Attaining Sustainability? The (Unintended) Consequences of Venture Capital Investments on Firms' Environmental Performance

Kenneth G. Huang[1], Michelle Xiaomin Fan[1], Jiaxing You[2]

Introduction

Using the context of the energy-intensive industry in China, we find: Strengthening of formal institutions for VC investment as a result of the top-down, major VC policy reform significantly increases the (air and water) pollution emissions intensity of target firms; Nevertheless, VC firms' greater experiences in energy-intensive industries and local governments' more robust environmental protection measures can mitigate such pollution; Thus, it is possible to benefit from improved VC investment institutions AND mitigate its (unintended) adverse impacts on environment under appropriate conditions (thus attaining sustainability).

Motivation

- Emerging economy of China has experienced rapid economic growth fueled by increasing energy consumption and (traditional) industrial processes but faces severe air and water pollution with major health and social implications
- As major consumers of energy and emitters of pollutants, firms in "energy-intensive" industries face challenges in satisfying the dual and (often) conflicting goals of improving profitability and reducing pollution emissions, esp. in such economies where environmental issues are vital
- VC investments and their institutional environment have improved significantly in China, and they can improve target firms' performance and innovation, but we know little about the consequences of VC policy/institutions on firms' environmental impacts, esp. for energy-intensive firms

Research Questions

- Whether and to what extent a strengthening of formal institutions for venture capital (VC) investments generate an (unintended) adverse consequence on the environment?
- How do the roles and attributes of the participating key stakeholders—investors and regulators—influence or mitigate such effects?

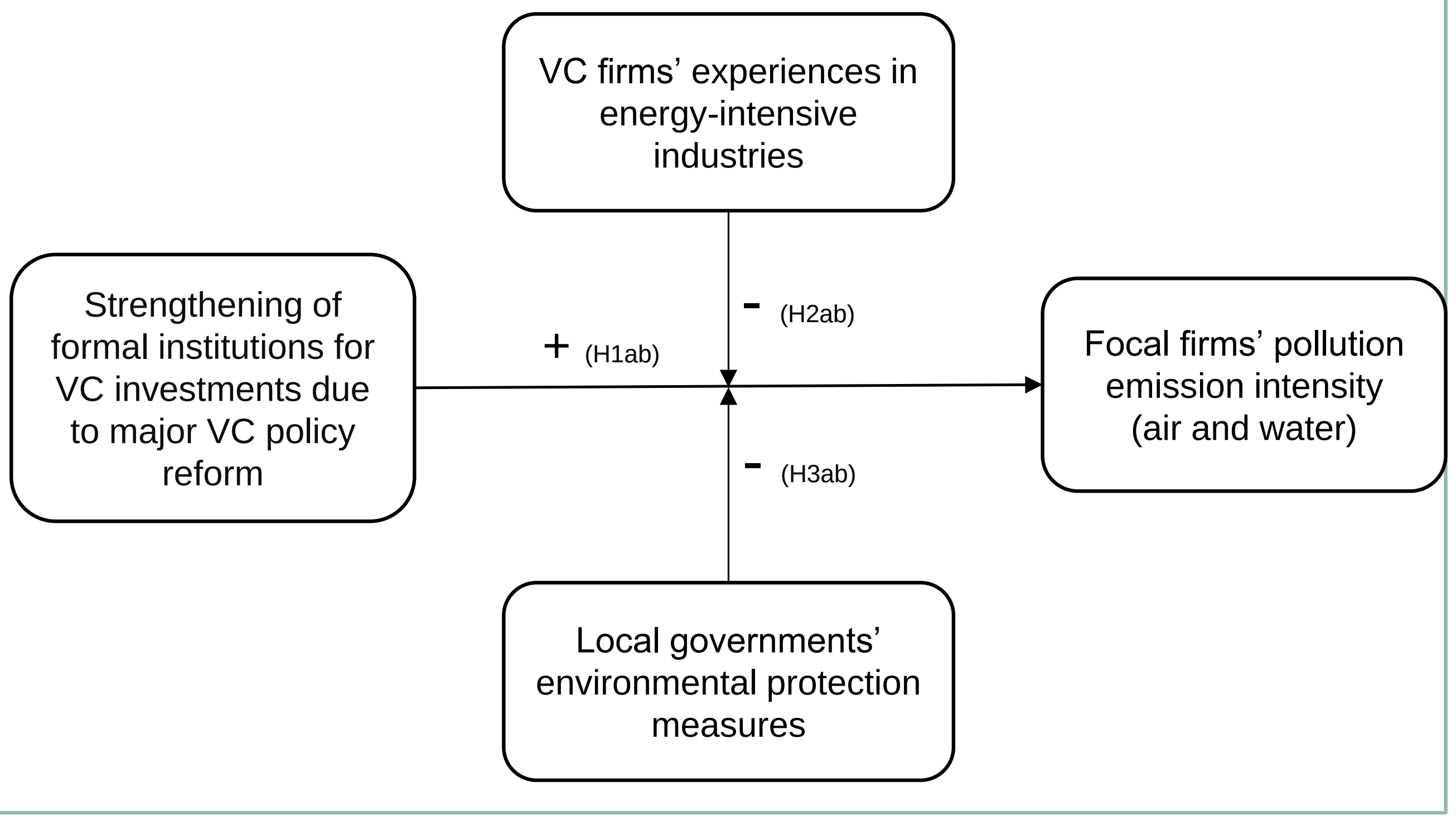
Conceptual background and theoretical framework

Entrepreneurial Finance and Firm Environmental Performance

- Prior studies suggest VC plays an important role in shaping target firms' operation, innovation, and eventual success
- Specifically, typical VC firms tend to adopt a shorter-term investment horizon and orientation, focusing on profitability and growth from their target firms
- But firms' environmental performance and sustainability often require a longer-term orientation and perspective taken by the VC investors

Strengthening of formal institutions for VC investment in China

- April 2009, Ministry of Finance (MF) and State Administration of Taxation (SAT) issued *Circular of Issues on Implementing the Preference Policy of Business Income Tax* (Tax [2009] No.69)
- June 2009, China Securities Regulatory Commission (CSRC) restarted granting IPOs
- **Oct. 2009, CSRC announced and established the Growth Enterprises Market (GEM) in the stock exchange**
- Local governments followed to establish favorable policies



VC firms' experiences in energy-intensive industries

Strengthening of formal institutions for VC investments due to major VC policy reform

Focal firms' pollution emission intensity (air and water)

Local governments' environmental protection measures

+ (H1ab)

- (H2ab)

- (H3ab)

Methodology

Focus on VC institutions change: Difference-in-differences (DID) estimation

- Use **plausibly exogenous**, major top-down VC policy reform announced and implemented in 2009 in China; Treatment Group: Firms in energy-intensive industries that VC firms tend to invest in **"VC-active" industries**; Control Group: Firms in energy-intensive industries typically not (or minimally) affected by VC firms' investment **"VC-inactive" industries**

Propensity score matching (PSM)

- Firm-level attributes on all the years before the policy reform: age, size, leverage, tangibility, ROA, R&D expenditure, and SOE

Data and sample

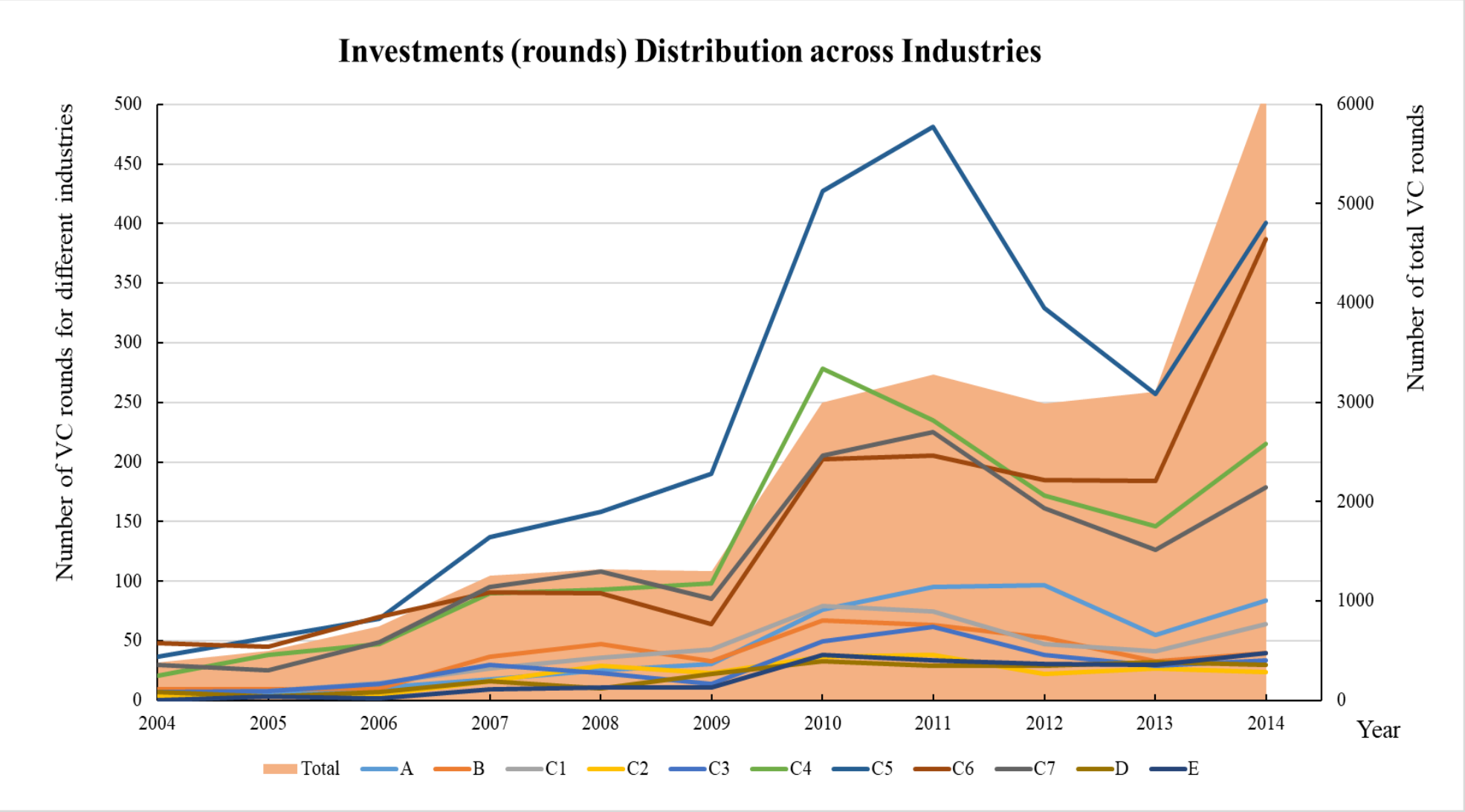
- Pollution Data: The Environmental Survey and Reporting (ESR); Financial Data: Annual Tax Survey (ATS); VC Data: CVSource
- **Final Sample**: 24,798 firms (2004-2014) after matching

Dependent variables

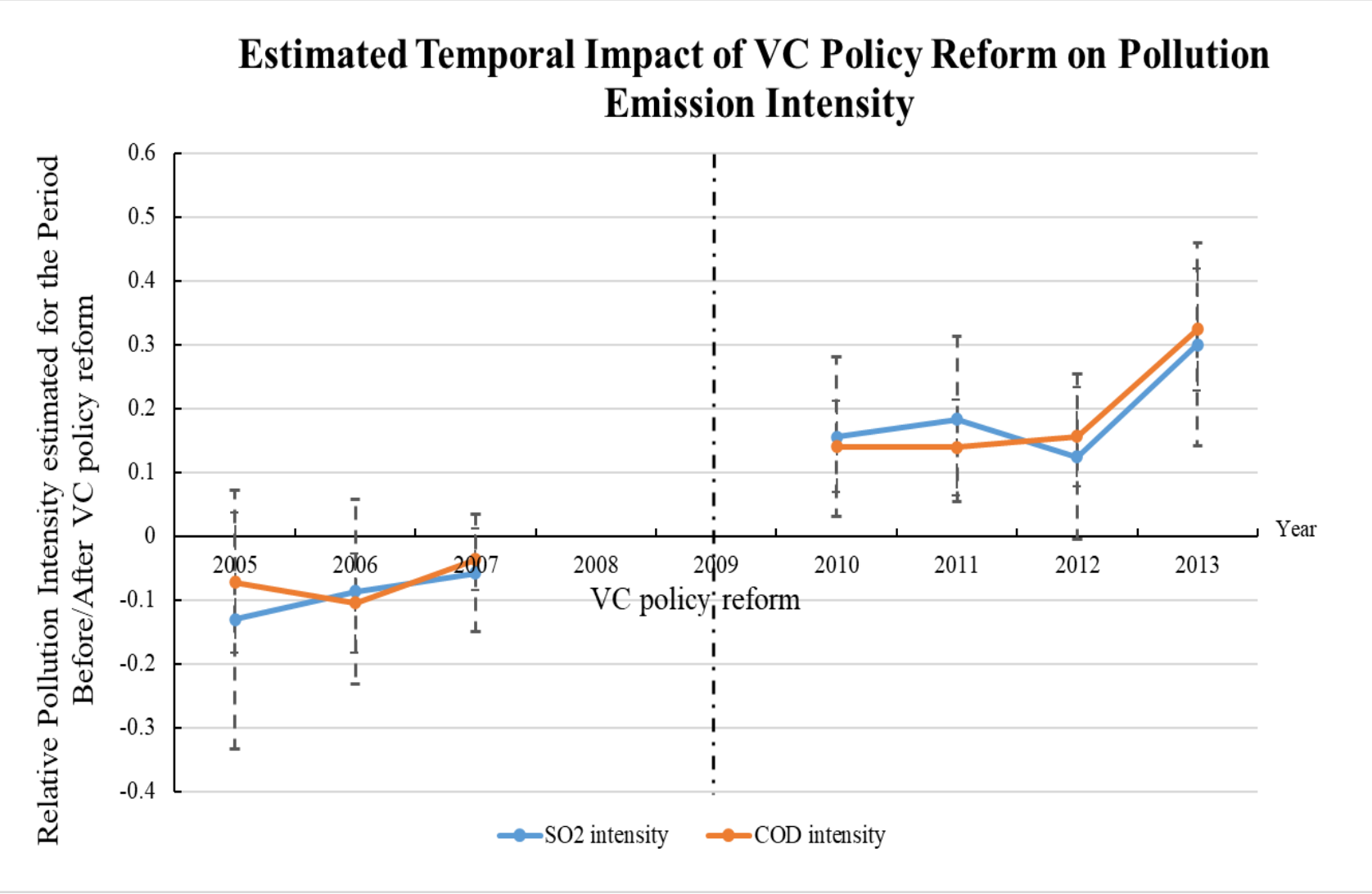
- Define the intensity of pollution emissions in the air, *SO2 intensity*, and in the water, *COD intensity* (kg/1,000 CNY), as the **total SO2 emission and COD emission respectively scaled by the actual output adjusted for inflation**, calculated based on the constant 2004 prices using CPI

Independent variables

- *Post-policy*: equals one if a focal firm belongs to an industry that VC firms actively invest in (i.e., treatment group) and during the VC policy reform year 2009 or later, and equals zero otherwise. For a focal firm in the control group, *post-policy* is always defined as zero



Investments (rounds) Distribution across Industries



Estimated Temporal Impact of VC Policy Reform on Pollution Emission Intensity

Contributions and Implications

- Extend prior literature on entrepreneurial finance and environmental sustainability by linking it to institutional theory
  - Decision-making by the focal firm depends on the participation and intervention of key stakeholders such as investors and regulatory agencies as each exerts its influence and the institutional regime in which the focal firm and these stakeholders are embedded in
  - Among the first study to investigate how the strengthening of institutions for VC investment could shape the target focal firms' (environmental) strategies and performance, and how the roles and salient attributes of these key stakeholders could jointly influence the focal firms' performance

- Dual roles of VC firms
  - We find support that VC investments enhance economic performance of target firms, including their profitability, growth and innovation
  - We provide new evidence on the "dark side" of VC investments institutions e.g., (unintended) adverse consequence on environment as VC investors and their target firms prioritize economic returns over social welfare and externalize adverse outcomes such as environmental pollution, especially in emerging economies with weak regulatory oversight and enforcement
  - Nevertheless, under the appropriate conditions, it is possible to reap economic return and mitigate the associated perverse outcomes through the roles played by key stakeholders involved in the decision process, such as investors and regulatory agencies

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Carbon Neutral Fuel Additives for Internal Combustion Engine

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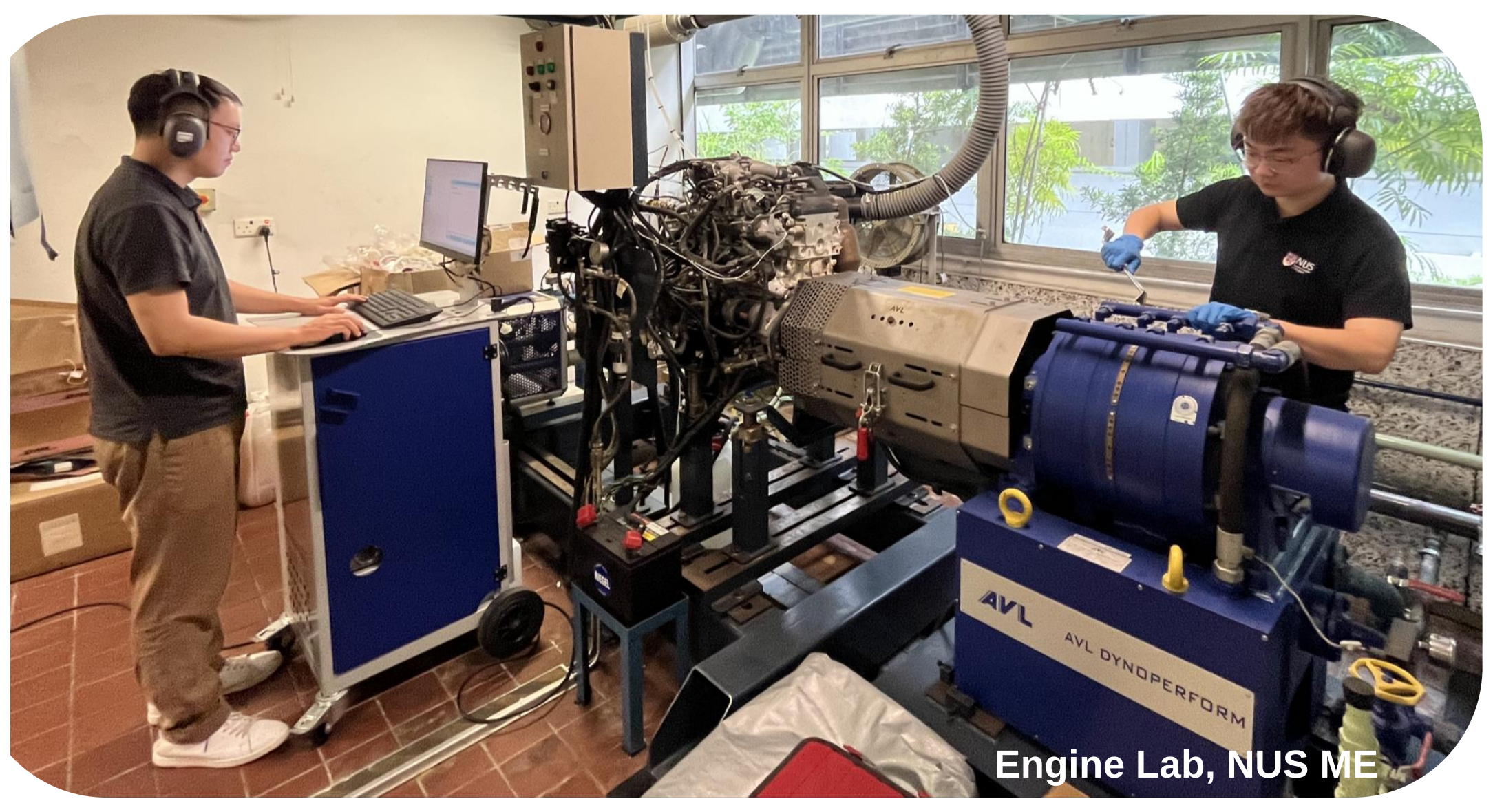
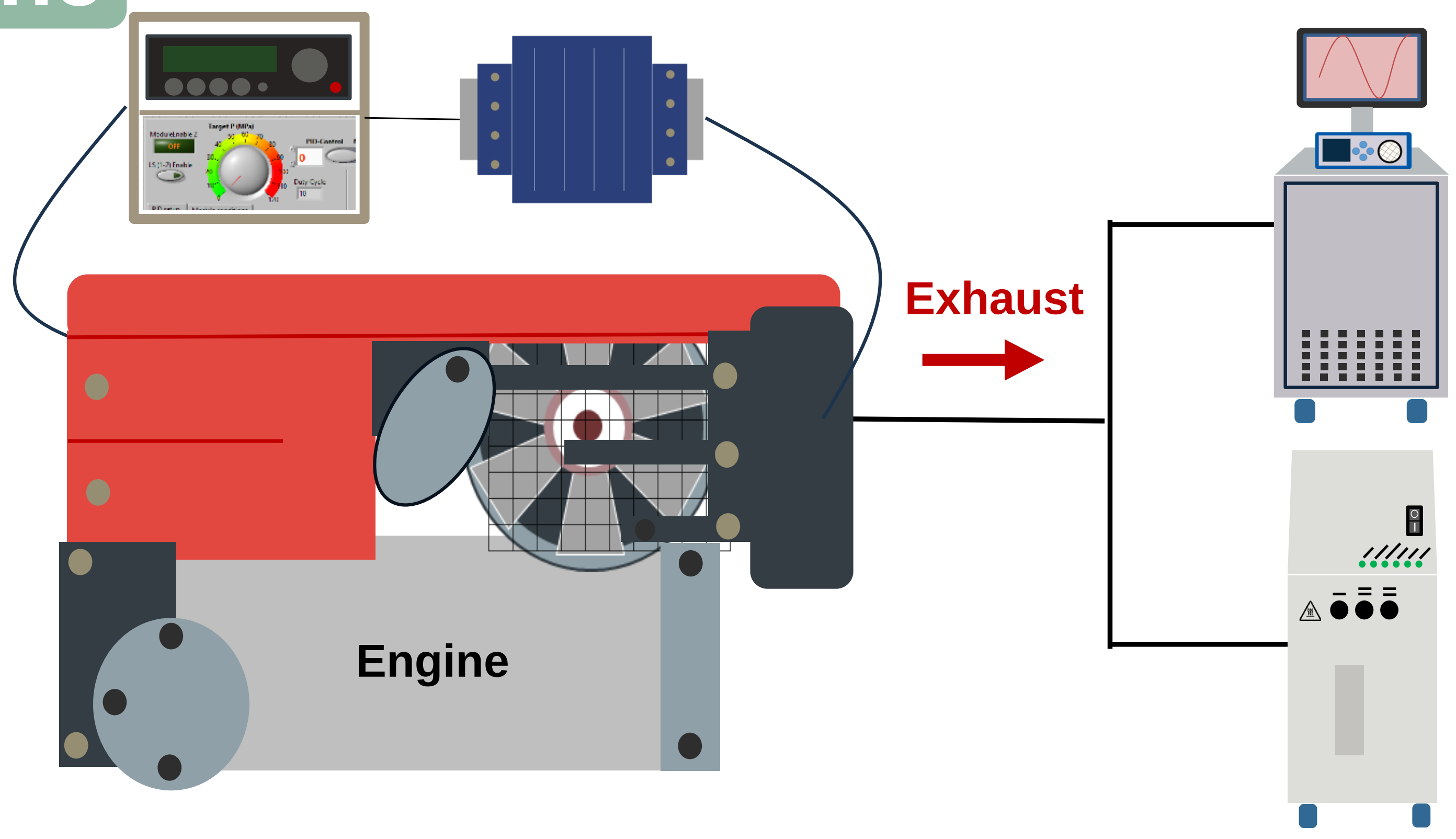


