Technische Universität Braunschweig

MaritimeMET I Workshop

Modelling of MeOH Dual-Fuel Combustion and Emissions Formation – Using Kinetic Mechanisms and Machine Learning Approach

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Agenda

- Motivation for Renewable Fuels in the Maritime Sector and for the Simulation of Combustion and Emissions
- Combustion Model for a Dual-Fuel Engine
- Using Kinetic Mechanisms and Machine Learning for Emissions Modelling
- Application of the Models in the Project MaritimeMET

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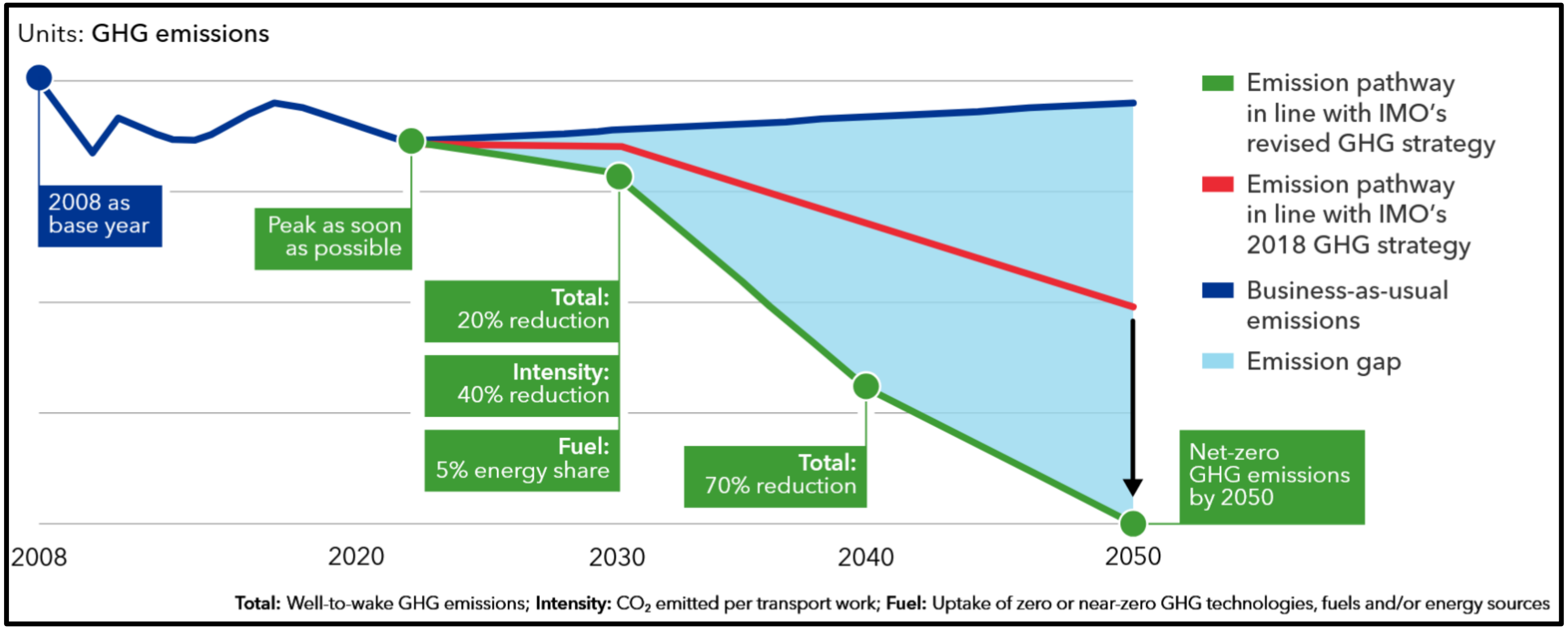
Motivation for Renewable Fuels in the Maritime Sector

- **Maritime transport:** Responsible for over 80% of global trade [1]
- **Shipping emissions:** Account for 11–15% of global transport CO_2 emissions [2]
- **International Maritime Organization:** Net-zero emissions from shipping by around 2050

