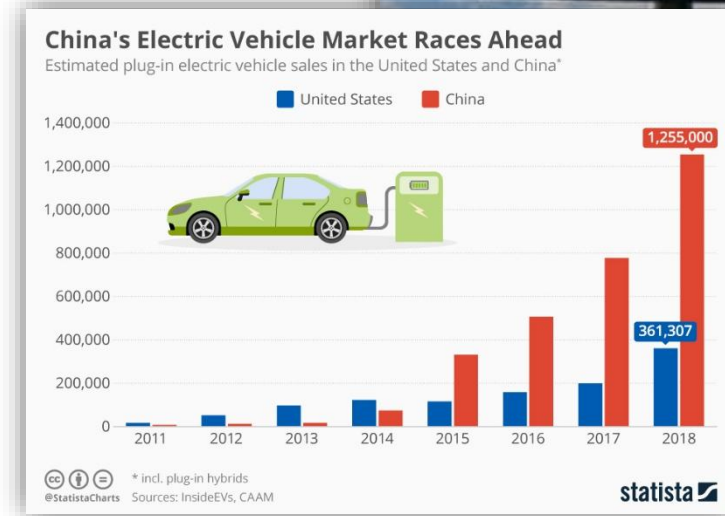
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Why?

- ICE decarbonization has been set forward by many international communities (EU, UK, China, etc.).
- Are battery-powered electric vehicles (BEVs) the only option?
- Using an alternative fuel could save the need for replacing the whole power plant.
- Hydrogen, as proposed, is difficult to transport and store [1, 2].
- Ammonia could achieve the same performance, without these issues.

www.greenammonia institute.cl



[1] P. Hu et al. *Nature Comm* 2015, DOI: 10.1038/ncomms7859.

[2] D. Zhao et al. *Energies*, DOI: 10.3390/en17102337.

Combustion of Ammonia

- Ammonia has ~3x volumetric energy density than compressed Hydrogen.
- When produced via renewable energies, it doesn't emit any GHG.
- However, it's combustion characteristics are far from those of fossil fuels.
- Low burning velocity, high auto-ignition pressure/temperature, etc.
- Ammonia is also highly toxic.

| Properties | Unit | Compressed Hydrogen | Liquid Hydrogen | Methanol | Liquid Ammonia |
|----------------------------------|-----------------------------------|---------------------|-----------------|---------------------------------------|---------------------------------------|
| Storage method | - | Compression | Liquefaction | Ambient | Liquefaction |
| Temperature | °C | 25 (room) | -252.9 | 25 (room) | 25 (room) |
| Storage pressure | MPa | 69 | 0.1 | 0.1 | 0.99 |
| Density | kg/m ³ | 39 | 70.8 | 792 | 600 |
| Explosive limit in air | %vol | 4-75 | 4-75 | 6.7-36 | 15-28 |
| Gravimetric energy density (LHV) | MJ/kg | 120 | 120 | 20.1 | 18.6 |
| Volumetric energy density (LHV) | MJ/L | 4.5 | 8.49 | 15.8 | 12.7 |
| Gravimetric hydrogen content | wt% | 100 | 100 | 12.5 | 17.8 |
| Volumetric hydrogen content | kg-H ₂ /m ³ | 42.2 | 70.8 | 99 | 121 |
| Hydrogen release | - | Pressure release | Evaporation | Catalytic decomposition T > 200 °C | Catalytic decomposition T > 400 °C |
| Energy to extract hydrogen | kJ/mol-H ₂ | - | 0.907 | 16.3 | 30.6 |