Introduction

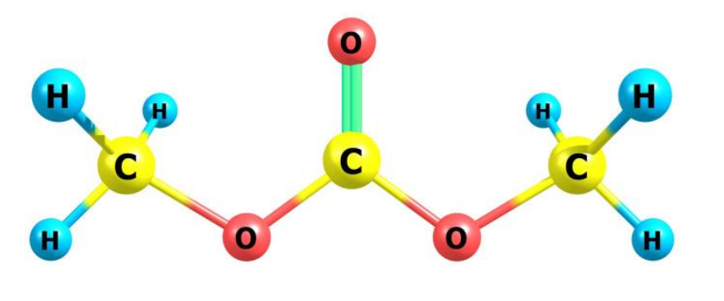
Decarbonizing the transportation sector by transitioning to low or zero-carbon fuels is essential for Singapore to achieve its 2050 net-zero emissions target and align with International Maritime Organisation (IMO) decarbonization goals for shipping industry. Researchers at CARES have been actively developing and testing carbon neutral fuel additives that can significantly reduce carbon, gas, and particulate emissions from internal combustion engines. Experiments have examined the impact of blending these additives with diesel and jet fuel on both combustion characteristics and emission profiles.

Internal Combustion Engine

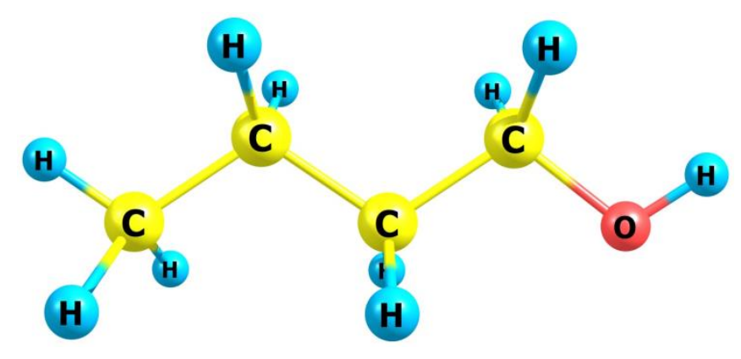
Parameters	Value
Bore	92 mm
Stroke	96 mm
Displacement	0.638 L
Compression ratio	17.7
Maximum torque	40 Nm (1200 rpm)
Maximum injection pressure	100 MPa



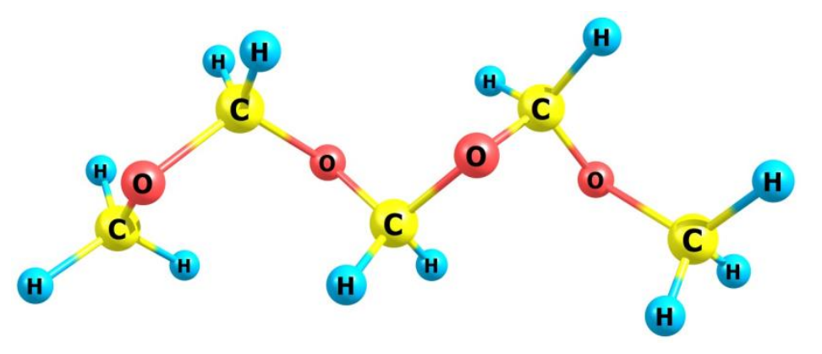
Fuel Additives



Dimethyl carbonate (DMC)



Butanol (BuOH)



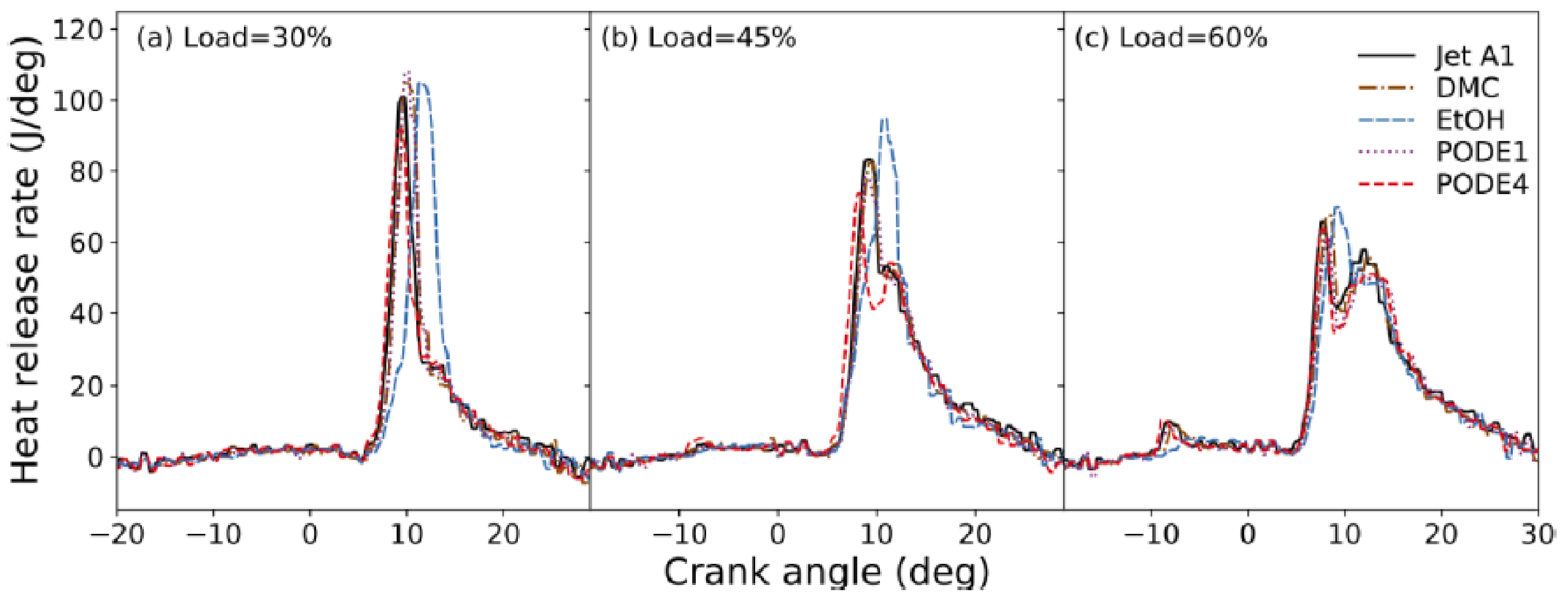
Polyoxymethylene dimethyl ether ($PODE_3$)

Combustion Performance

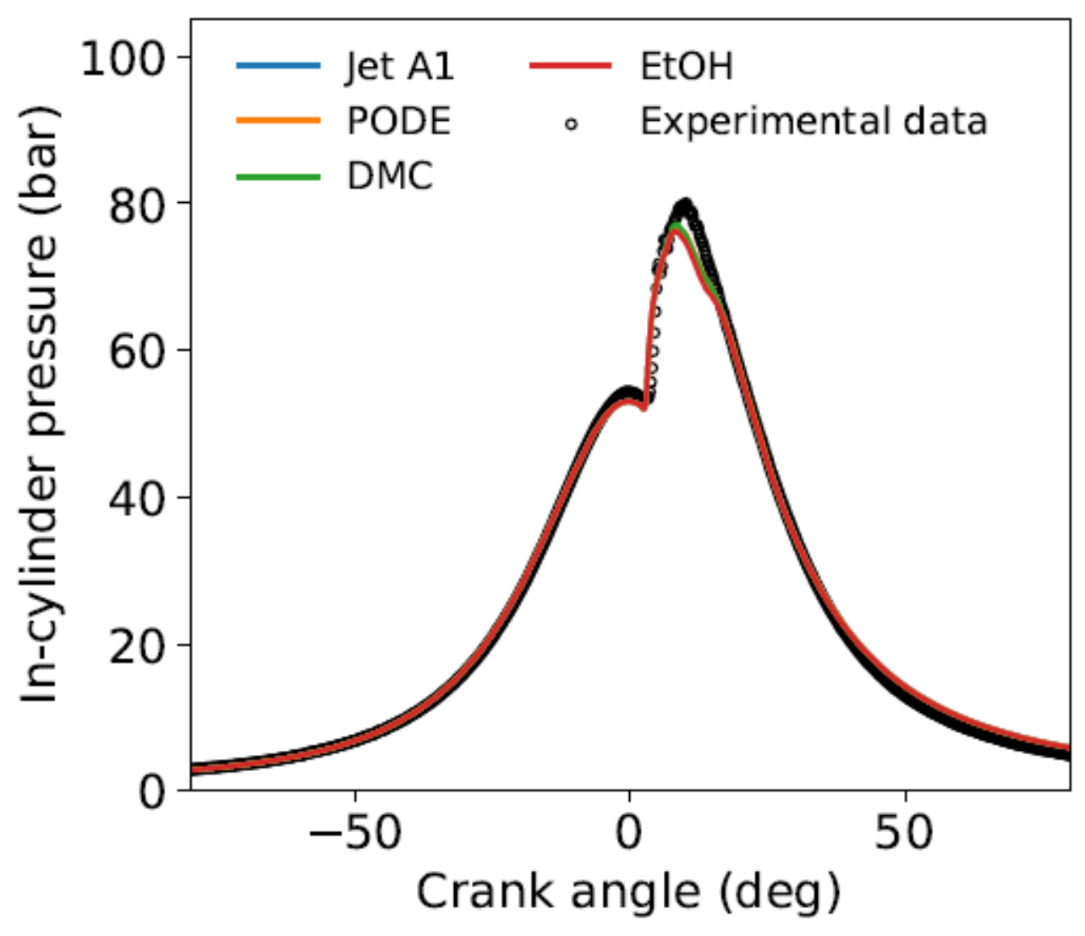
Apparent heat release rate (AHRR)

$$AHRR = \left[\left(\frac{\gamma}{\gamma-1}\right)P\frac{dV}{dt}\right] + \left[\left(\frac{1}{\gamma-1}\right)V\frac{dP}{dCA}\right]$$

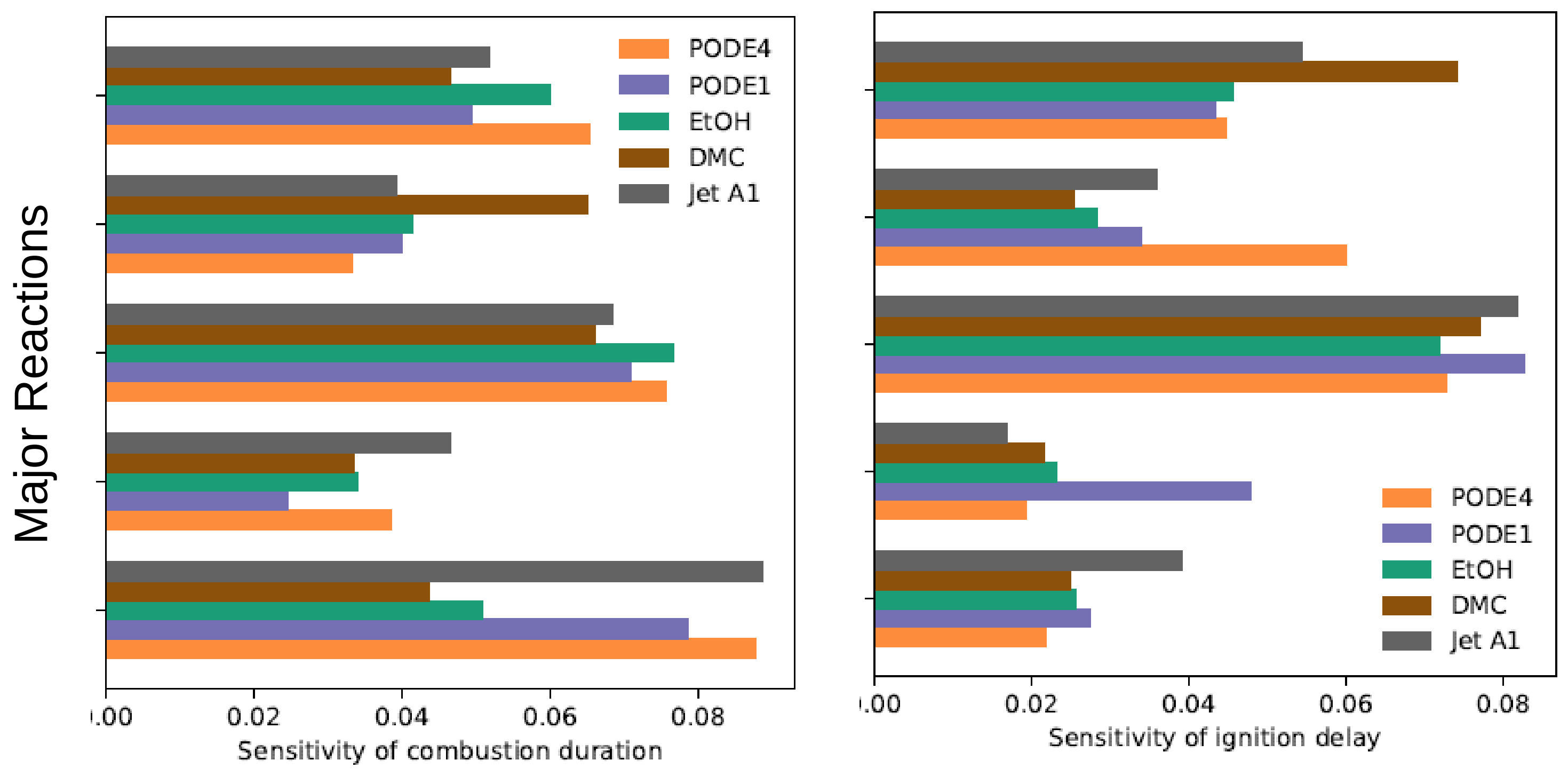
where *CA* is the crank angle.