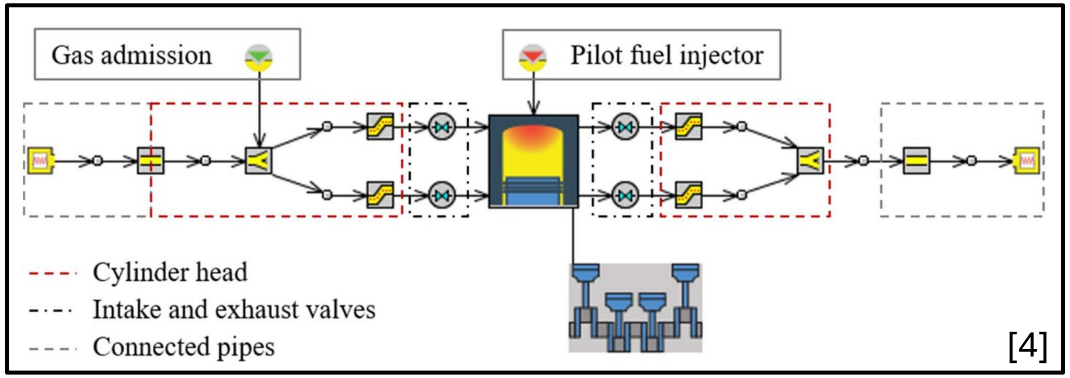


[3]

Motivation for Simulation

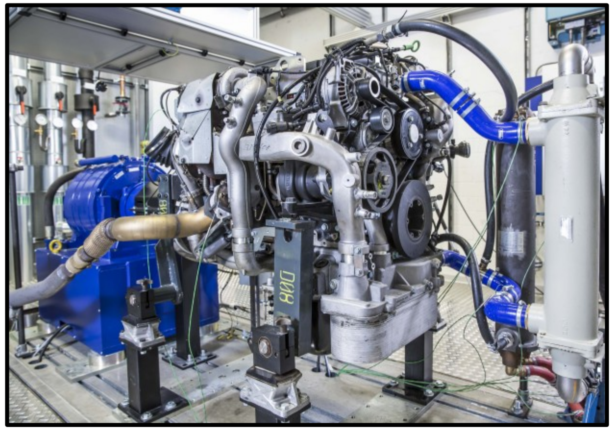
Simulation

- Can be fast and cost-efficient
- Testing of multiple scenarios
- Suitable early in the development process
- Modelling reality with simplifications



Test bench

- Reflects real system behaviour
- Validation and calibration of simulations
- Limited test flexibility



Simulation can deliver fast and cost-efficient results, while test benches provide realistic validation