Source: Extracted from M. Aziz et al. *Energies* 2020, DOI: 10.3390/en13123062

| Species | Ammonia | Methanol | Hydrogen | Methane | Gasoline |
|--|-----------------|--------------------|----------------|-----------------|----------|
| Formula | NH ₃ | CH ₃ OH | H ₂ | CH ₄ | - |
| Storage | Liquid | Liquid | Compressed | Compressed | Liquid |
| Storage temperature (K) | 300 | 300 | 300 | 300 | 300 |
| Storage pressure (MPa) | 1.1 | 0.1 | 70 | 25 | 0.1 |
| density @ storage conditions (kg.m ⁻³) | 600 | 784.6 | 39.1 | 187 | ~740 |
| FL in air (vol.%) | 15-28 | 6.7-36 | 4.7-75 | 5-15 | 0.6-8 |
| LBV @ stoichiometry (m.s ⁻¹) | 0.07 | 0.36 | 3.51 | 0.38 | 0.58 |
| Auto-ignition T (K) | 930 | 712 | 773-850 | 859 | 503 |
| Research Octane Number | 130 | 119 | >100 | 120 | 90-98 |
| LHV (MJ/kg) | 18.8 | 19.9 | 120 | 50 | 44.5 |

Source: Extracted from C. Mounaim-Rousselle et al. *Energies* 2021, DOI: 10.3390/en14144141

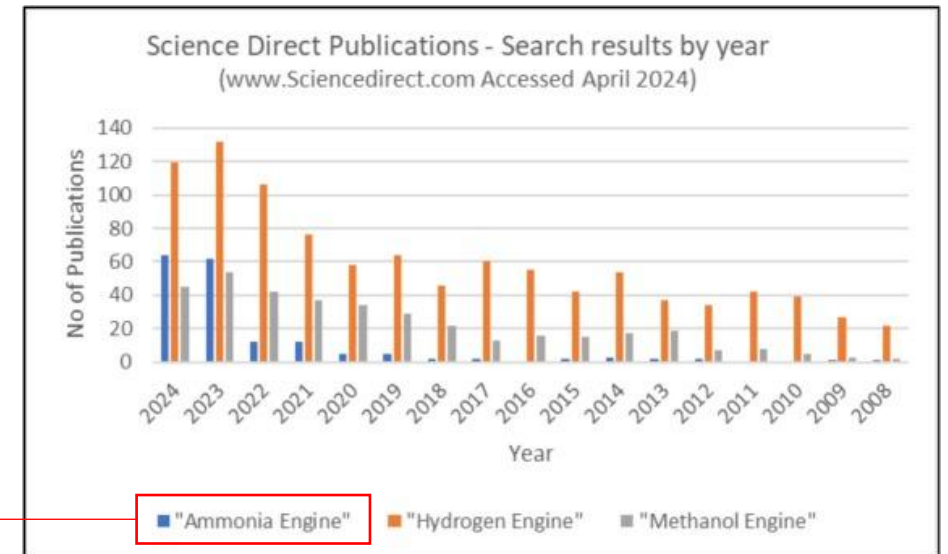
Cases of Use

- Slow burning could be negated in slowly rotating engines (e.g., marine).
- Dedicated manufacturers have explored this possibility (MAN, Wärtsilä).
- Due to its toxicity, ammonia is not considered safe for (public) road vehicles.
- Possible alternative for non-public roads and off-road (mining, gensets, etc.).



Research

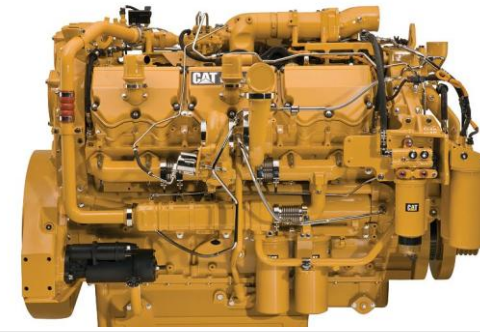
- Investigation into alternative fuels has been ramping up in academia and industry.
- Ammonia now has an important share of research among other fuels.
- What do these studies focus on?
- Mainly, small-scale (road vehicles) and marine-scale engines.
- Little to no research on off-road, heavy-duty engines.