Engine Simulation

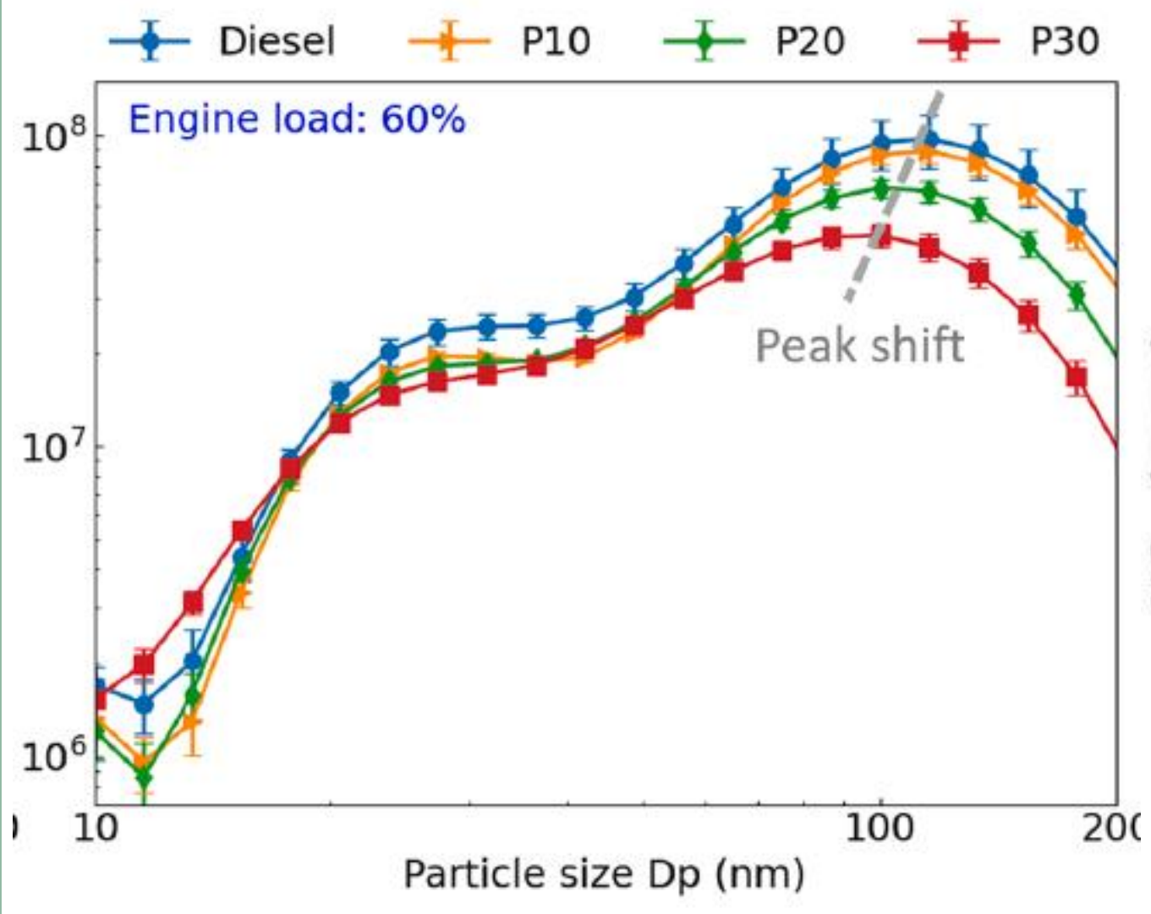


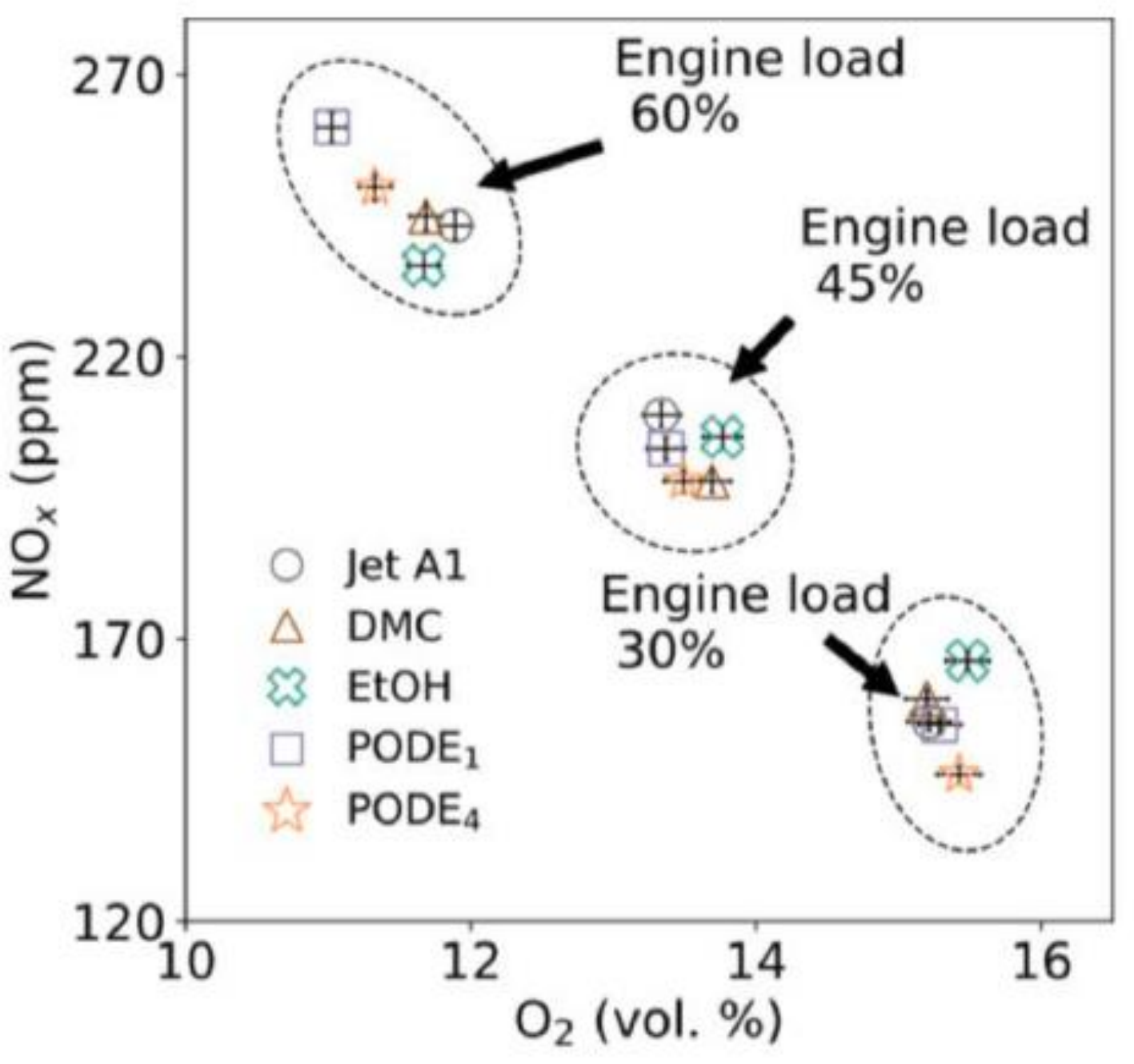
The simulation work is performed in SRM Engine Suite and Model Development Suite (MoDS) workflows from *CMCL Innovations* for combustion model calibration and global sensitivity analysis.

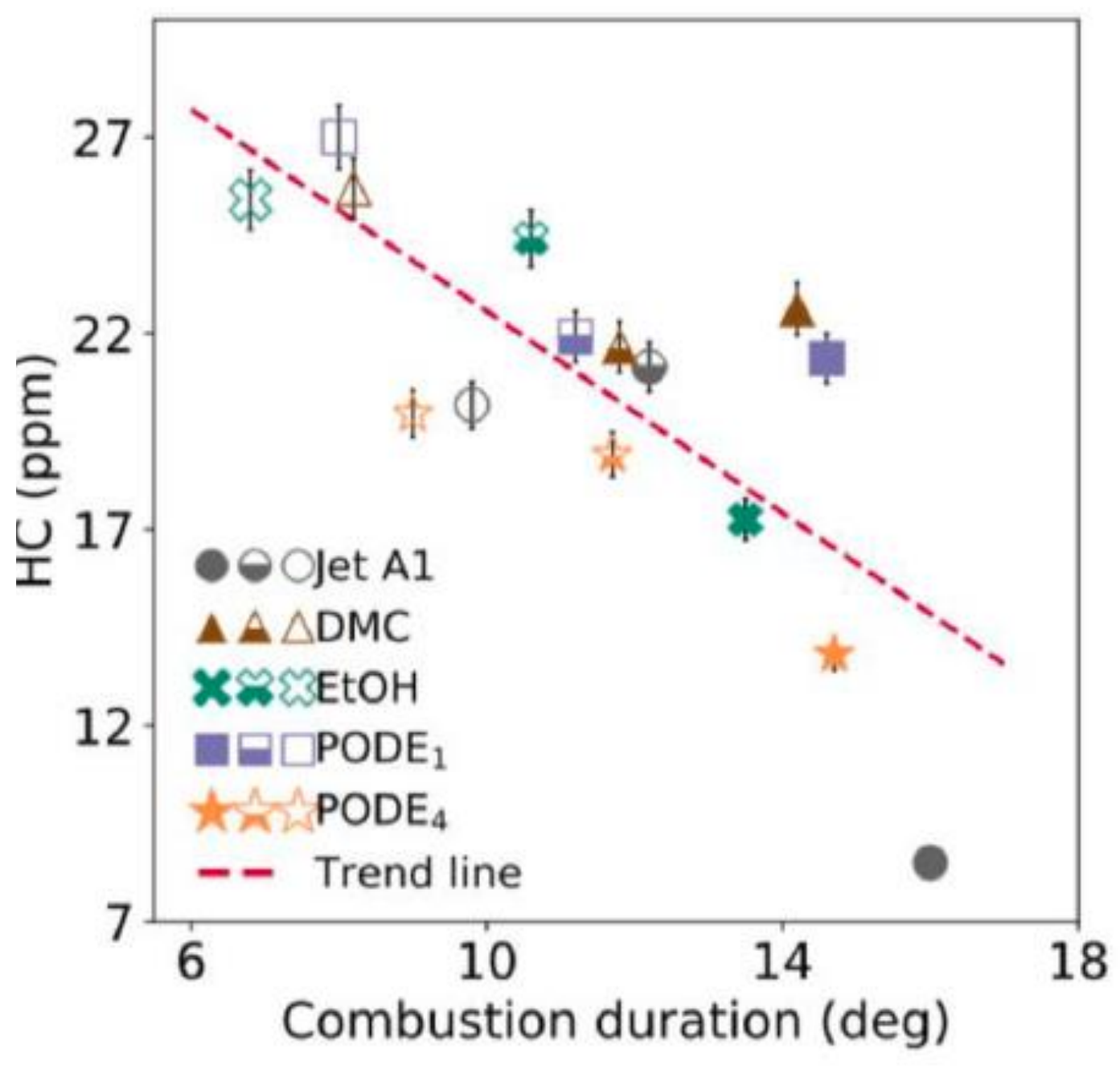


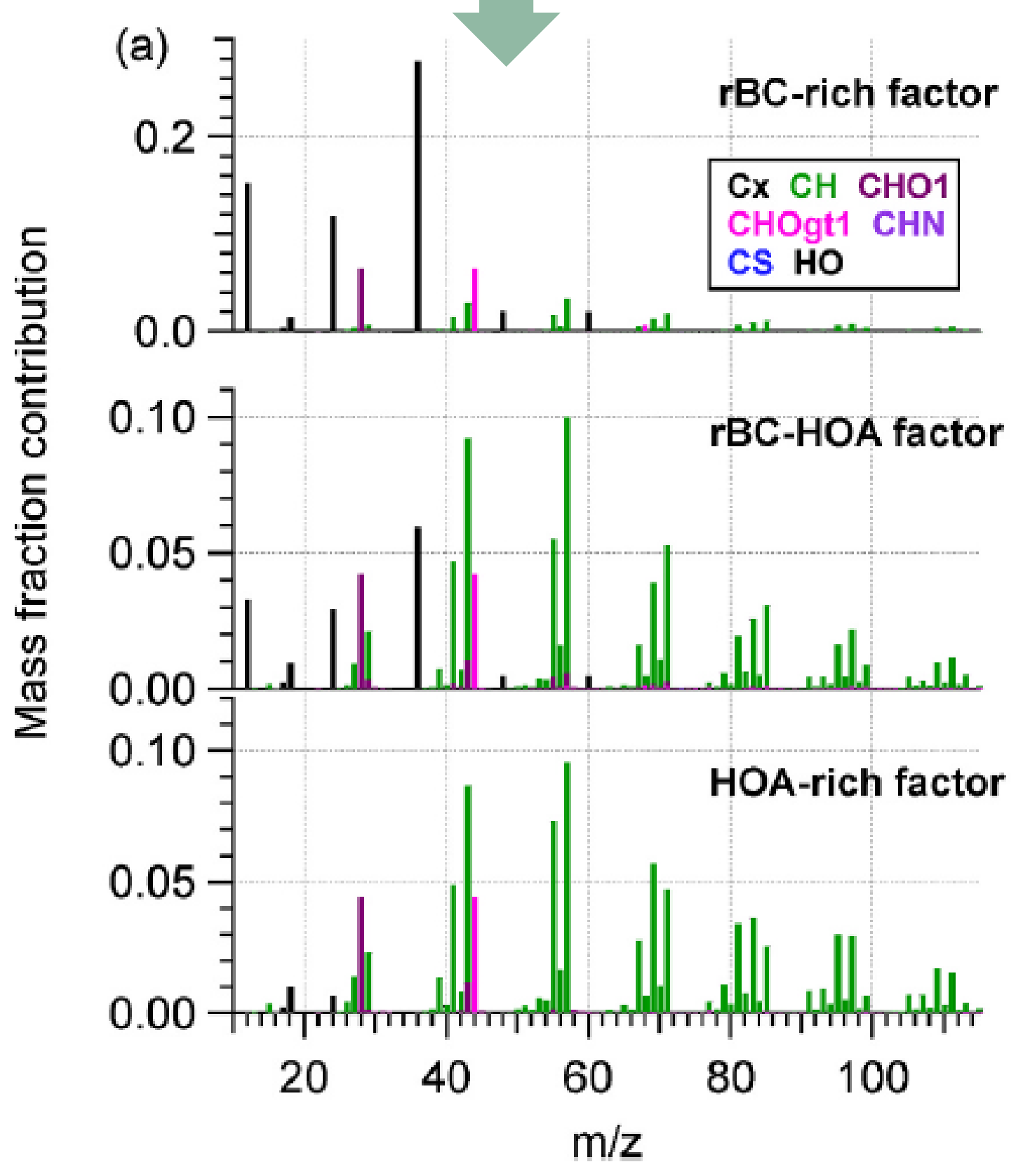
Emission Measurement

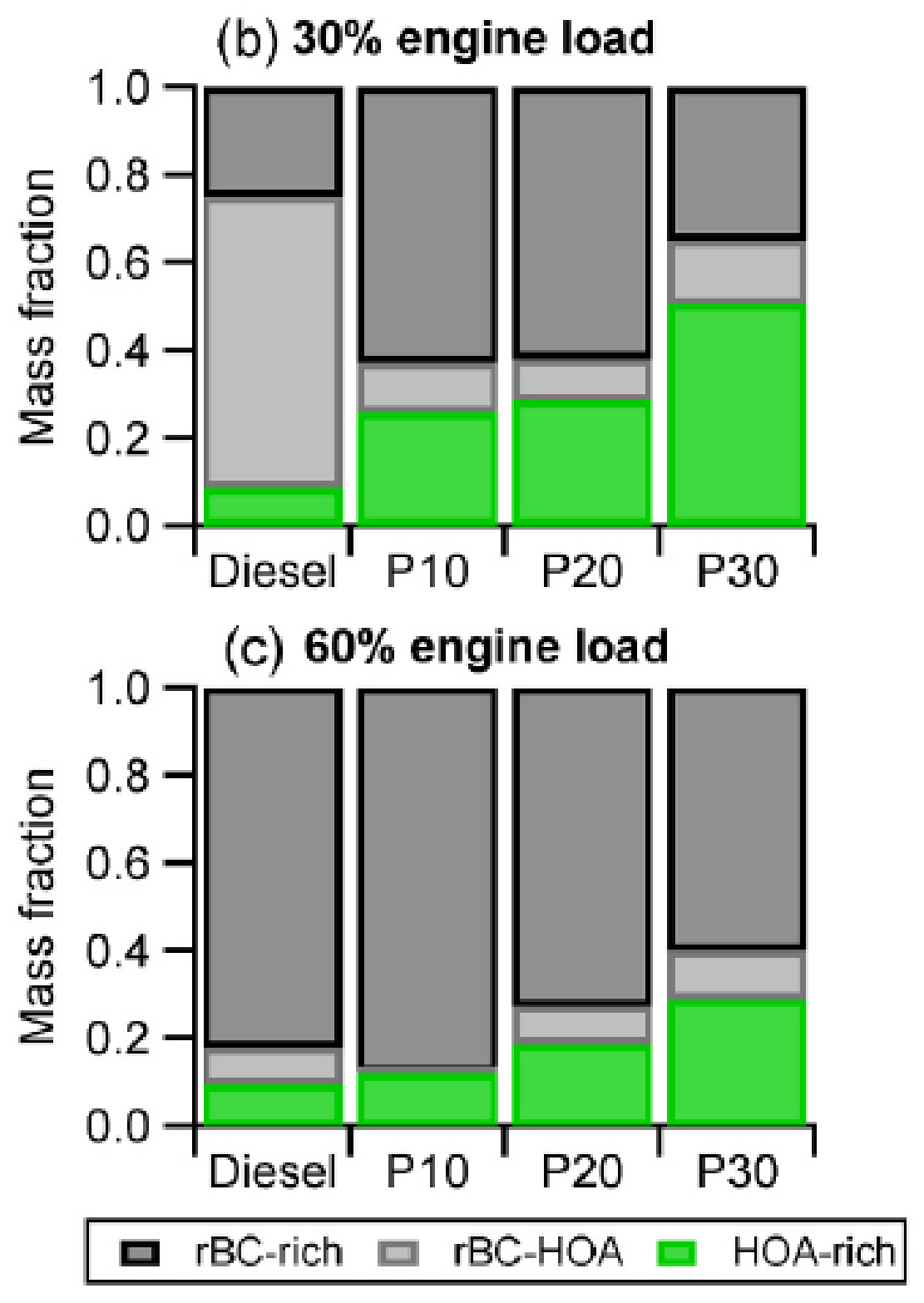
- ☐ Particulate emission. Both particle peak size and number concentration decrease when the blending ratio of $PODE_3$ in diesel is increased.
- ☐ NO_x emission. The data shows clustering based on different engine loads.
- ☐ Unburned hydrocarbon (HC) emission. The data shows a trendline against combustion duration for different fuel blends.



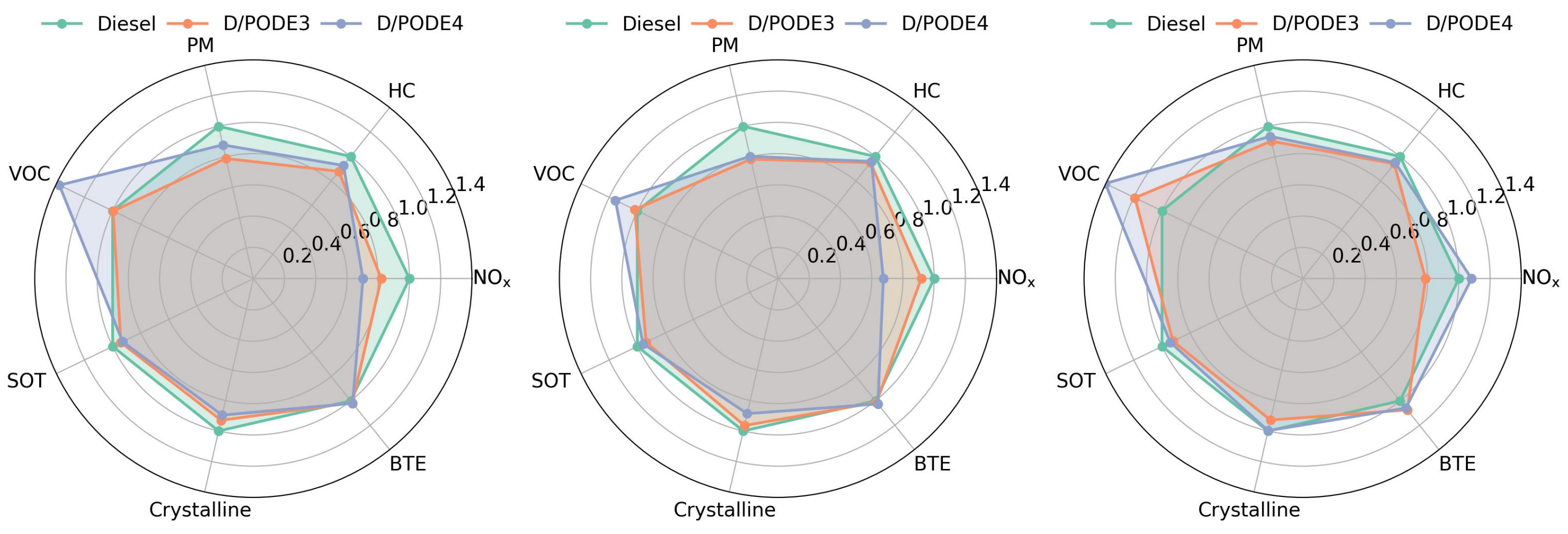


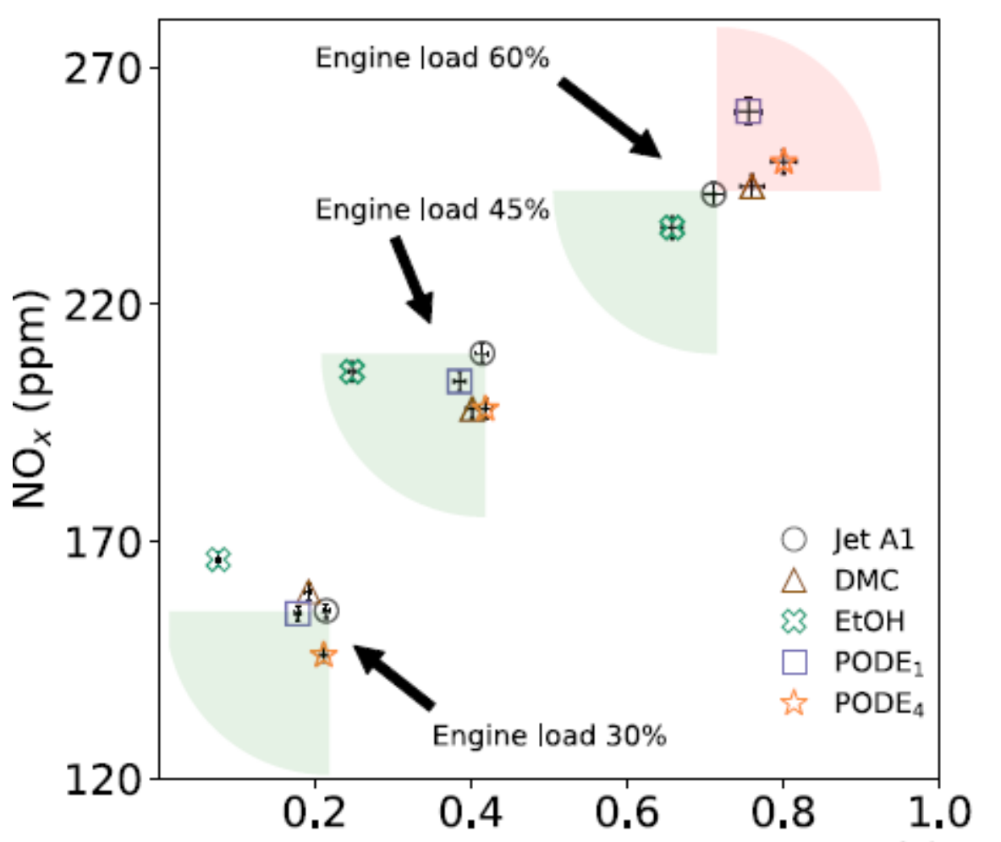






- ☐ Brown carbon (BrC) is found in emission analysis using aerosol mass spectrometer and aethalometer.
- ☐ Comparison of the engine performance and emissions of various fuel blends under different injection pressures.