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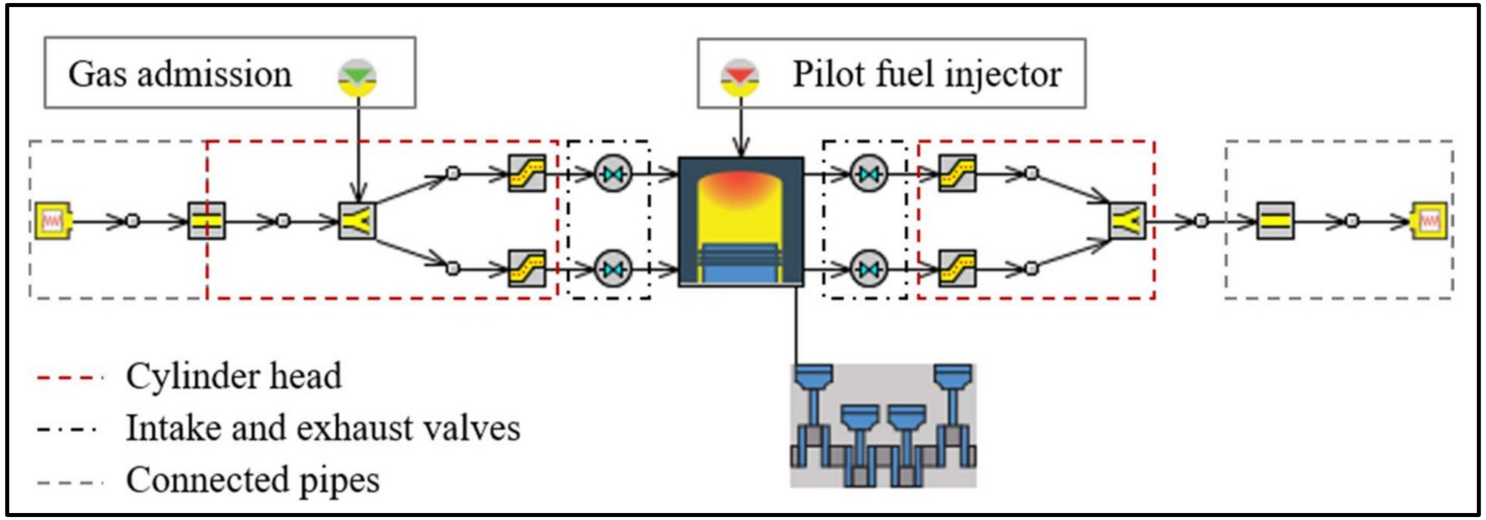
Modelling of Combustion

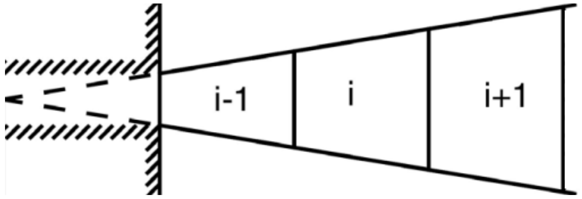
- **Single cylinder engine model**: Developed in GT-Power an engine simulation software
  - ➢ 1D flow simulation from the intake manifold through the valves to the exhaust
- **Combustion simulation:** Implementation of the combustion model in the cylinder
  - ➢ Model for dual-fuel engines (methanol and n-heptane) for the calculation of the ignition and the flame propagation in the cylinder



Single cylinder engine model in GT-Power [4]

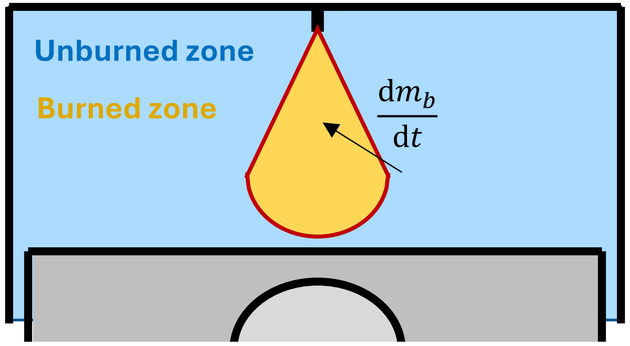
Submodels of the Combustion Model

- **Models for the ignition timing**
  - ➢ 1D spray model → liquid fuel distribution
  - ➢ Evaporation model → temperature distribution
  - ➢ Ignition delay using reaction kinetics



Schematic view of the 1D spray model [4]

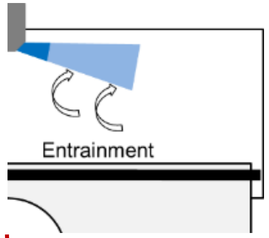
- **Models for the combustion**
  - ➢ Pilot spray
  - ➢ Homogeneous methanol/air mixture

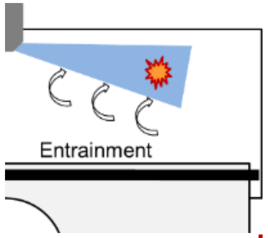


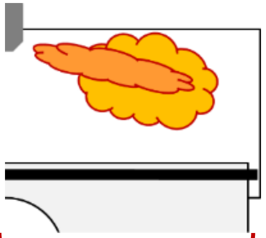
$\frac{dm_b}{dt}$: Implementation in the flame front