Source: Extracted from D. Heaton, and A. Cairns. *Fuel*, 2025. DOI: 10.1016/J.FUEL.2024.133538

Off-road Engines

- Underserved in research, but tightening of standards on off-road vehicles (EPA Tier 5, EU Stage V) urges for diminishing CO₂ emissions.
- The same operating principle as road vehicles (usually Diesel fuel).
- Larger displacement, power ratings, and emission figures.
- Large size and cost make acquisition for research difficult (but not impossible).



| | |
|-------------------------------|--|
| Manufacturer and Model | CAT C32 |
| Configuration | V12, 4 stroke, direct injection diesel |
| Rated engine speed | 1800 rpm |
| Bore × stroke | 145 mm × 162 mm |
| Displacement | 32.1 L |
| Aspiration | Turbocharged after cooled aspiration |
| Engine power (bkW) | 994 |
| Compression ratio | 15 |

Source: Extracted from [4]

CATERPILLAR C32 For Sale 1 - 23 of 23 Listings

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Show Closest First:

2023 CATERPILLAR C32
Engine



USD \$251,797.00

USD \$251,797.00 + VAT = USD \$289,566.55
(VAT applies to buyers in South Africa)


Condition: New

Location: Kensington, Gauteng, South Africa

Email Seller [+27 11 083 5554](#)

Seller: Hole Tech (Pty) Ltd

2008 CATERPILLAR C32
Engine



USD \$159,500.00

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2006 CATERPILLAR C32
Engine



USD \$136,000.00

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Condition: Used

Location: Washington, North Carolina

Email Seller [\(888\) 707-6740](#)

Seller: Gregory Poole Equipment Company

CATERPILLAR C32
Engine



USD \$99,995.00

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Condition: Rebuilt

Location: Chicago, Illinois

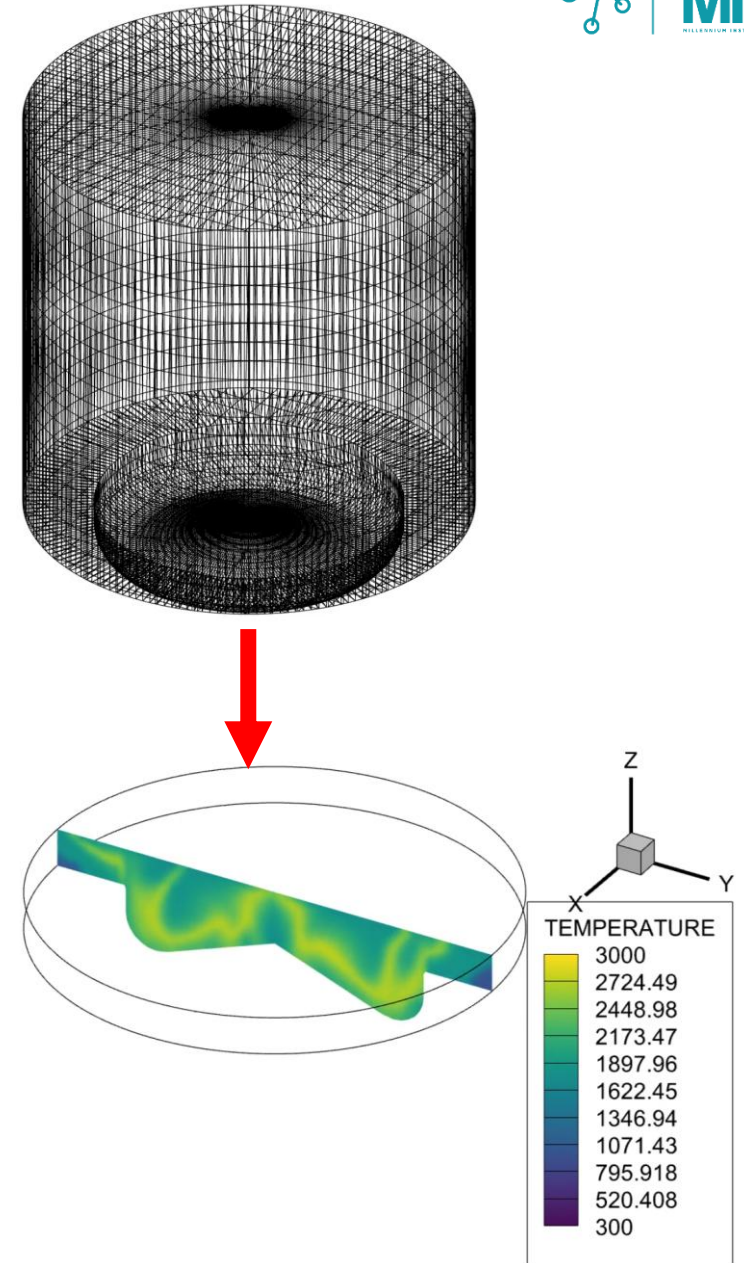
Email Seller [\(312\) 631-7996](#)