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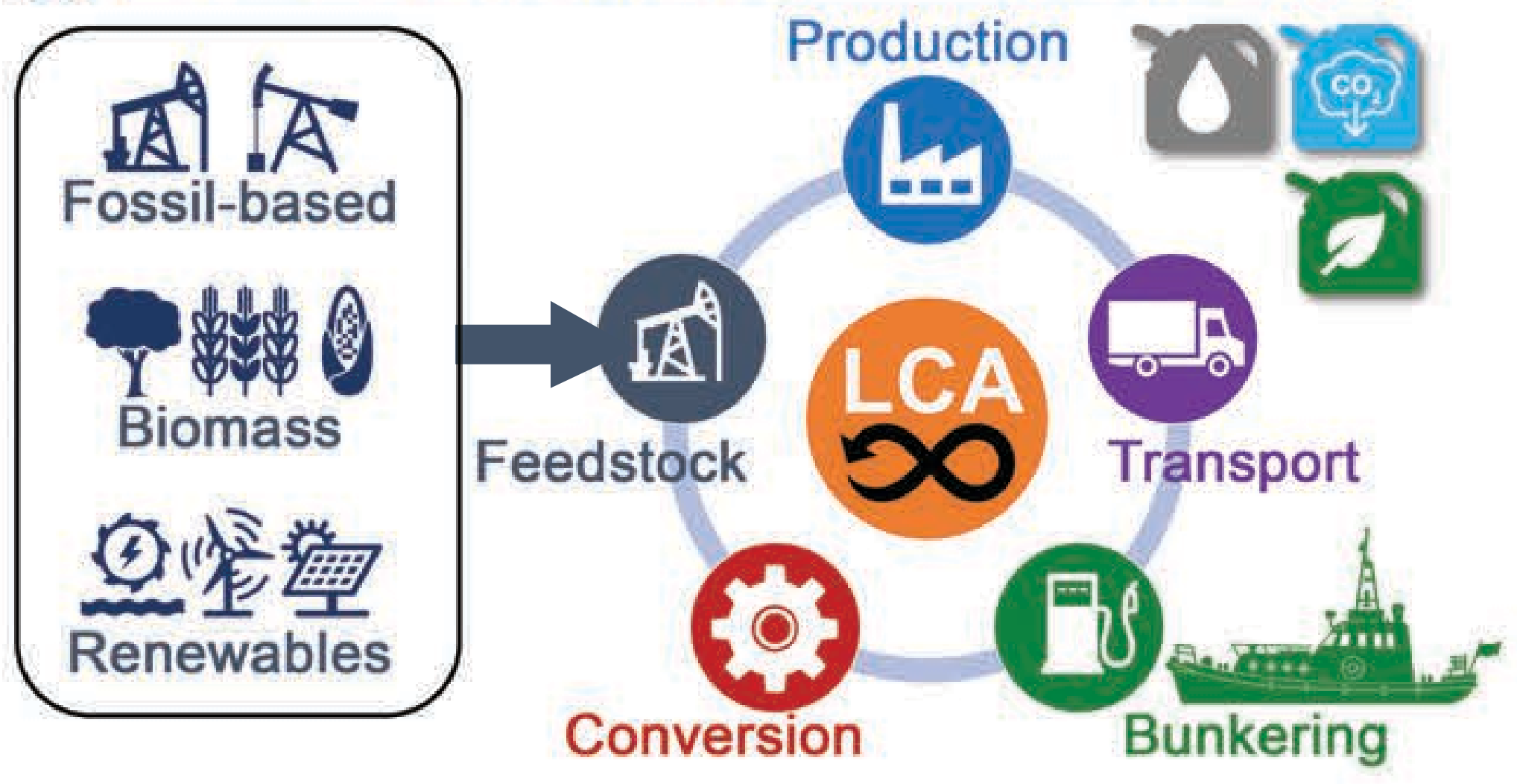
Decarbonising Maritime Transport (1)

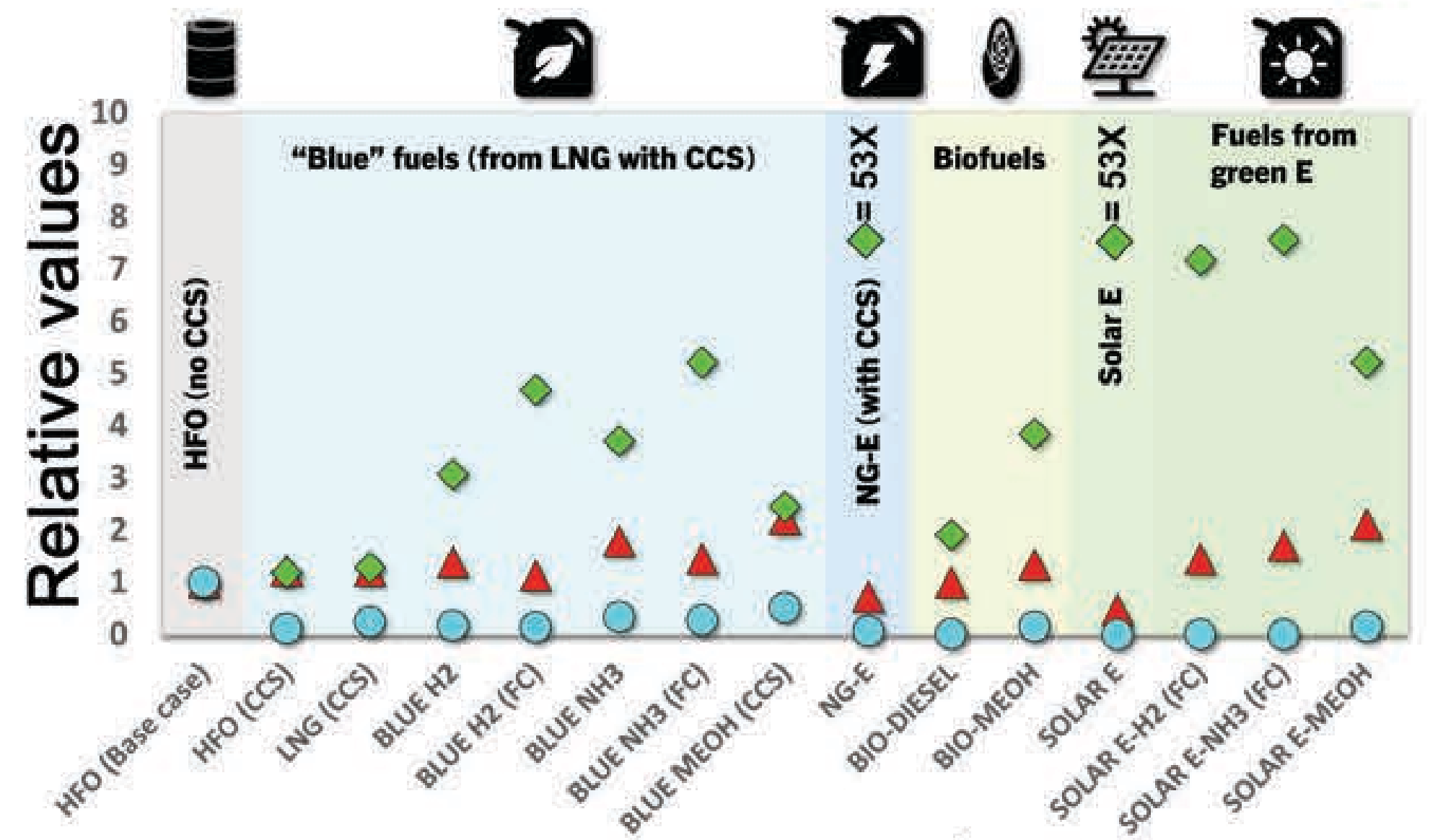
[Li Chin Law[1], Jessie R. Smith[2], Epaminondas Mastorakos[1,2] , Stephen Evans[1,2]]

Introduction

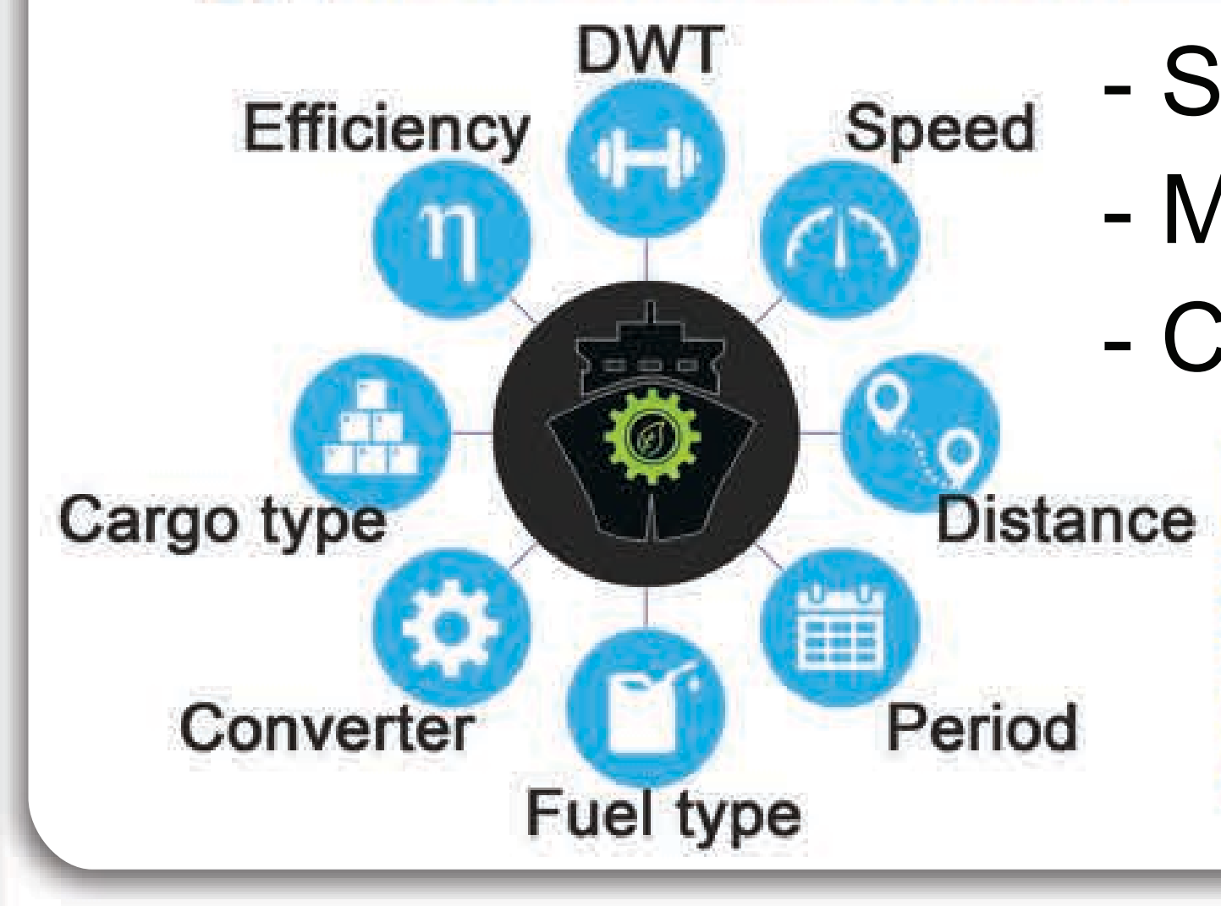
Shipping decarbonisation can be achieved through alternative fuels. An analysis of the lifecycle of each option reveals total emissions, energy and cost, and a future ship can be designed considering ship type, size, weather conditions, voyage profiles, and fuel properties. Comparative studies among the various fuels enable realistic comparisons and assist in making informed decisions.

LCA assessment → Fuel Data



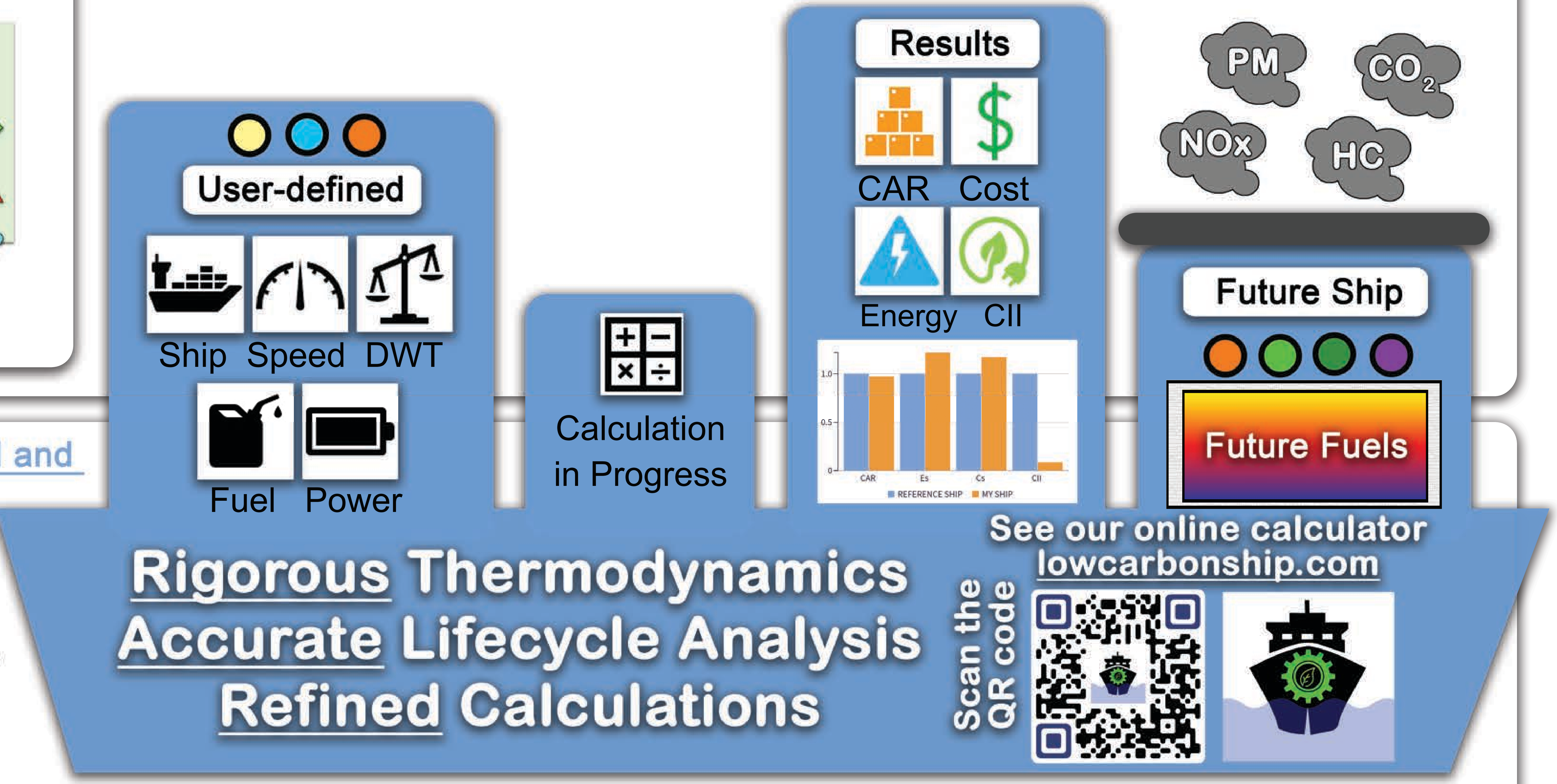


Fleet assessment → Ship Data



- Ship dimensions
- Mass & volume dist.
- CAR

Weather & Voyage



Rigorous Thermodynamics
Accurate Lifecycle Analysis
Refined Calculations

See our online calculator
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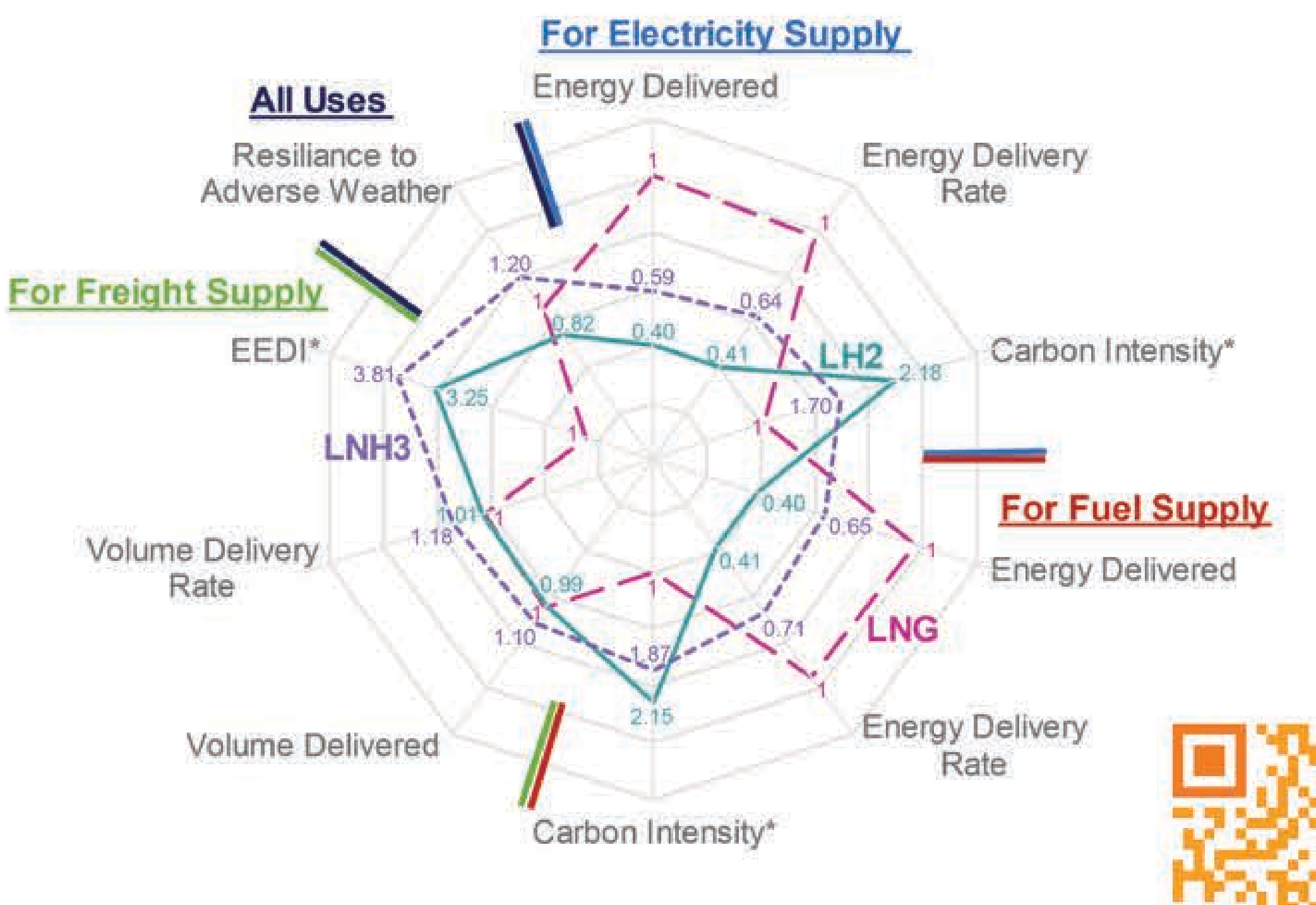
Scan the QR code

Fuel comparison in electricity, fuel and freight supply:

- CI: LH2 < LNH3 < LNG
- EEDI: LNH3 < LH2 < LNG
- Freight supply (volume): LNH3 (best)
- Resilient to weather: LNH3 (best)
- Electricity supply: LNG (best)
- Fuel supply: LNG (best)

Normalised Relative Ship Properties in 2050
(High Scores Are Favorable, Beaufort Number = 5)