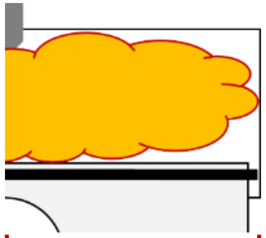
The model describes the combustion process, including pressure, temperature, and mass flow rate from the unburned zone to the burned zone

Schedule of the Submodels of the Combustion Model









Ignition timing

- Spray propagation in the combustion chamber
- Consideration of ignition delay for the precise determination of the ignition timing

Combustion of the pilot spray
(methanol + n-heptane)

Combustion of the homogeneous methanol/air mixture

SOI

SOC

Time

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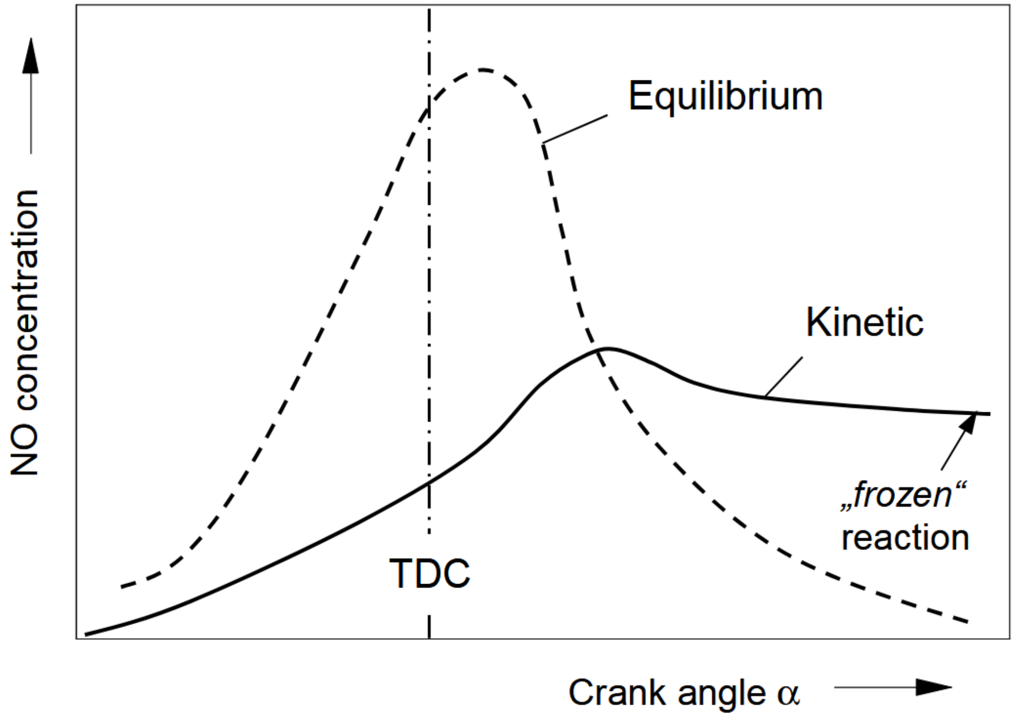
Kinetic Mechanism for the Calculation of the Emissions

- **Combustion model describes the burning progression**
  - ➢ Temperature, pressure and composition of the burned zone in chemical equilibrium

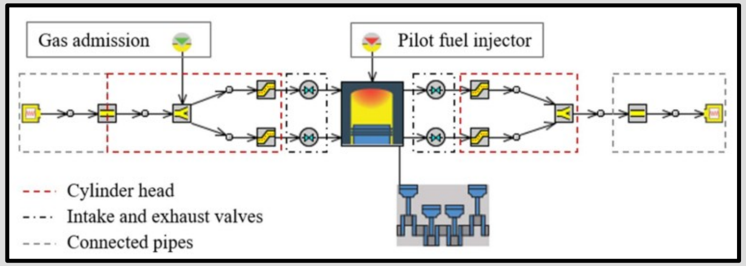
- **Simulation of emissions formation in Cantera**
  - ➢ Cantera is an open-source collection of object-oriented software tools for chemical kinetics, thermodynamics and transport processes [5]
  - ➢ Input: Results from the combustion model
  - ➢ Output: Kinetically controlled emission formation over the engine cycle