Seller: Diesel Sales

Source: powersystemstoday.com

Numerical Research

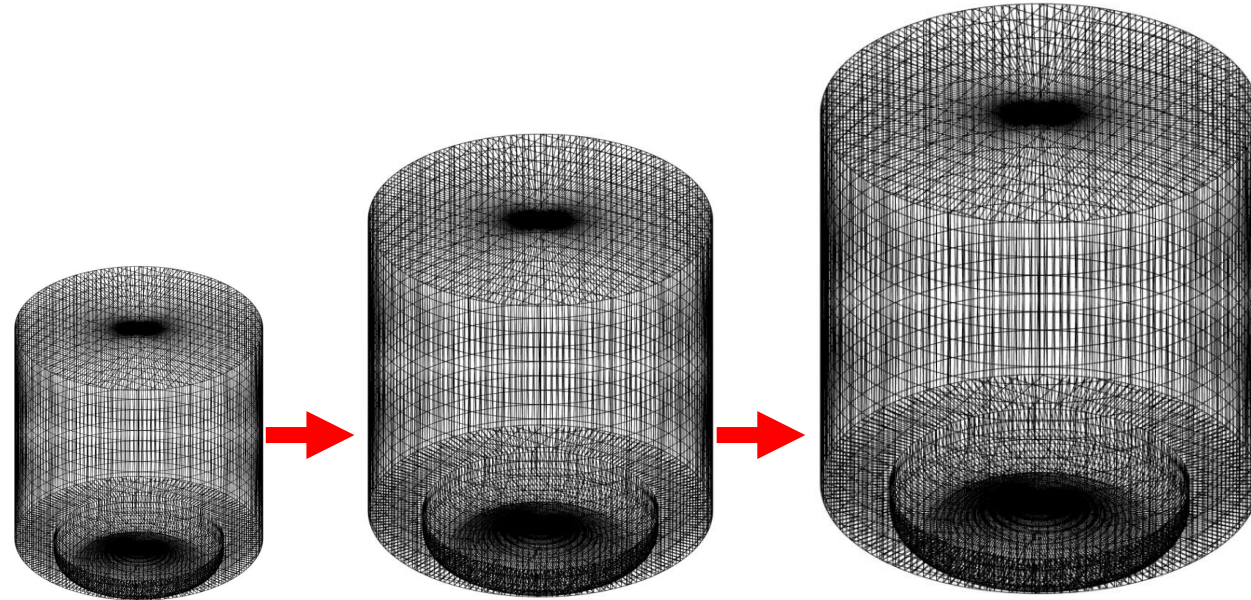
- Numerical simulation can save time and expenses related to operating a physical ICE.
- Thermodynamic, chemistry and CFD analyses are performed to simulate their operation.
- Validation is often found by comparing a numerical model to experimental data for a similar setup.