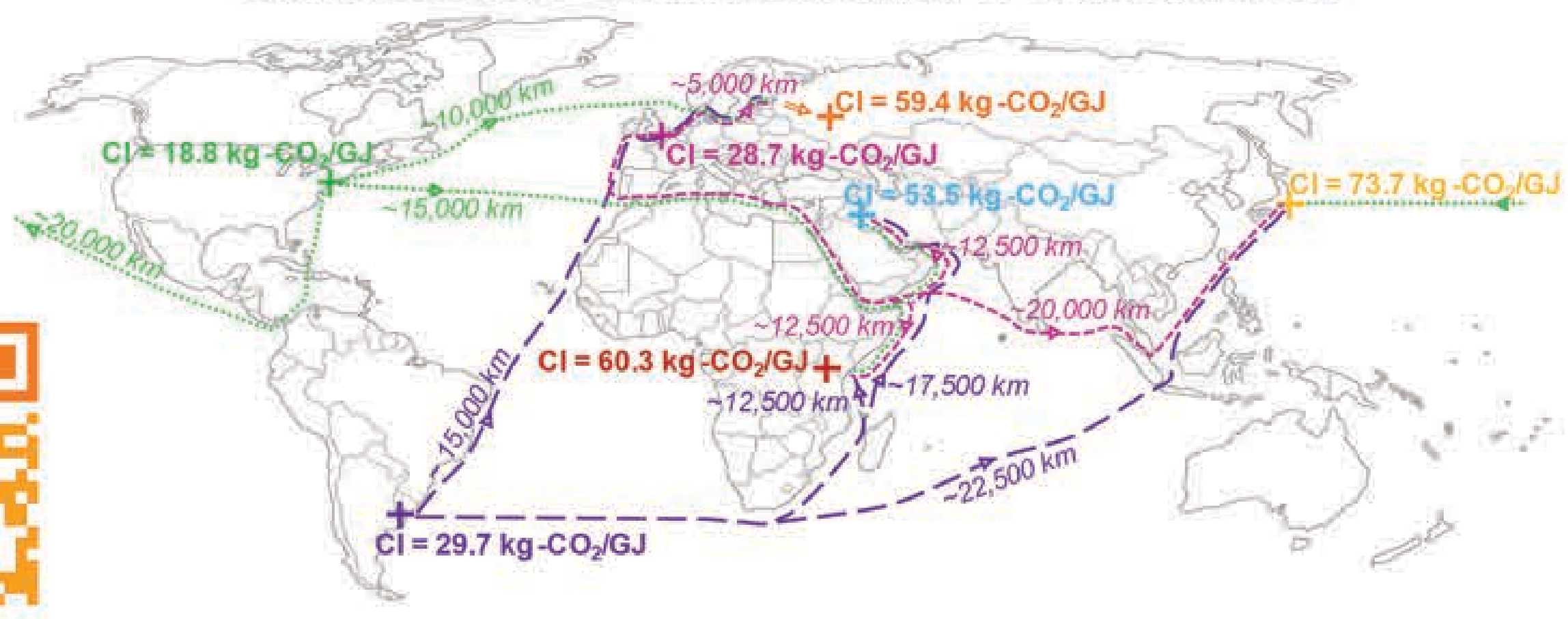


* Electricity Origin = North America Grid

Ship routes length and region-specific CI

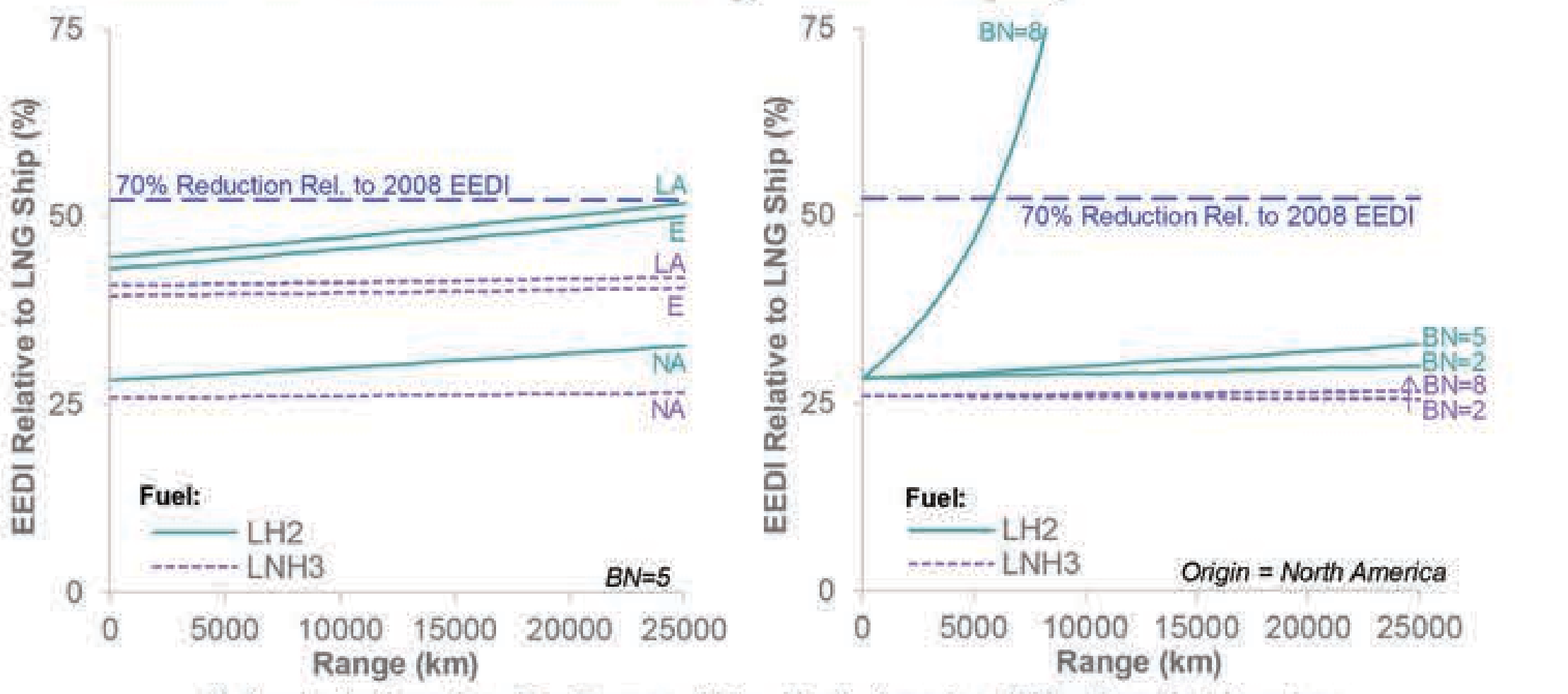
- Renewable energy is unevenly distributed
- This effects the feasibility of electricity, fuel and freight transport using LH2 and LNH3

Ship Routes And Carbon Intensity (CI) of Origin Electricity



EEDI relative to the IMO2050 target (70% reduction relative to 2008 EEDI)

- LNH3 ship meets the target, even in rough weather conditions
- LH2 ships do not meet the target in rough weather conditions (fuel loss)



*LA = Latin America, E = Europe, NA = North America, BN = Beaufort Number

*Abbreviation: $ = Cost, CAR = Cargo Attainment Rate, CI = Carbon Intensity, EEDI = Energy Efficiency Design Index (CO2 per unit volume-km), LH2 = Liquefied Hydrogen, LCA = Lifecycle Assessment, LNG = Liquefied Natural Gas, LNH3 = Liquefied Ammonia, WTW = Well-to-Wake (Lifecycle),

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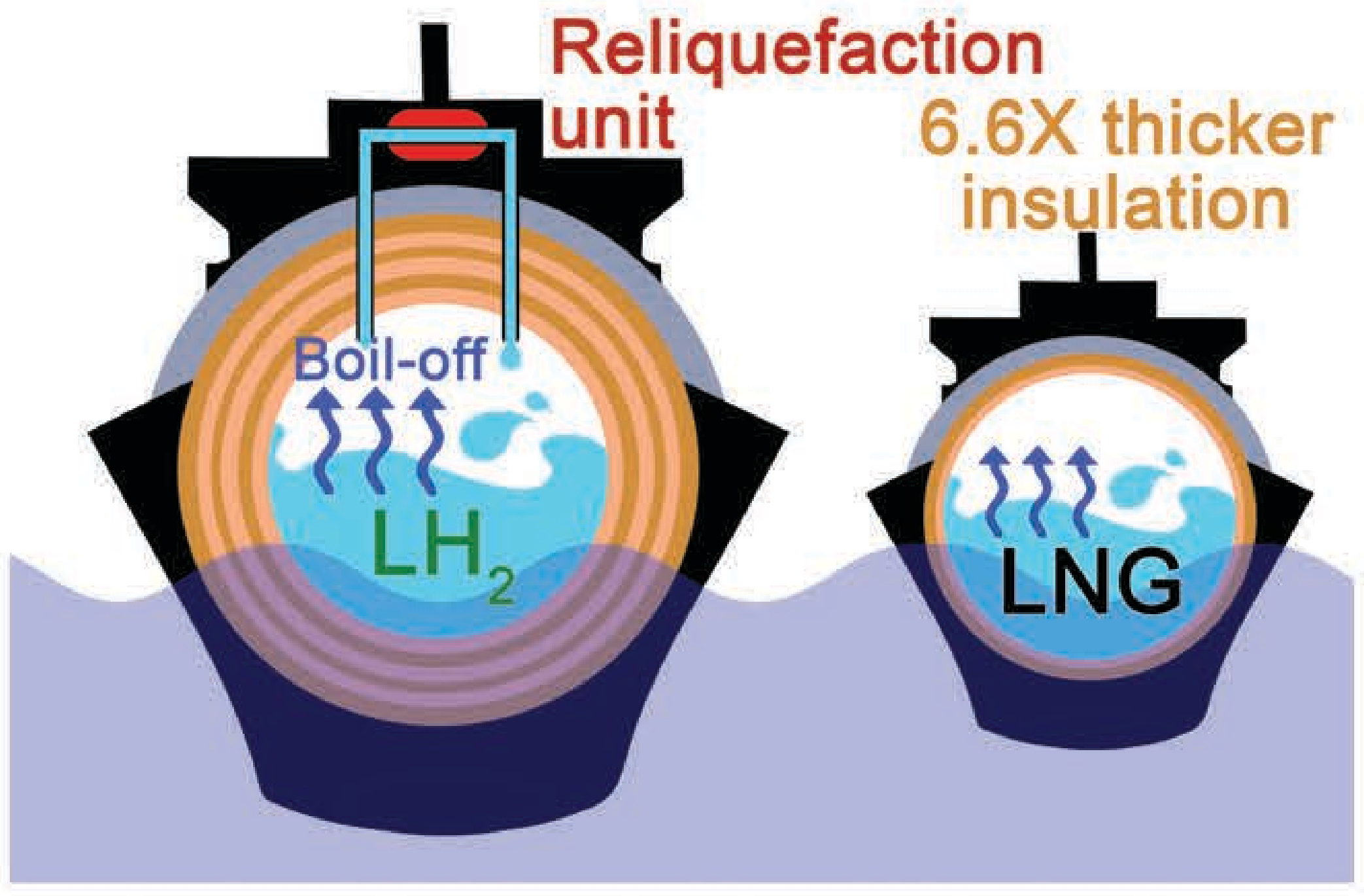
Decarbonising Maritime Transport (2)

[Li Chin Law[1], Savvas Gkantonas[2], Jessie R. Smith[2], Epaminondas Mastorakos[1,2]]

Introduction

The maritime industry is embracing a multi-fuel future. Unlocking their potential needs comprehending the thermodynamics of each of the alternative marine fuels. This study delves deeply into the design of ships powered by alternatives such as hydrogen, ammonia, methanol, biofuels, and onboard Carbon Capture and Storage; by employing rigorous thermodynamic analysis to ensure the suitability of these fuels, enhance ship safety and achieve an optimized ship design.

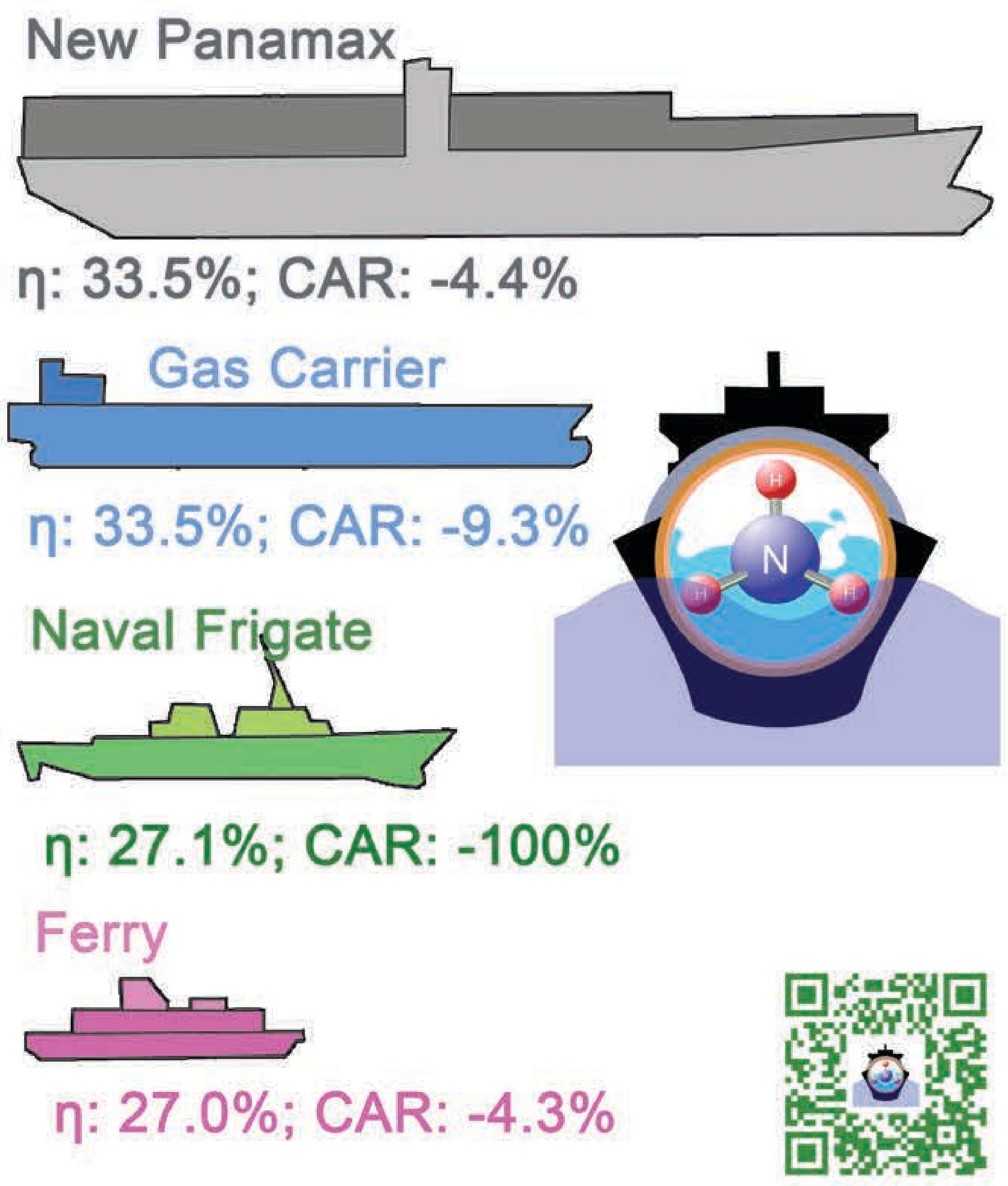
(H2-Ship) BOR and sloshing model



Same storage & insulation:
- Energy: LH_2 0.4X of **LNG**
- Boil-off: LH_2 9X of **LNG**
- Sloshing: LH_2 2X of **LNG**

Hence, for equivalent energy:
- Reliquefaction unit: Required
- Size: LH_2 1.7X of **LNG**
- Insulation: LH_2 6.6X of **LNG**

(NH3-Powertrain Model)