Qualitative NO concentration over crank angle for chemical equilibrium and kinetically controlled NO formation [6]

Structure of the Models

Combustion model



Input layer

$T_{ox}(\varphi)$, $p_{Cyl}(\varphi)$

Combustion Products
e.g. *H_2O, N_2, O_2, CO, H_2, O, H, OH*

Cantera
Kinetic calc. of emissions formation

Reactants

Products

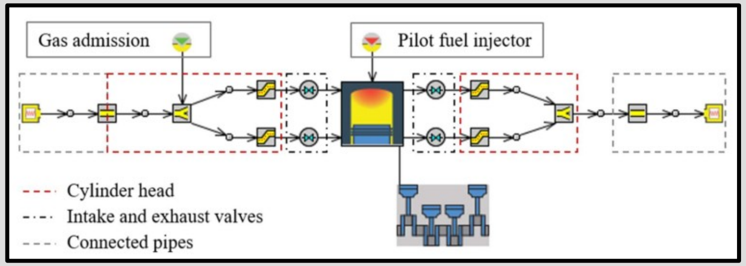
Mole fractions

- $x_{\mathrm{NO,EVO}}$
- $x_{\mathrm{CO,EVO}}$
- …

The combustion model provides input data to Cantera, which then calculates the rate of change of emissions

Structure of the Models

Combustion model



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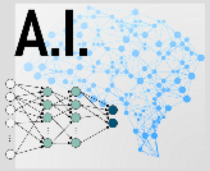