Source: Author

Challenges

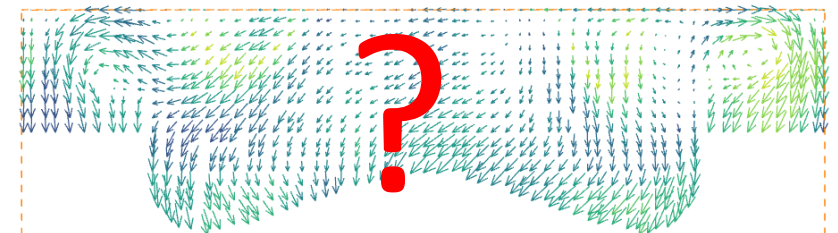
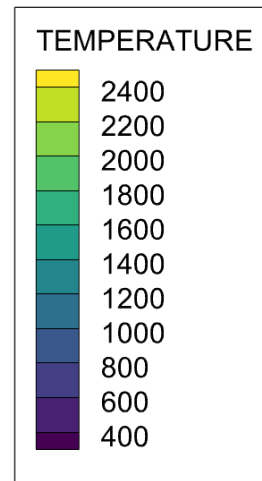
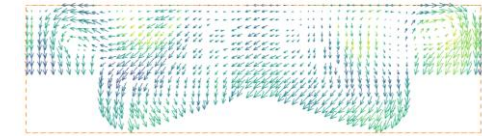
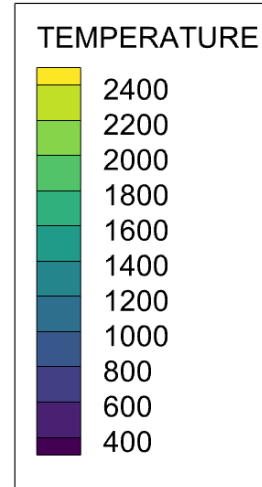
- Limited direct experimental validation.
- Not only does size change when compared to conventional research:
 - Turbulence phenomena is distinctly different for an upscaled geometry.
 - Chemical mechanisms must be validated or adapted.
- Therefore, nothing assures that ammonia engine results on small engines scale accordingly with size.



Source: Author

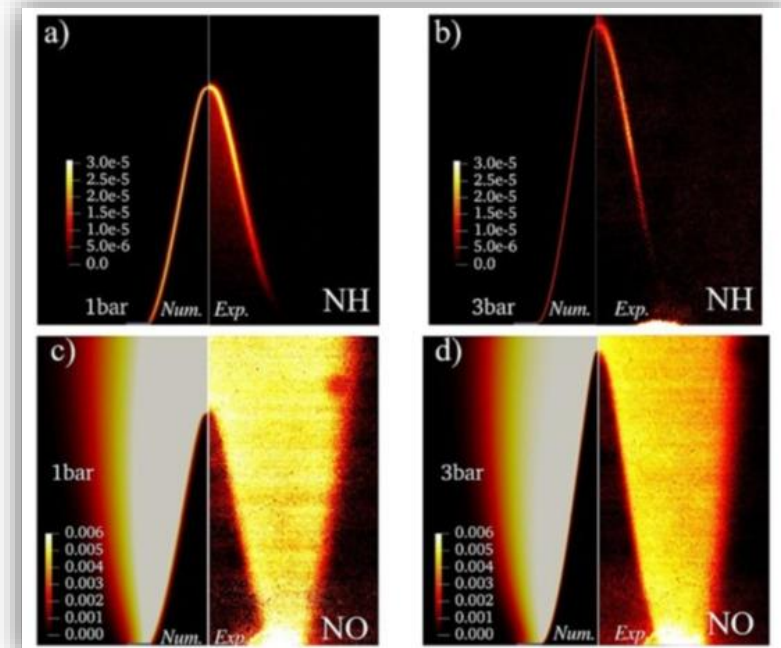
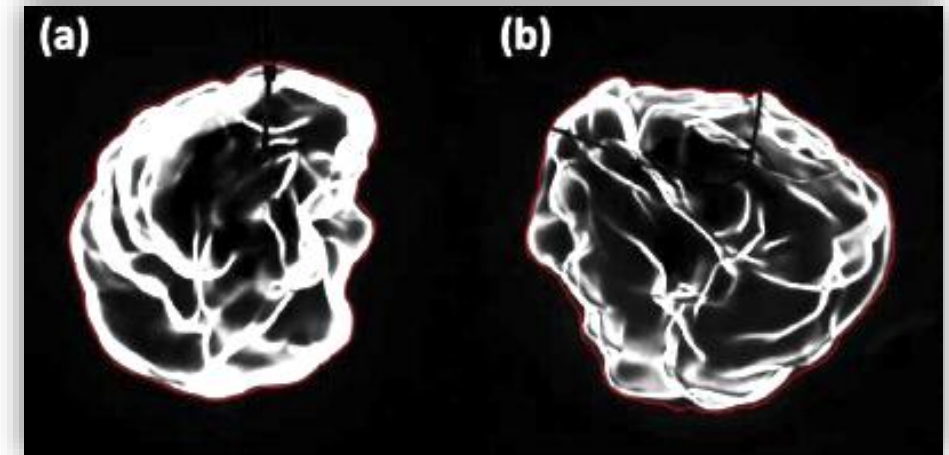
Challenges