New Panamax

η: 33.5%; CAR: -4.4%

Gas Carrier

η: 33.5%; CAR: -9.3%

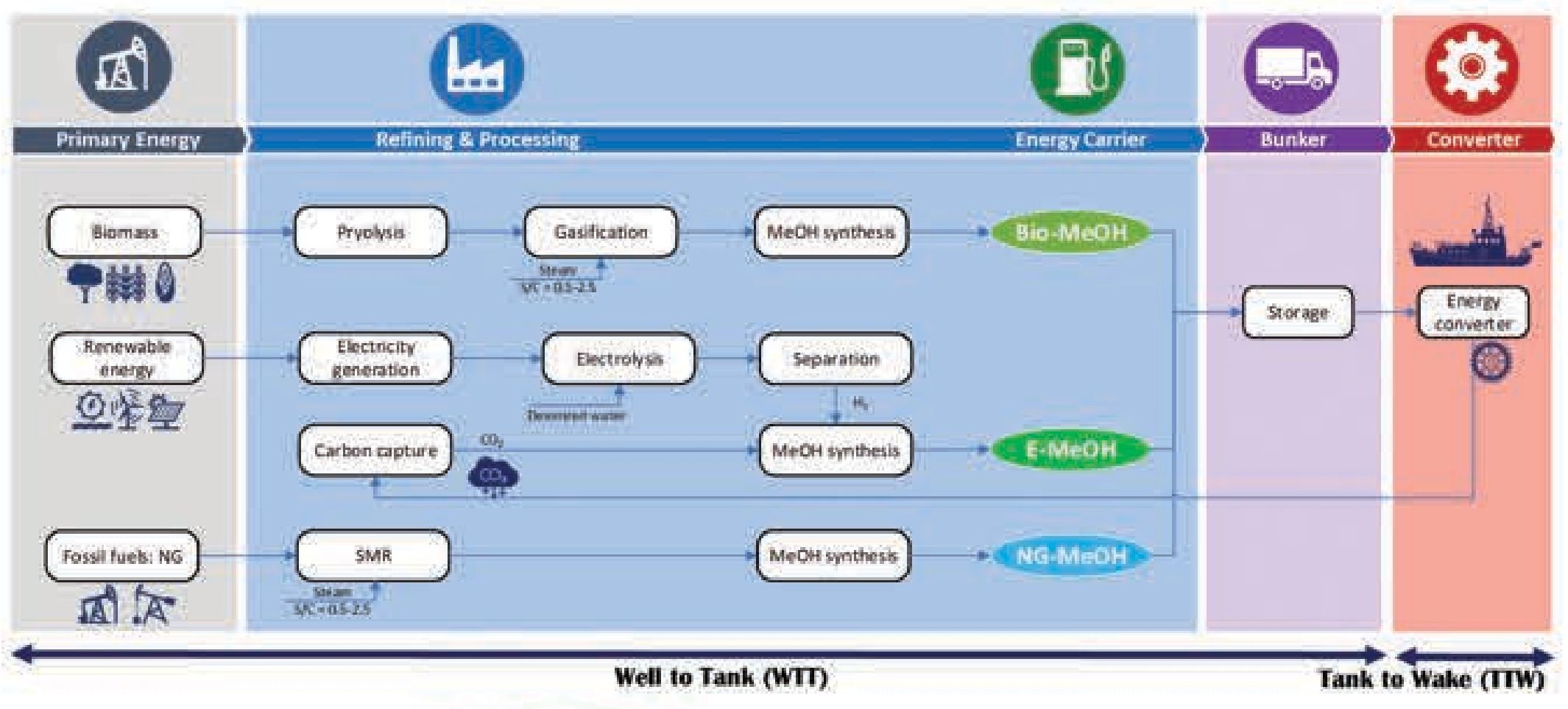
Naval Frigate

η: 27.1%; CAR: -100%

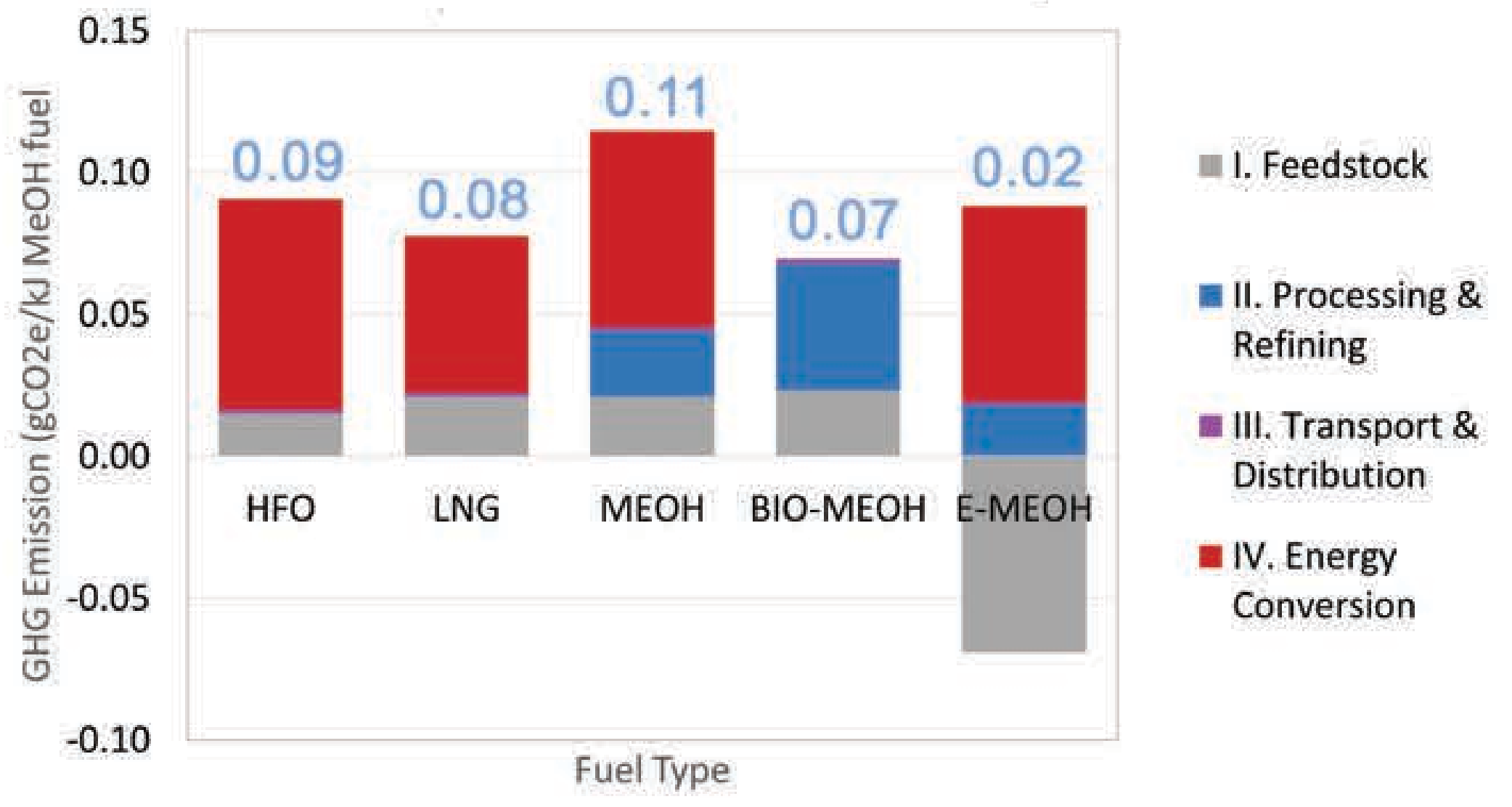
Ferry

η: 27.0%; CAR: -4.3%

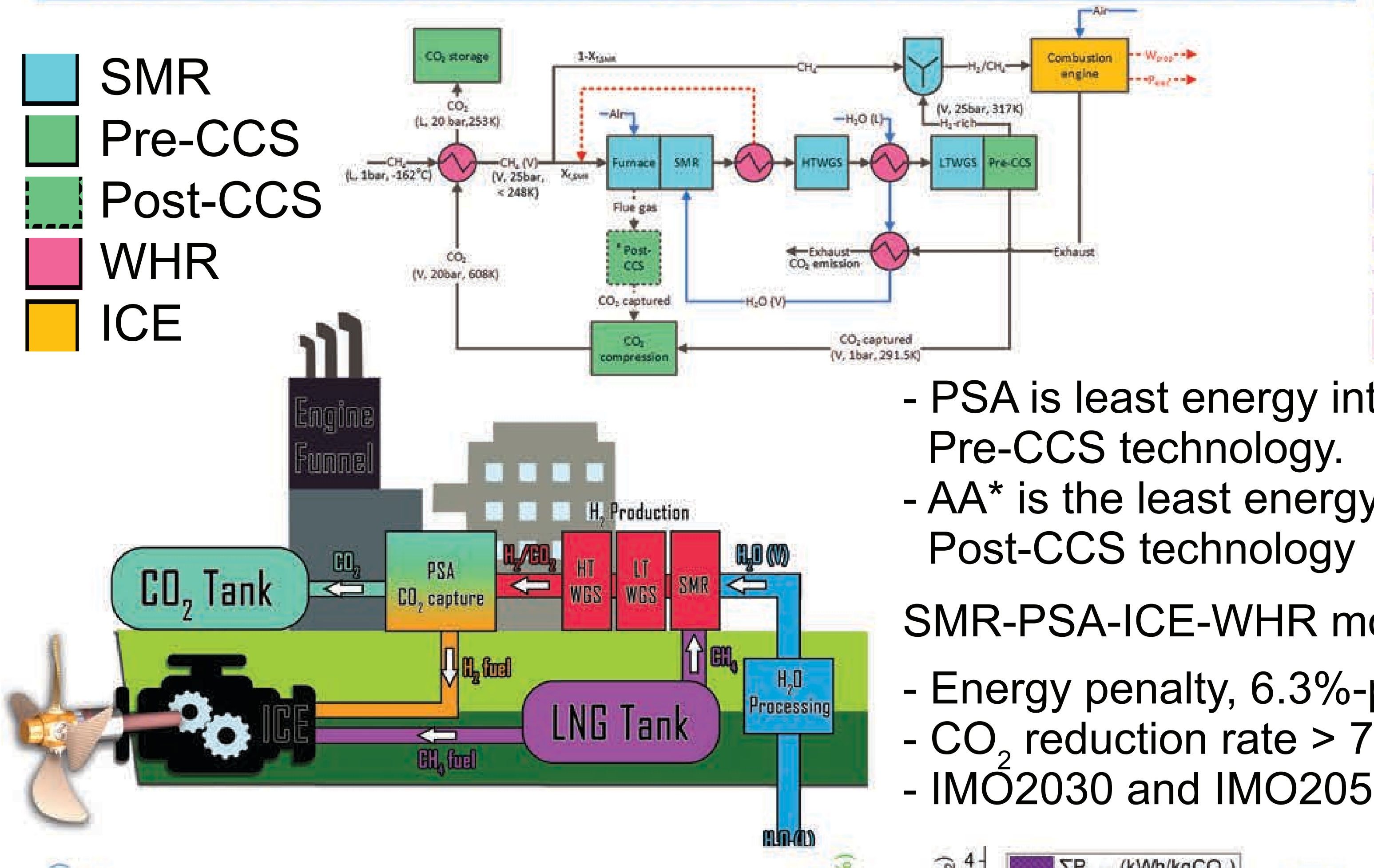
(MeOH-Ship Lifecycle Model)



- Energy: **LMEOH** 2.5X of **LNG**
- Boil-off: **LMEOH** 0.1X of **LNG**
- Insulation: **LMEOH** not required



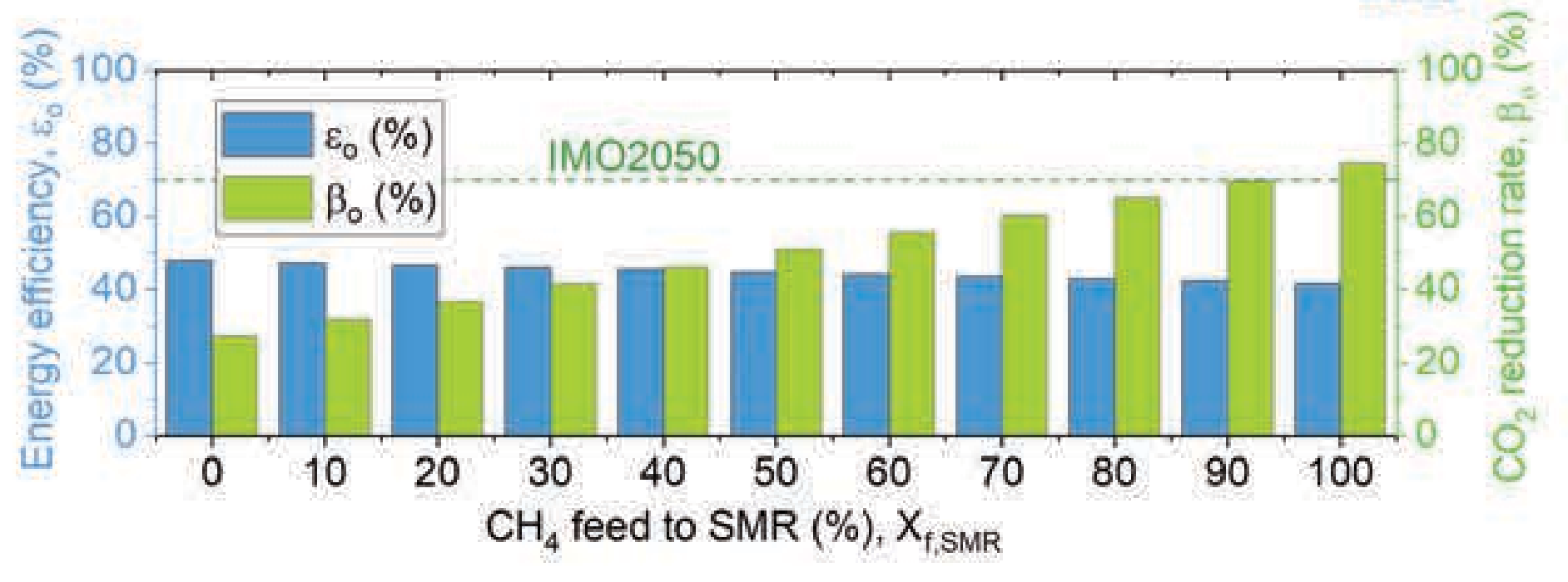
Onboard CCS with WHR Model (Pre-CCS & Post-CCS)

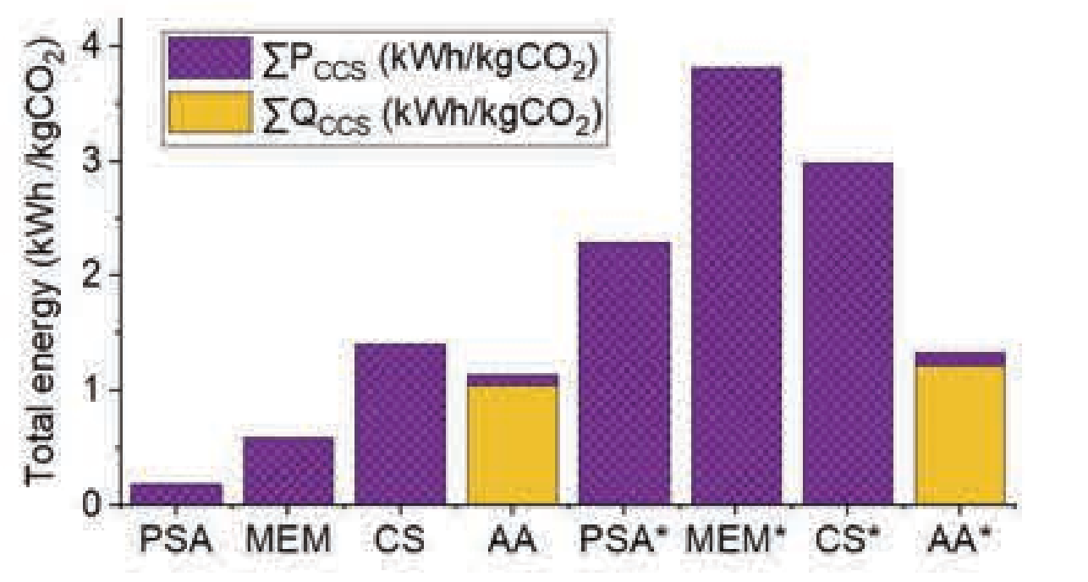


- PSA is least energy intensive Pre-CCS technology.
- AA* is the least energy intensive Post-CCS technology

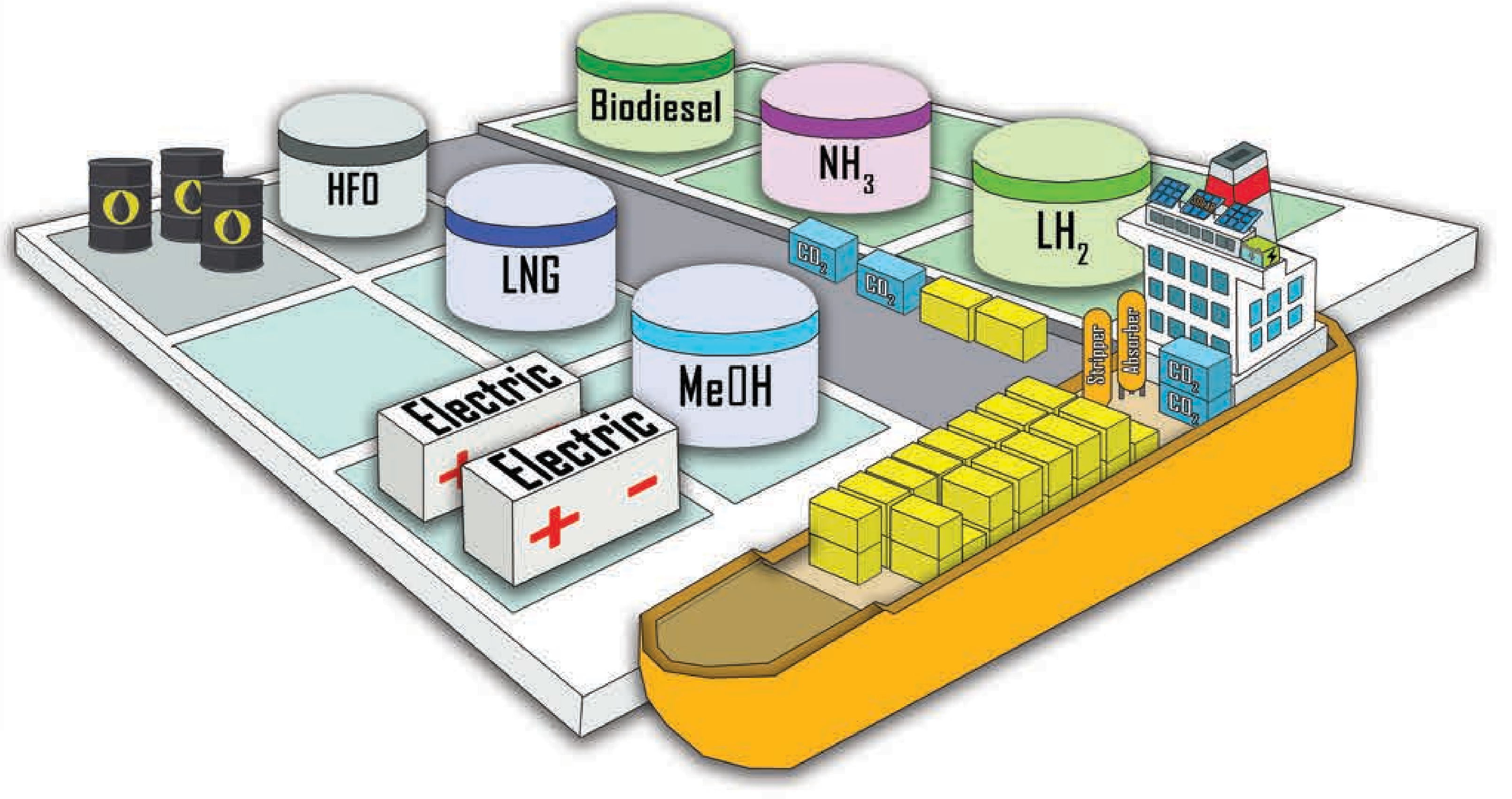
SMR-PSA-ICE-WHR model

- Energy penalty, 6.3%-points.
- CO_2 reduction rate > 70%
- IMO2030 and IMO2050 are met.





The Multi-fuels Future of Maritime Industry



*Abbreviation: **η = Energy Efficiency,** AA = Amine Absorption; CAR = Cargo Attainment Rate, CS = Carbon capture & storage, CS = Cryogenic CCS, H2 = Hydrogen, ICE = Internal combustion engine, LNG = Liquefied Natural Gas, MEM = Membrane, MeOH = Methanol, NH3 = Ammonia, Pre-CCS = Pre-combustion CCS, Post-CCS = Post-combustion CCS, PSA = Pressure Swing Adsorption, SMR = Steam methane reformer, WHR = Waste heat recovery,

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https://lowcarbonship.com/

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C4T
LOW CARBON SHIP

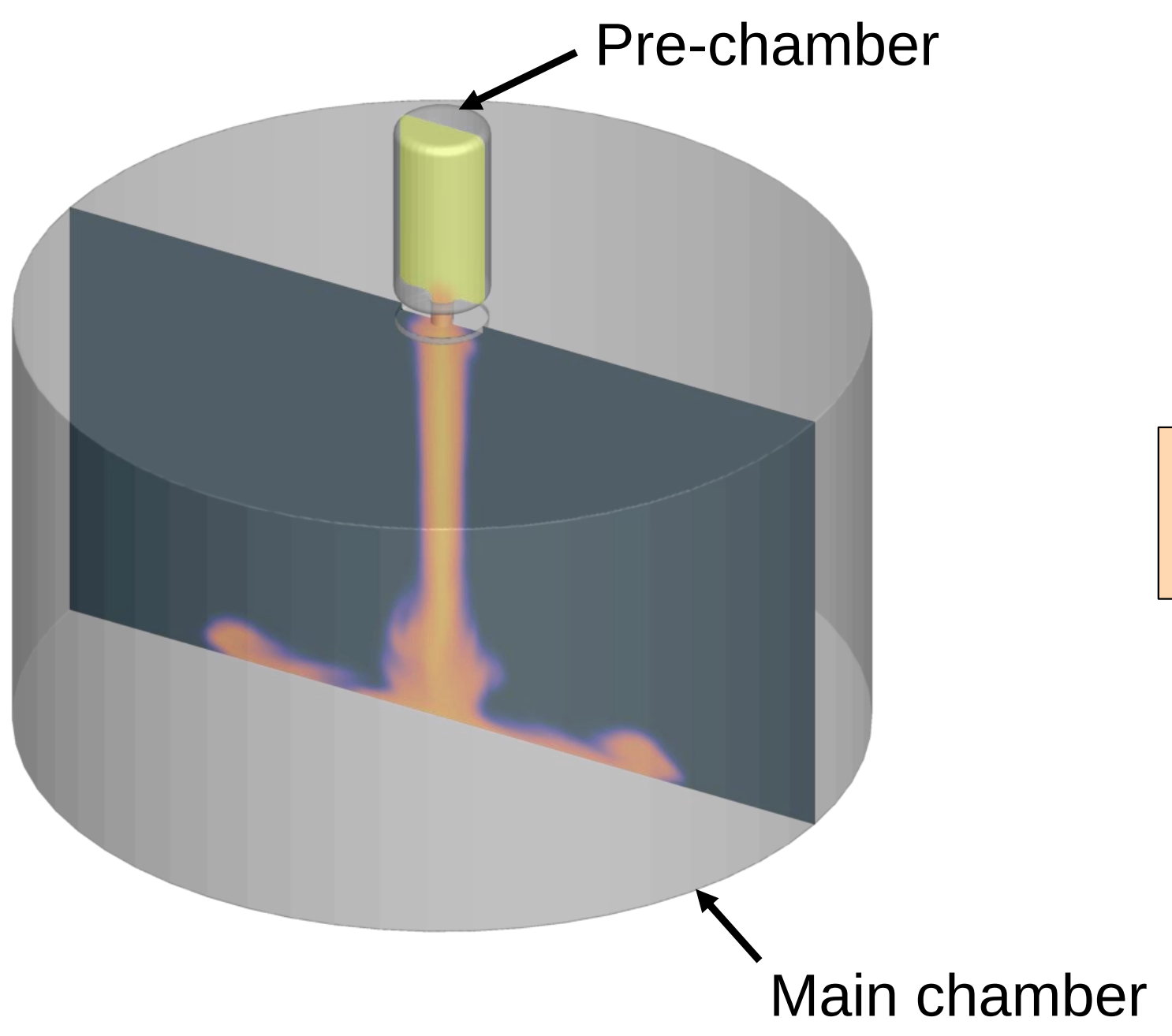
Engine emissions simulations with complex chemistry