ML calculate emissions formation

Reactants

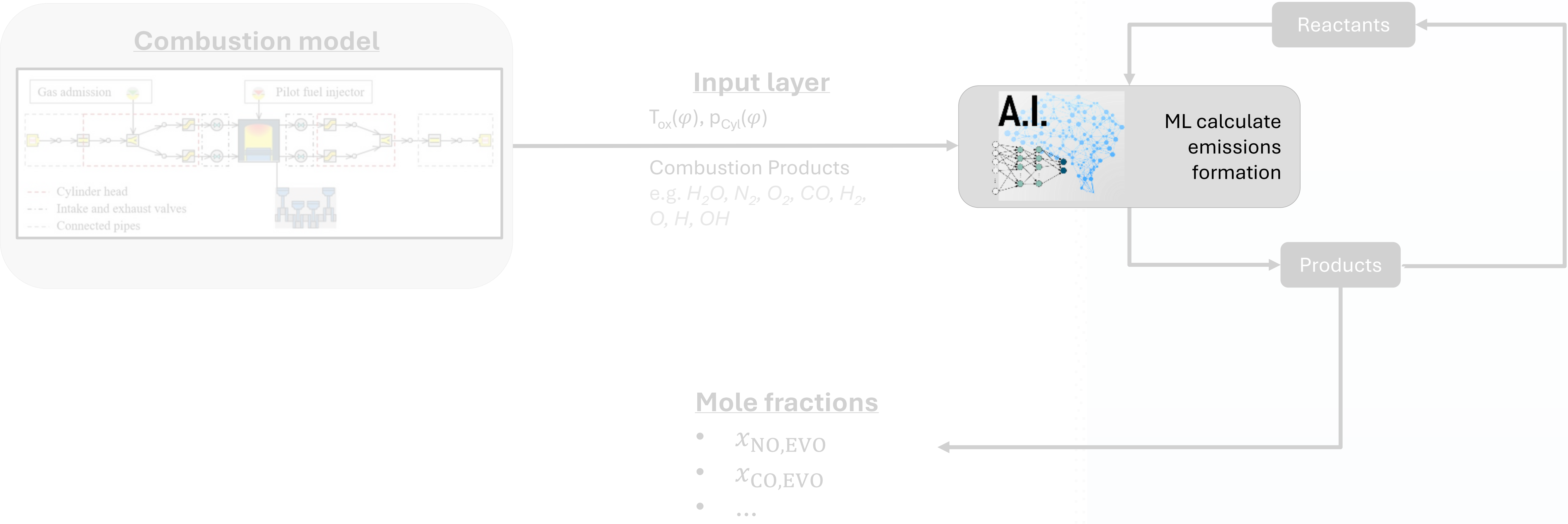
Products

Mole fractions

- $x_{\mathrm{NO,EVO}}$
- $x_{\mathrm{CO,EVO}}$
- …

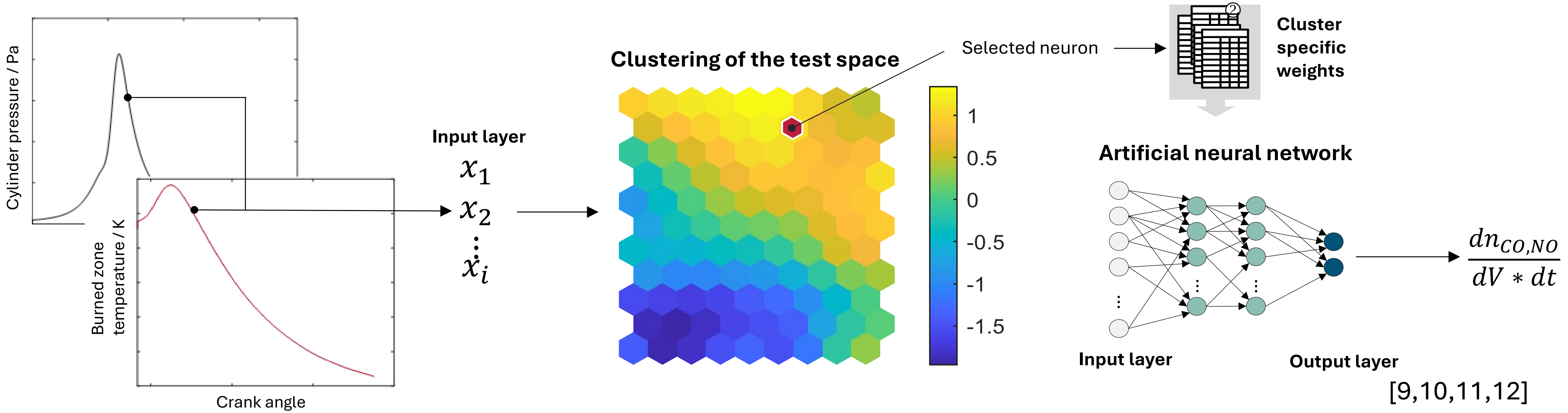
The machine learning model is being trained using Cantera data with the aim of replacing it

Structure of the Models



The machine learning model is being trained using Cantera data with the aim of replacing Cantera.

- **The model learns the formation of the relevant species over volume and time from a large training dataset**
  - ➢ Not enough measurements can be taken → synthetic generation of data points
- **The test space is derived from the evaluation of measurement data**
- **The test space is divided using machine learning into sub-spaces, each covering a range of pressure, temperature and relevant species**
  - ➢ A specialized artificial neural network is trained for each sub-space