- More research is needed to develop models that predict the behaviour of heavy-duty engines.
- E.g., A comparison of turbulence measurements for different sizes of the same cylinder geometry.
- How do turbulent structures change with respect to size?



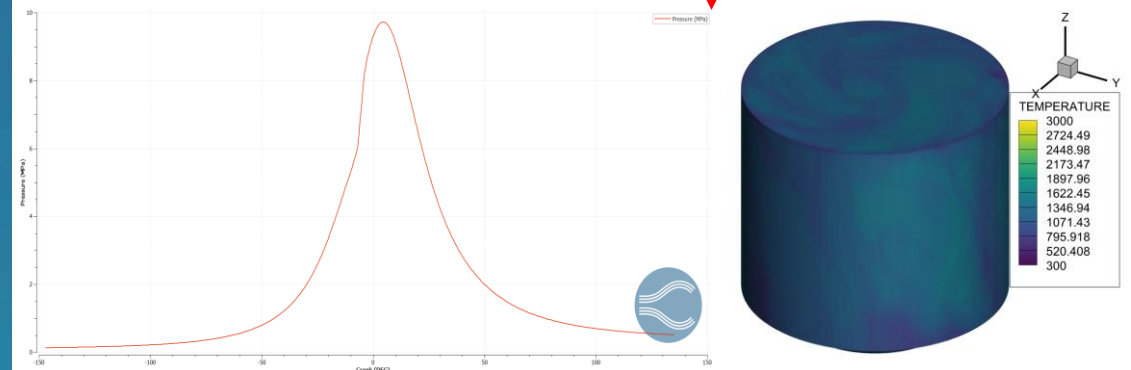
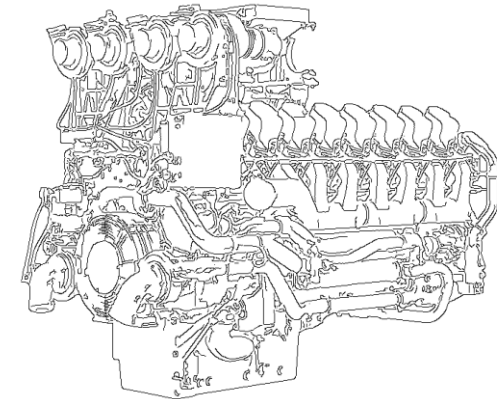
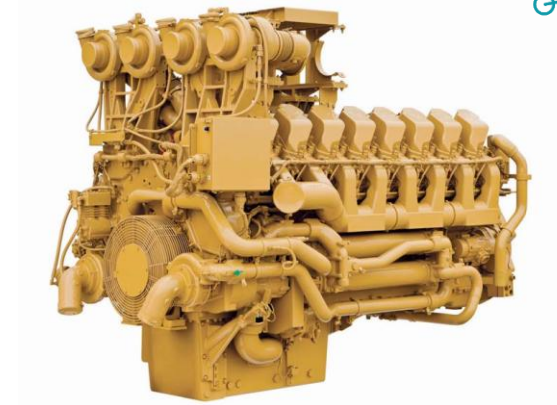
Challenges