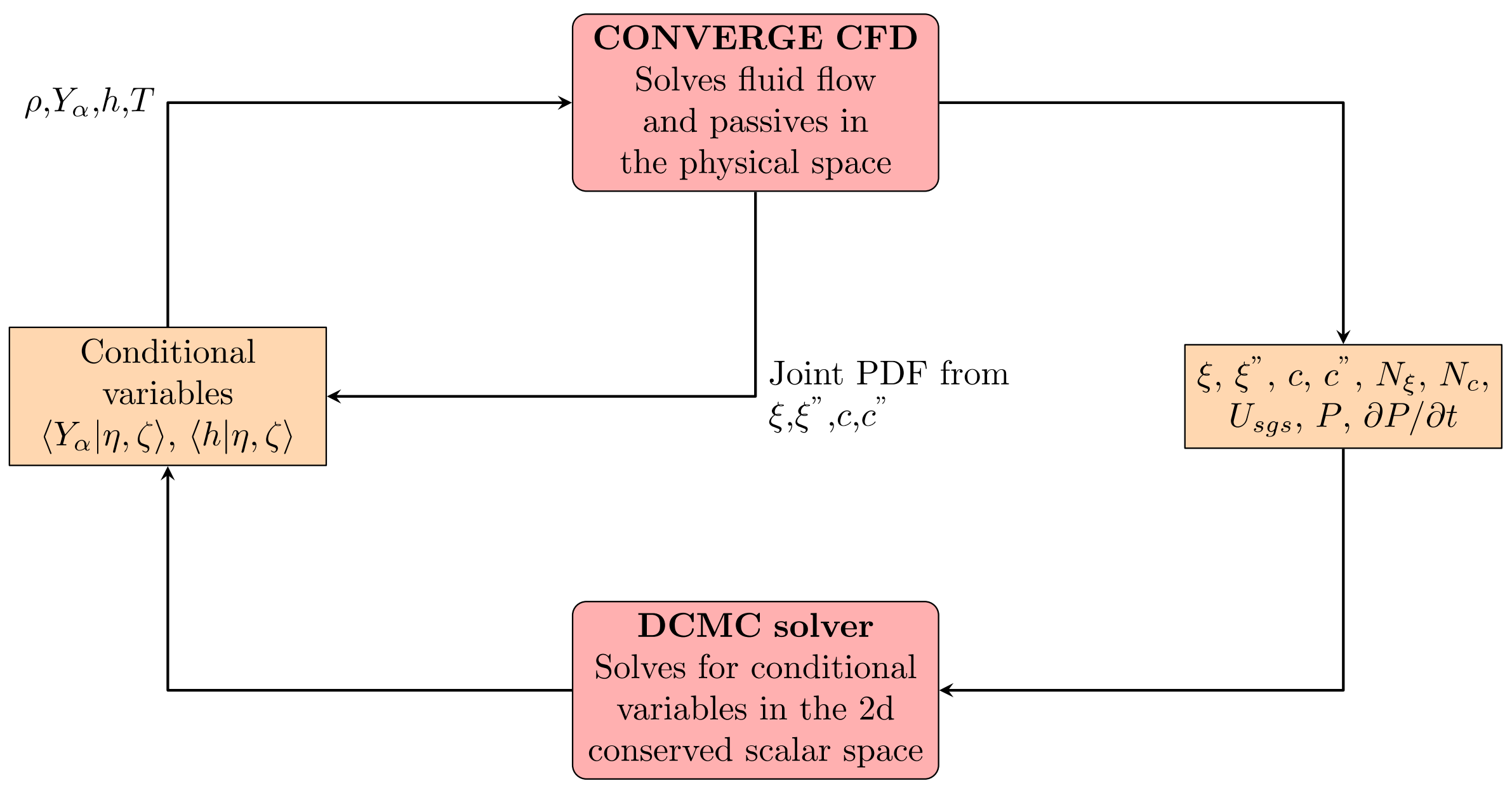
B Harikrishnan[1], Savvas Gkantonas[2], Epaminondas Mastorakos[1,2]

Introduction

The shipping industry must decarbonise and shift to low-/zero-carbon fuels like ammonia or methanol and lean-burn engines. Due to the low flammability of methanol and ammonia, dual-fuel combustion concepts are considered by industry so that a highly-reactive fuel is used to ignite the fuel with low reactivity. However, the conventional models used in industry for engine design cannot handle such complexities, needing novel approaches that treat the fluid mechanics and the chemistry together. Large-Eddy Simulations coupled with the Doubly Conditioned Moment Closure (LES-DCMC), an advanced turbulent reacting flow modelling framework, were used in this project to explore the physics of dual-fuel combustion and to develop better computational engine simulation tools.

Methodology





ρ,Y_α,h,T

CONVERGE CFD
Solves fluid flow and passives in the physical space

Joint PDF from ξ,ξ'',c,c''

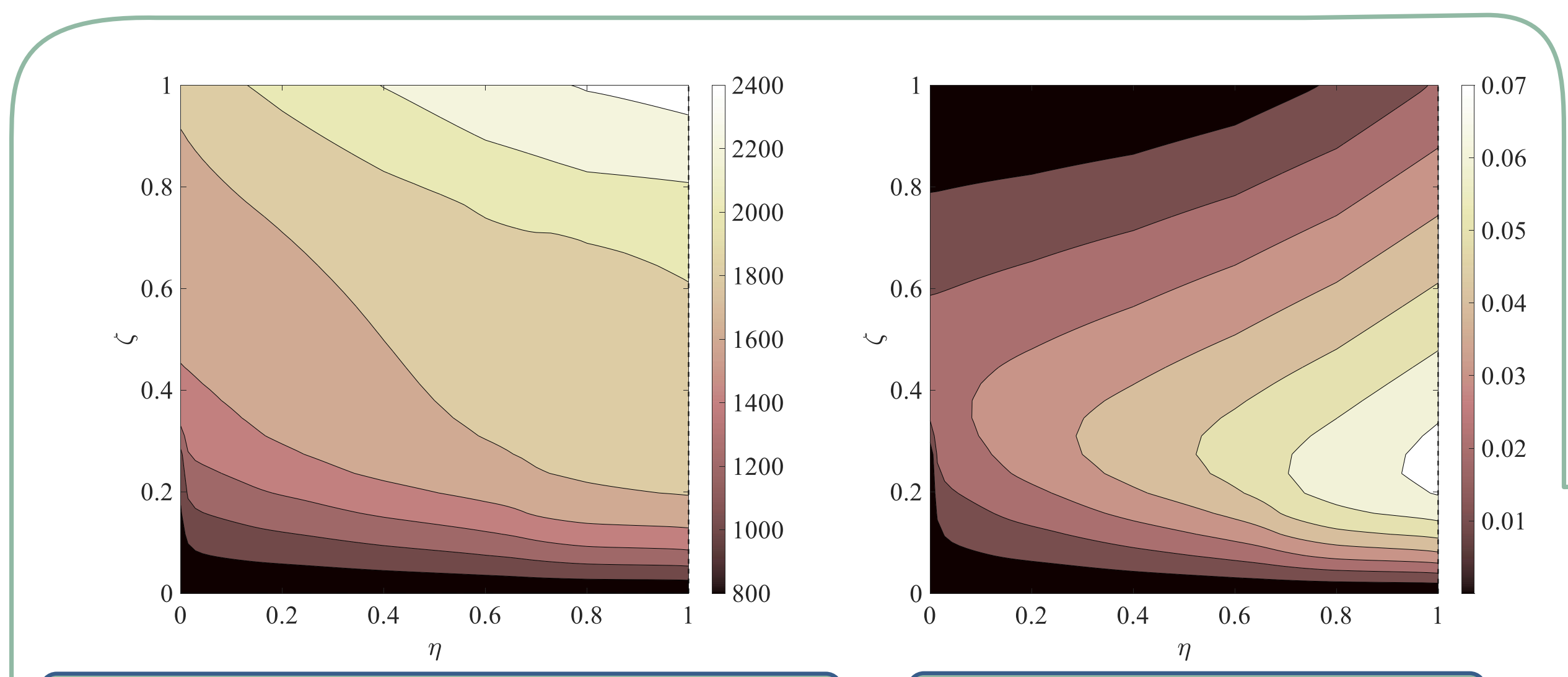
ξ, ξ'', c, c'', N_ξ, N_c, U_{sgs}, P, $\partial P/\partial t$

Conditional variables $\langle Y_\alpha|\eta,\zeta\rangle$, $\langle h|\eta,\zeta\rangle$

DCMC solver
Solves for conditional variables in the 2d conserved scalar space

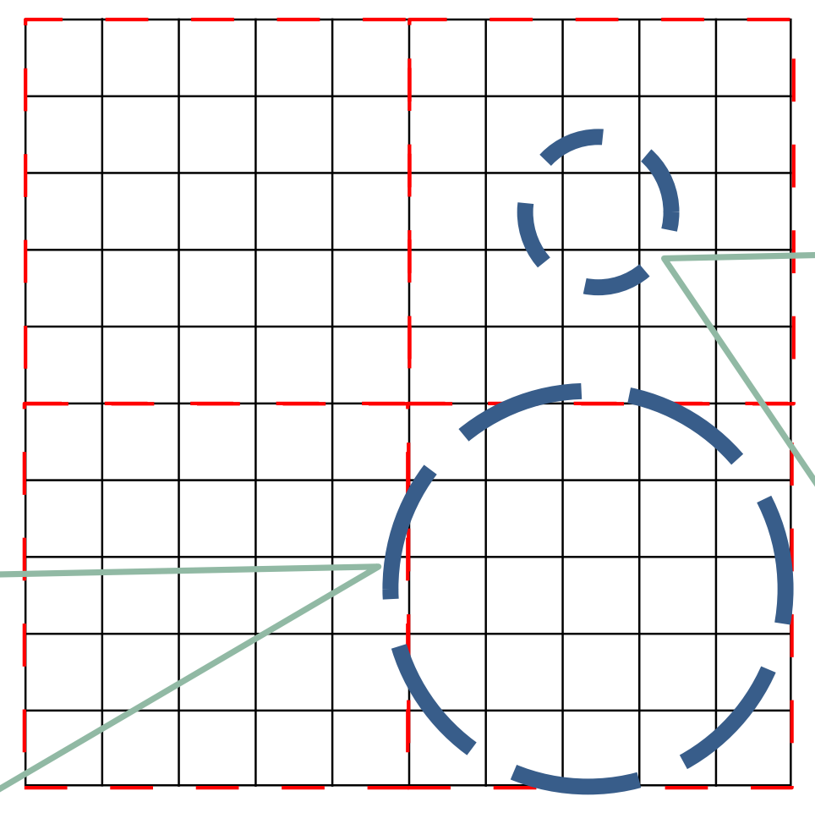
- DCMC solves for conditionally filtered reactive scalars conditioned on mixture fraction ξ and progress variable c
- Coarse mesh for DCMC, so complete chemistry at low computational cost
- $k-\epsilon$ large eddy simulation (LES) is chosen as the turbulence model
- Adaptive mesh refinement (AMR) for complex geometries

Results



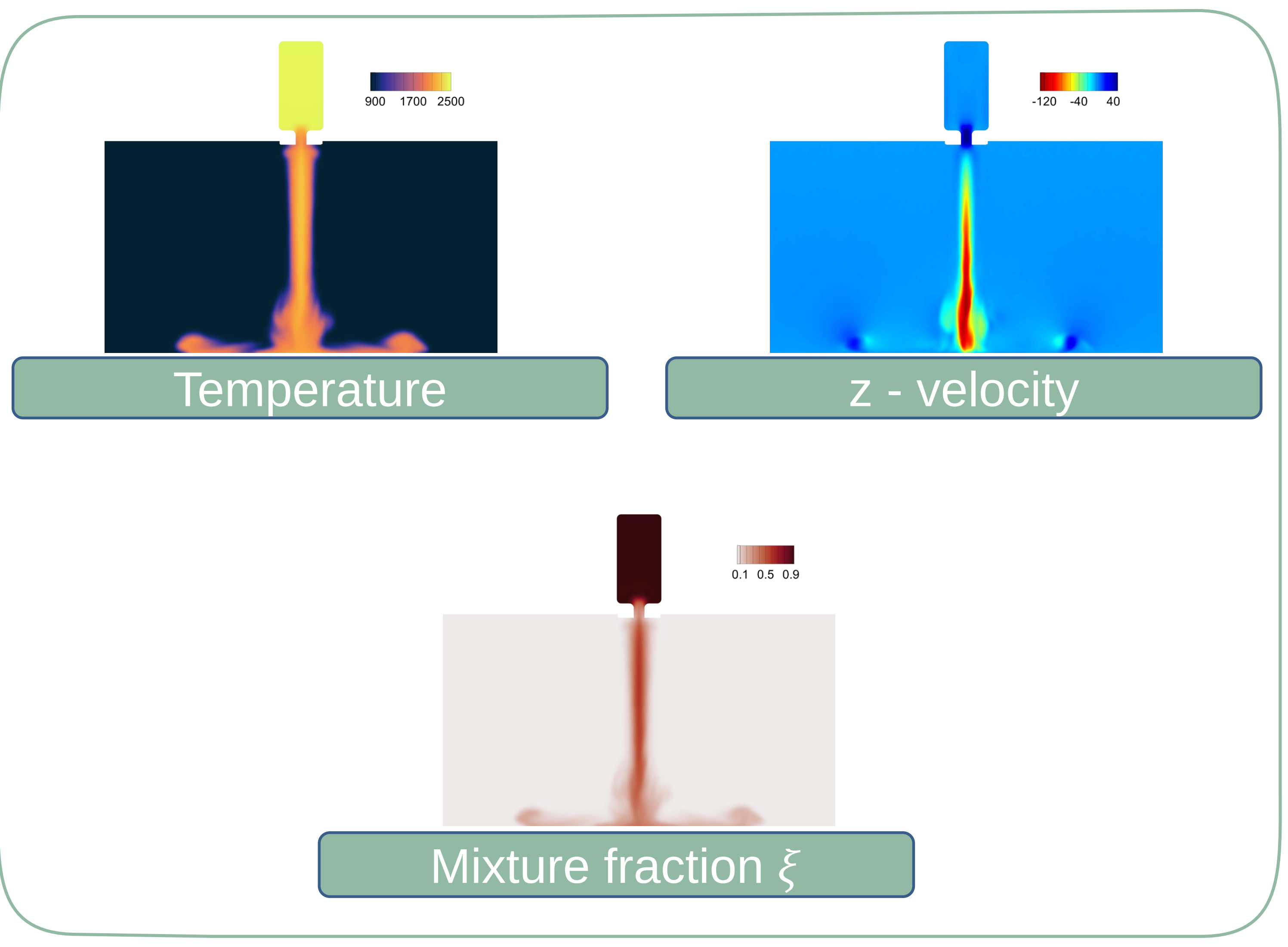
Conditional temperature

$\langle Y_{co}|\eta,\zeta\rangle$



☐ CFD cell

▭ DCMC cell

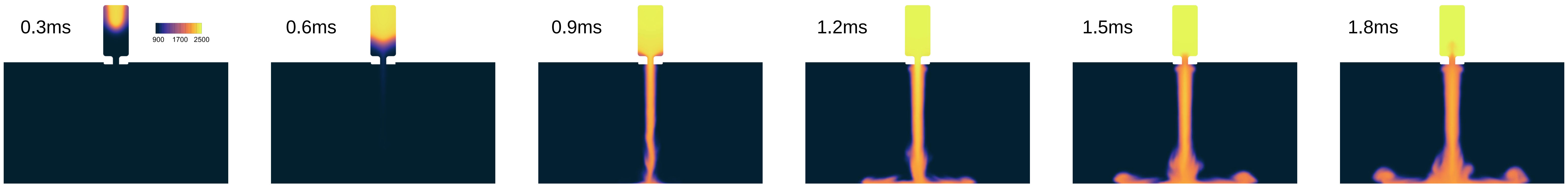


Temperature

z - velocity

Mixture fraction ξ

- Insights from both the η - ζ space and the physical space
- Online chemistry calculations with DCMC equations captures complex turbulence-chemistry interactions



Various modes of combustion as the flame propagates from the pre-chamber to the main chamber

Conclusions and future work

- LES-DCMC combines adaptive mesh refinement with complete chemistry
- Dual-fuel jet or pilot ignition with new fuels such as ammonia, methanol and hydrogen
- Emission analysis for improving their compliance to the standards

Kongsberg Maritime / Viridis Bulk Carriers

Contact: em257@eng.cam.ac.uk, bh540@cam.ac.uk

References

B Harikrishnan, Gkantonas,S., Mastorakos, E., AIAA Scitech Forum (2024)

[1] Cambridge Centre for Advanced Research and Education in Singapore Ltd.
[2] Hopkinson Laboratory, University of Cambridge

"This research project is funded by the National Research Foundation (NRF) Singapore under its Campus for Research Excellence and Technological Enterprise (CREATE) programme."

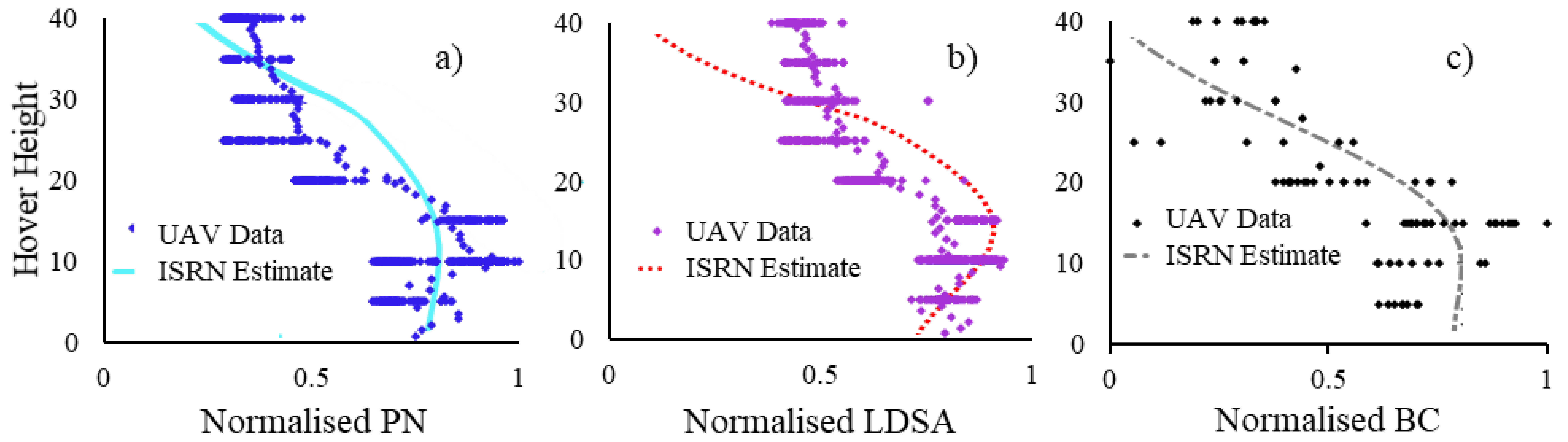
Ship-scale emissions dispersion: measurements

Molly J. Haugen[1*], Savvas Gkantonas[1], Ingrid El Helou[1], Rohit Pathania[1], Adam M. Boies[1,2], and Epaminondas Mastorakos[1,2]

Introduction

The University of Cambridge made novel measurements on maritime particle emissions using an unmanned aerial vehicle (UAV) and handheld particle sensors in Rafina, Greece building on previous studies that considered complications of using UAVs for gaseous data collection in maritime applications. This work adds particle data to the knowledge base of maritime emissions and gives insight to how using UAVs for particle measurements can be improved and standardised.

- 3 particle instruments gathered information for plume emissions
- At 90 cm from the centre of the UAV, the sampling location is outside the downwash created by the rotors, ensuring particles captured were minimally influenced by the drone's movements



- UAV/plume interaction studied
- Real-time monitoring of multiple particle characteristics
- Ability to incorporate coagulation and mixing into plume estimates (ISRN)

With a more standardized and robust measurement and data collection processes, UAV measurements can be directly comparable between studies, contributing to international maritime emission inventories for at-sea emissions, lending to regulatory, research, and industrial sectors.

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References

Frederiksen, M. H., & Knudsen, M. P. (2018). Drones for offshore and maritime missions: Opportunities and barriers. SDU Centre for Integrative Innovation Management, April.

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"This research project is funded by the National Research Foundation (NRF) Singapore under its Campus for Research Excellence and Technological Enterprise (CREATE) programme."