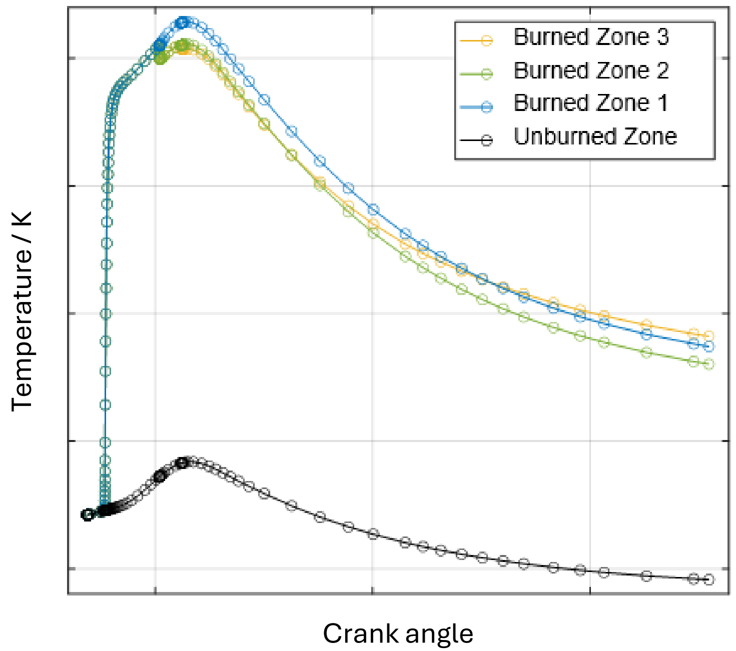


[9,10,11,12]

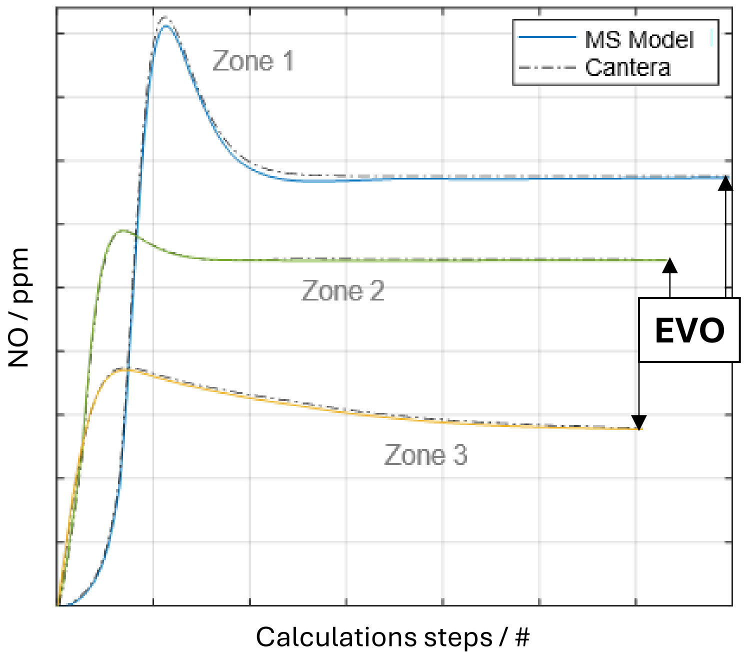
Model Results for the Calculation of Entire Engine Cycles

- **The combination of clustering and artificial neural network makes it possible to calculate the reaction kinetics much faster**

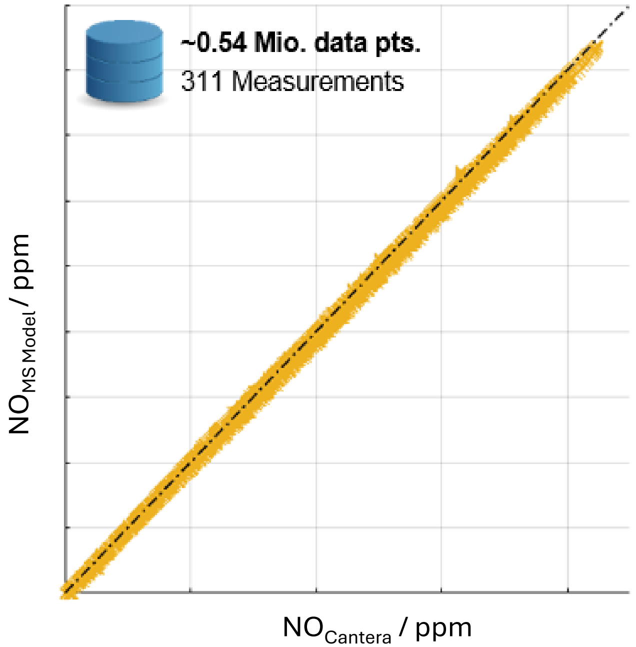
4-Zone: Temperature traces



NO formation in the burned zones



Regression: NO formation



The machine learning approach provides NO formation over an engine cycle comparable to Cantera