- Performance of chemical mechanisms at increasing cylinder size & ammonia content.
- Does a particular mechanism predict properties accurately on various domains/eq. ratio/operating conditions?
- Can be validated using combustion chambers of different sizes. No need for full engine!



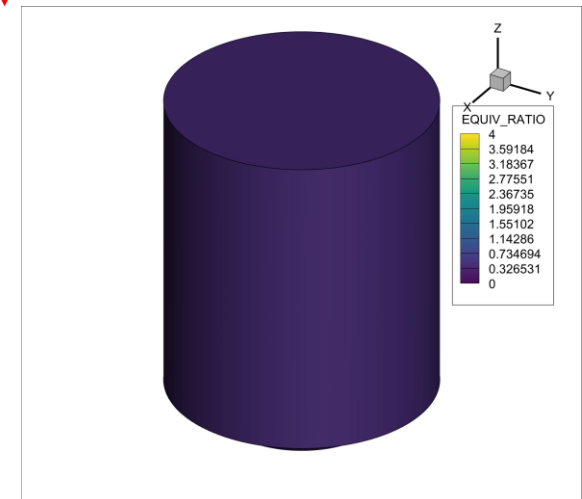
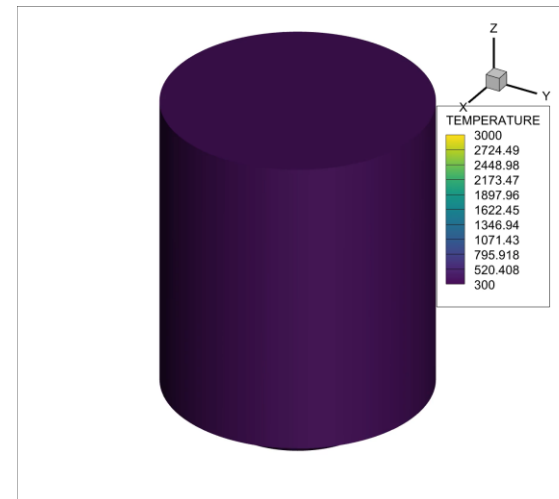
Challenges

- Is validation with a physical engine possible?
- Sure, if you can find one.
- Then, you can validate the CFD, chemistry, etc. directly.
- After this, simulation is still important, as all variables can be analyzed for sensibility.
- Check out our work in the future for more on this!



Our work

- Caterpillar C32 Engine, used in 777G Mining Truck, from PowerTrain Technologies.
- To be refitted for diesel/ammonia use.
- Numerical simulation to be compared with similar (smaller) physical engines.
- Pave the way for physical trials + expand on obtained results after validation.
- Hopefully, help decarbonize the mining industry, one step at the time.



Conclusions

- **Off-road, heavy-duty ICEs are an integral part of the industrial world. However, research in alternative fuels for these engines is not as advanced as in other engine segments.**
- **Numerical simulation can (somewhat) cover the lack of research in heavy-duty off-road ICEs, with adequate validation.**
- **Validation of these results is not trivial. When direct validation (using a physical engine) is not possible, indirect measurements can be extrapolated to include the studied case.**
- **Work is in progress to make experimental data available for validation of numerical simulations.**

ACKNOWLEDGMENT

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