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Application of the Models in the Project MaritimeMET

- **Calibration of the combustion model for methanol and n-heptane using measurement data from the Danish Technological Institute (DTI)**

- **Train the existing in-house machine learning approach for emission calculations**

  1. The GT-Model calculates the combustion process with input data from the test bench

  2. The information from the measurement data will be used to derive the test space for machine learning and the results from the GT-Model as input for a Cantera model used for emission calculations

  3. Training and validation of the machine learning approach, which is intended to learn the chemical mechanism and thereby replace Cantera

The goal is to enable efficient and accurate emission prediction using machine learning

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https://www.linkedin.com/showcase/maritimemet-project/about/

Kiitos.

Tak skal du have

Děkuju. Danke.

Merci ! Thank you.

Tack så mycket

Hartelijk dank.

Teşekkür ederim.

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References

[1] Shipping data: UNCTAD releases new seaborne trade statistics | UN Trade and Development (UNCTAD) [WWW Document], 2025. URL https://unctad.org/news/shipping-data-unctad-releases-new-seaborne-trade-statistics (accessed 7.21.2025).

[2] Global CO2 emissions from transport by sub-sector in the Net Zero Scenario, 2000-2030 – Charts – Data & Statistics [WWW Document], n.d. . IEA. URL https://www.iea.org/data-and-statistics/charts/global-co2-emissions-from-transport-by-sub-sector-in-the-net-zero-scenario-2000-2030-2 (accessed 7.21.2025).

[3] Maritime Forecast to 2050, 2023 edition (DNV) [WWW Document], n.d. URL https://www.dnv.com/publications/maritime-forecast-to-2050-edition-2023/ (accessed 02.28.2026).

[4] Frerichs, J., Küçükay, F., Eilts, P., Bargende, M., 2022. Development of a Combustion Model for Medium Speed Dual-Fuel Engines. Berichte aus dem ivb. Shaker Verlag, Düren. https://doi.org/10.24355/dbbs.084-202203271148-0

[5] Cantera [WWW Document], 2026. URL https://cantera.org/ (accessed 4.10.2026).

[6] Scholl, F., 2017. Study of premixed combustion induced by controlled hot surface ignition in stationary gas engines. Universidad de Valladolid. https://doi.org/10.35376/10324/28664

[7] Chindaprasert, N. Thermodynamic based prediction Model for NOx and CO Emissions from a Gasoline Direct Injection Engine. (Universität Rostock, 2007)

[8] Karvountzis-Kontakiotis, A. & Ntziachristos, L. Improvement of NO and CO predictions for a homogeneous combustion SI engine using a novel emissions model. *Applied Energy* 162, 172–182 (2016).

[9] Zhou, L., Song, Y., Ji, W. & Wei, H. Machine learning for combustion. *Energy and AI* 7, 100128 (2022).

[10] An, J., He, G., Luo, K., Qin, F. & Liu, B. Artificial neural network based chemical mechanisms for computationally efficient modeling of hydrogen/carbon monoxide/kerosene combustion. *nternational Journal of Hydrogen Energy* 45, 29594–29605 (2020).

[11] Franke, L. L. C., Chatzopoulos, A. K. & Rigopoulos, S. Tabulation of combustion chemistry via Artificial Neural Networks (ANNs): Methodology and application to LES-PDF simulation of Sydney flame L. 185, 245–260 (2017).

[12] Chi, C., Janiga, G. & Thévenin, D. On-the-fly artificial neural network for chemical kinetics in direct numerical simulations of premixed combustion. *Combustion and Flame* 226, 467–477 (2021).