Ship-scale emissions dispersion: calculations

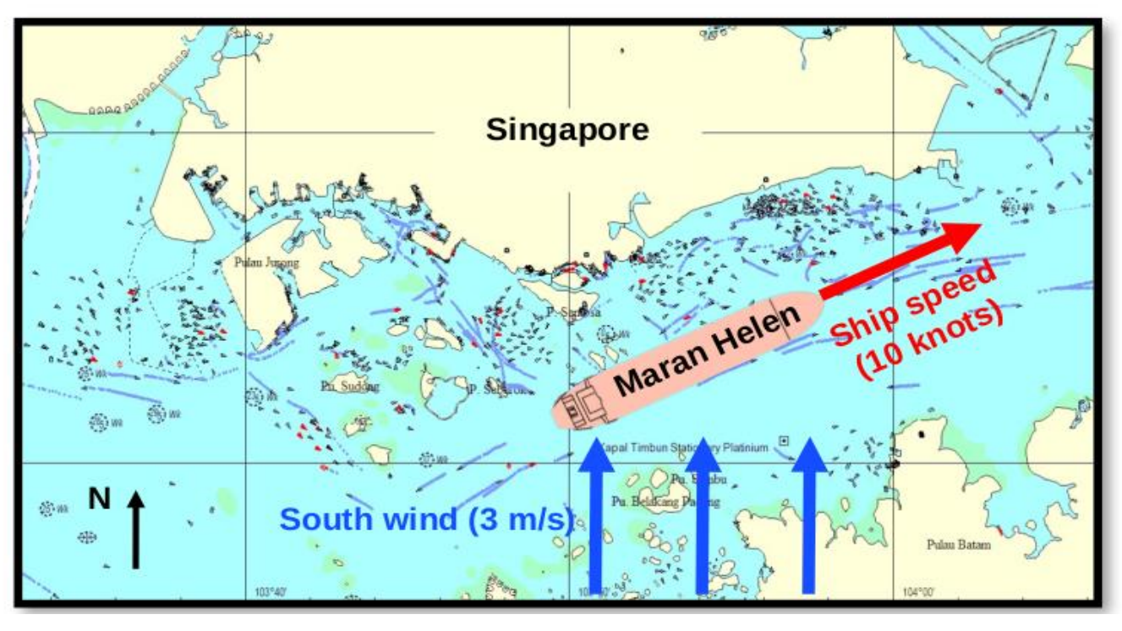
Ramesh Kolluru[1], Yangyang Liu[1], Savvas Gkantonas[2], Epaminondas Mastorakos[1,2]

Shipping Emissions and Leak Dispersion Studies

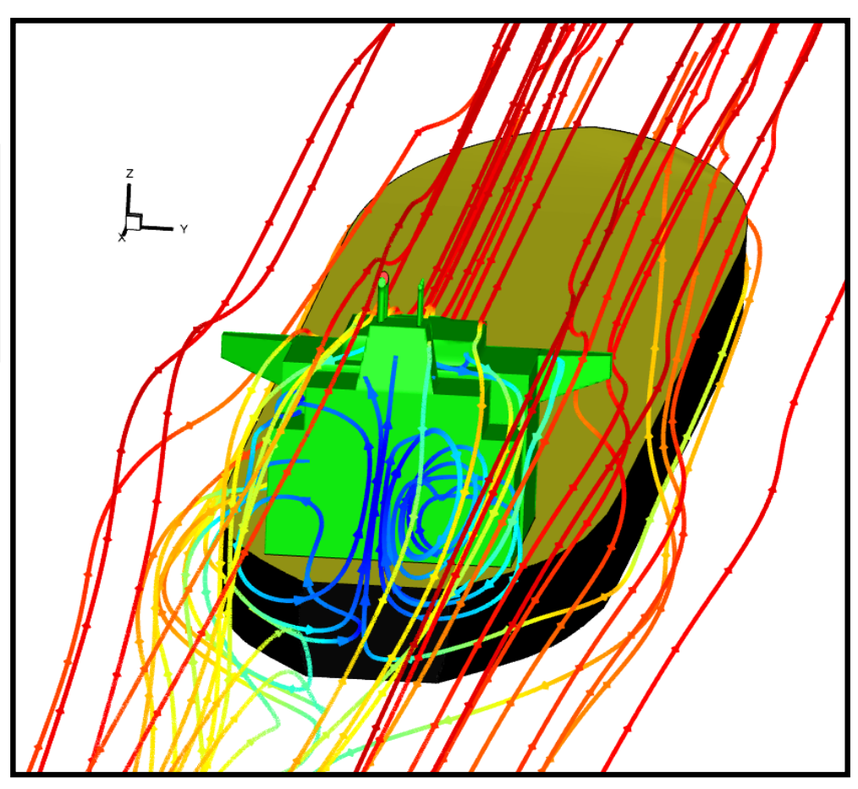
Ship-scale emissions dispersion calculations and assessment for accidental ammonia leakage are critical aspects for todays and future shipping. These calculations involve sophisticated modelling techniques to assess how emissions from ships disperse in the atmosphere, helping authorities and ship operators mitigate their environmental impact. Additionally, understanding dispersion behaviour for ammonia leakage during bunkering is essential for guaranteeing personnel safety and safeguarding marine ecosystems. Numerical simulations play a pivotal role in these assessments and are performed in this research with a combination of multi-dimensional Computational Fluid Dynamics and advanced turbulent reacting flow theories that include the effects of mixing on the chemical evolutions of the emitted species.

Enhancing Pollution Modelling: CFD-ISRN Investigations of mixing Effects in Plumes

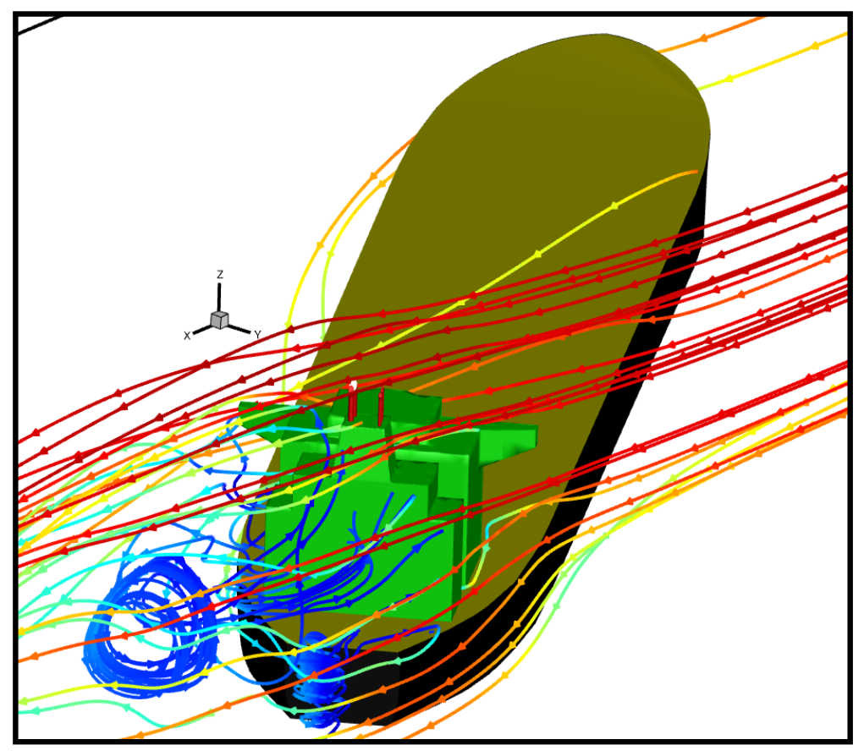
Scenario and cases under consideration



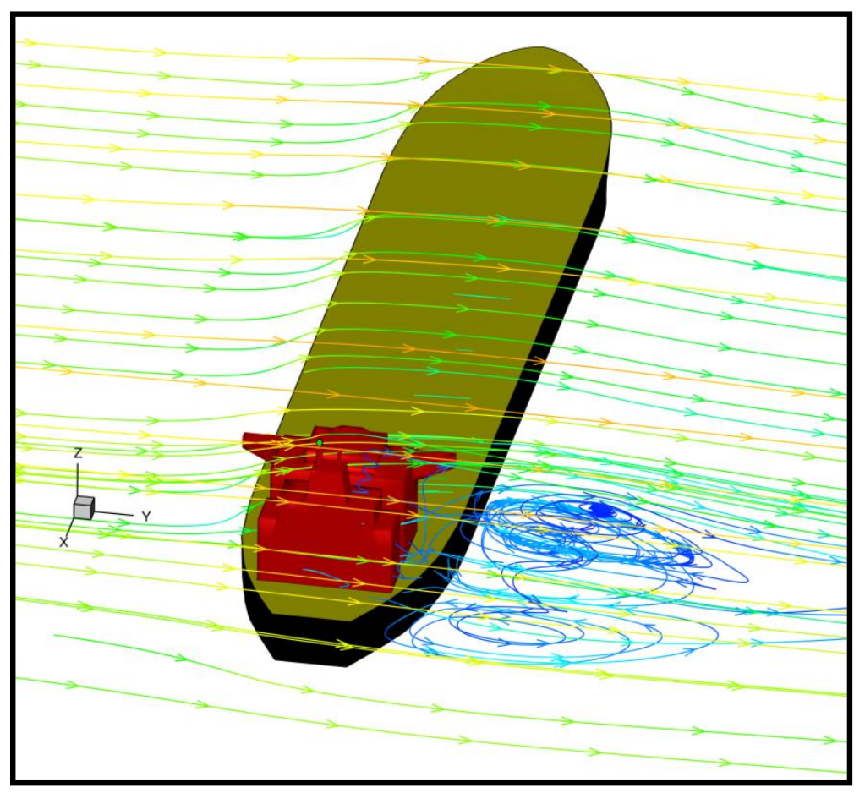
Head Wind



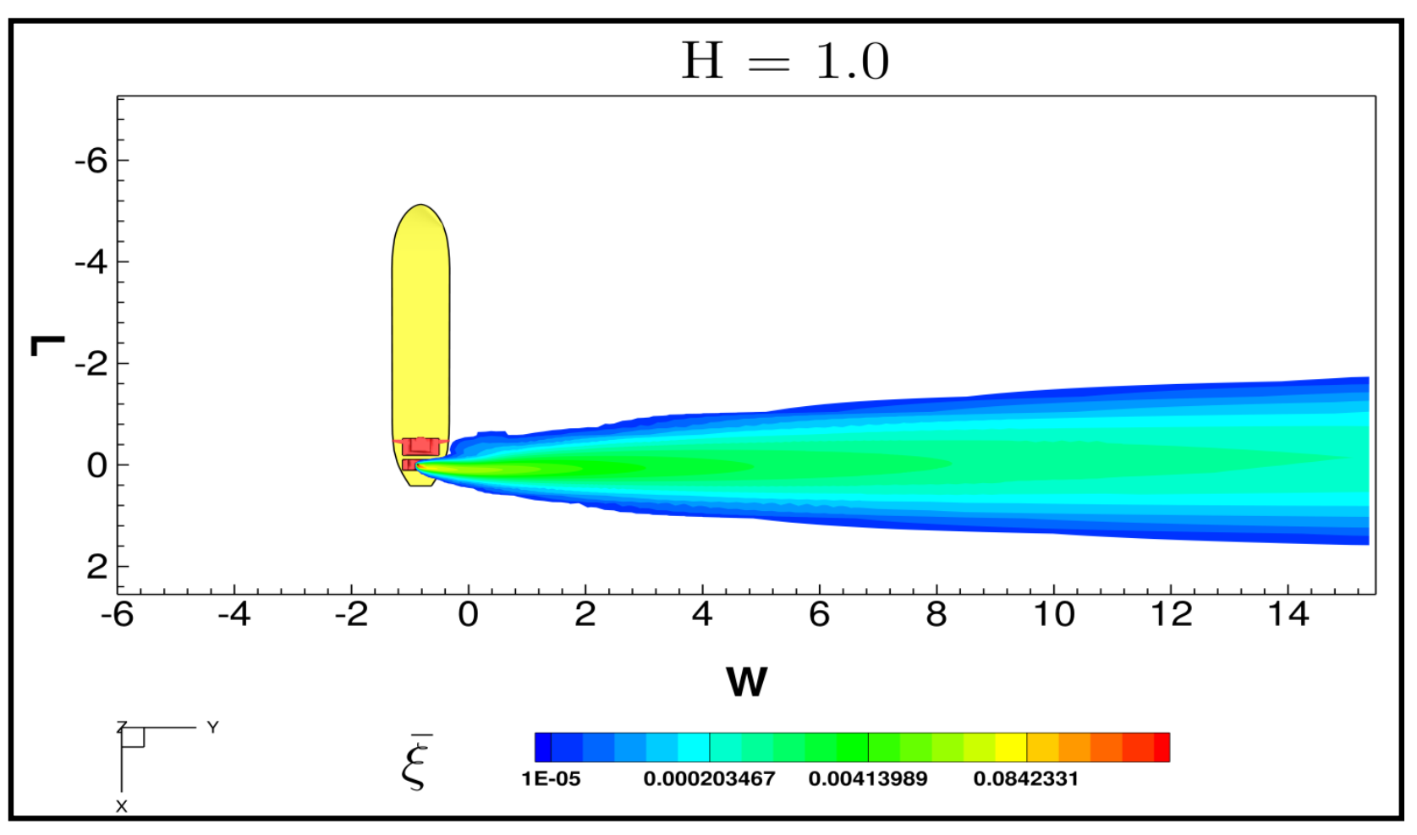
Inclined Wind Flow approaching ship at 30^0



Cross Wind



Evolution of passive scalar from the main engine stack using CFD



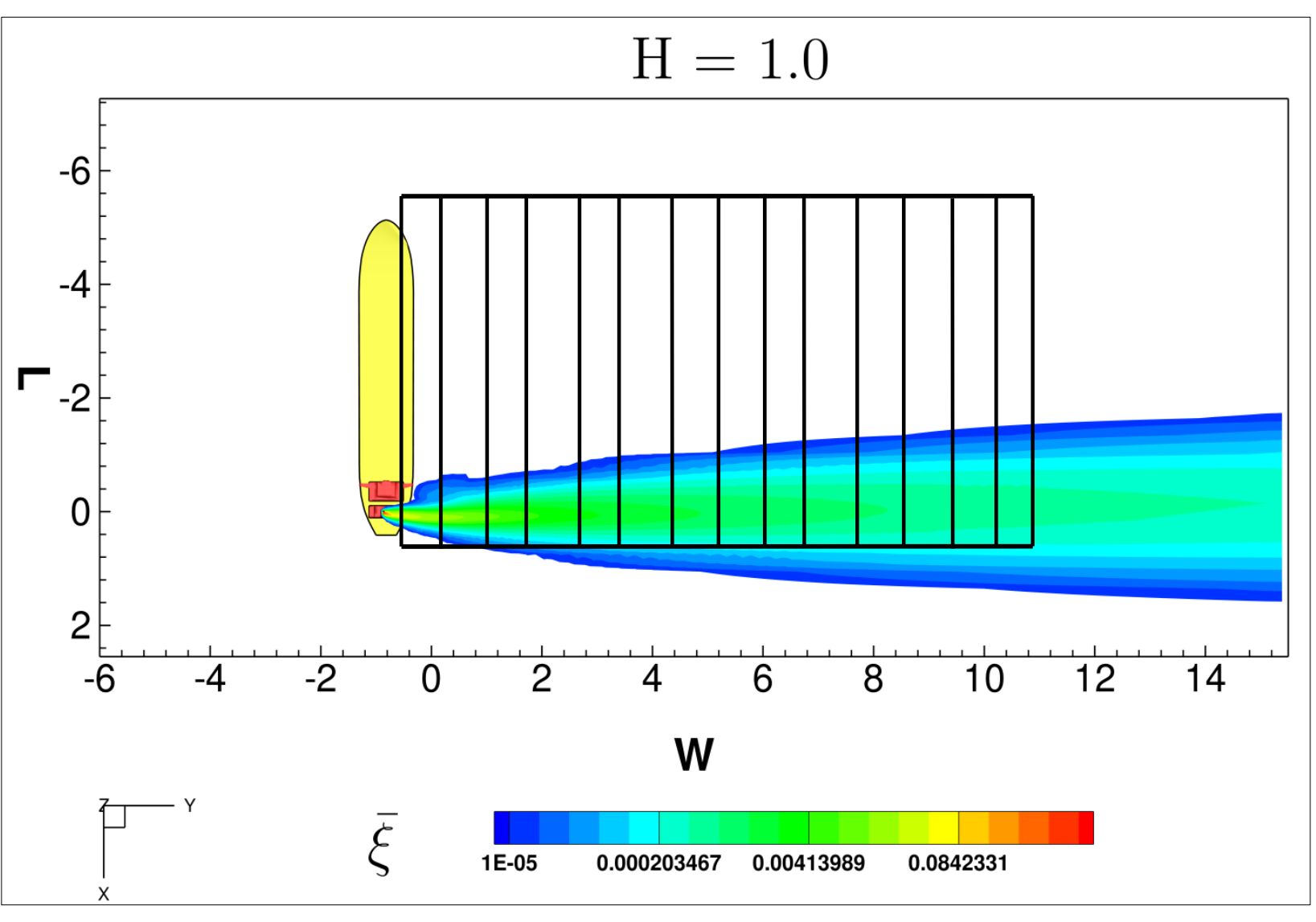
ISRN Simulation Details

- CBM IV Mechanism is used for Chemistry
- Solved in mixture fraction space η ϵ [0,1].
- 240 ISR cells are used in the mixture fraction space.
- Table below - Boundary conditions of species in the mixture fraction space

Species	Concentration in ppb	Concentration in ppb
	@ Exhaust	@ Background
Nitric Oxide (NO)	1111.148	0.182
Nitrogen Di Oxide (NO2)	-	0.018
Ethene(ETH)	1.871	-
Xylene(XYL)	0.220	0.35
Toluene (TOL)	0.538	0.35
Carbon Monoxide (CO)	58.016	130.0
Methane (CH4)	68.353	0.0
Sulpher dioxide (SO2)	43.974	0.0
PAN	-	0.135
Ozone O3	0.0	20.3

Distribution of ISR Cells in η space

CFD TO ISRN



ISRN TO CFD

ISRN can be thought of as like CMC, but specifically tailored for post-processing tasks.

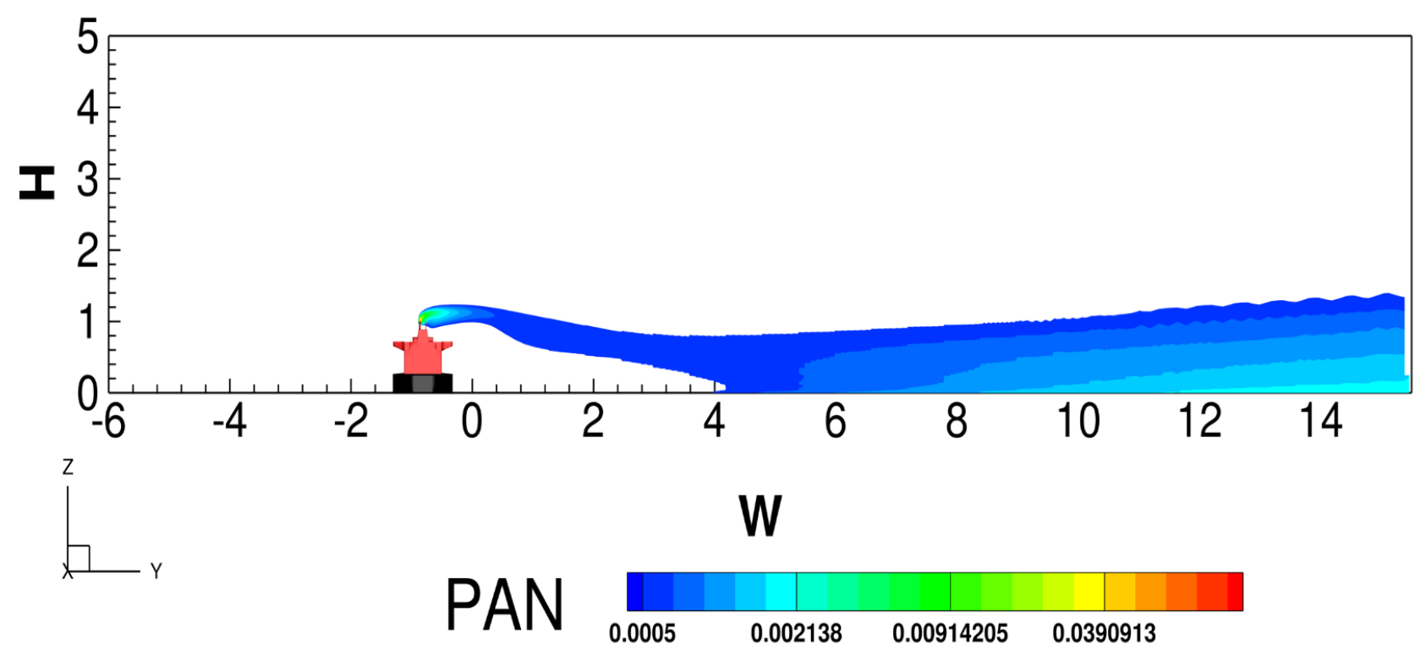
$$\frac{\partial Q_a}{\partial t} + \underbrace{\langle u_i|\eta\rangle \frac{\partial Q_a}{\partial x_i} = \frac{\partial}{\partial x_i}\left(D_t \frac{\partial Q_a}{\partial x_i}\right)}_{\text{Transport in physical space}} + \underbrace{\langle N|\eta\rangle \frac{\partial^2 Q_a}{\partial \eta^2}}_{\text{Micro-mixing}} + \underbrace{\langle \dot{\omega}_\alpha|\eta\rangle}_{\text{Reaction}}$$

$$\langle N|\eta\rangle = \left\langle D \frac{\partial \xi}{\partial x_i} \frac{\partial \xi}{\partial x_i} \middle| \eta \right\rangle \text{ - Scalar dissipation rate}$$

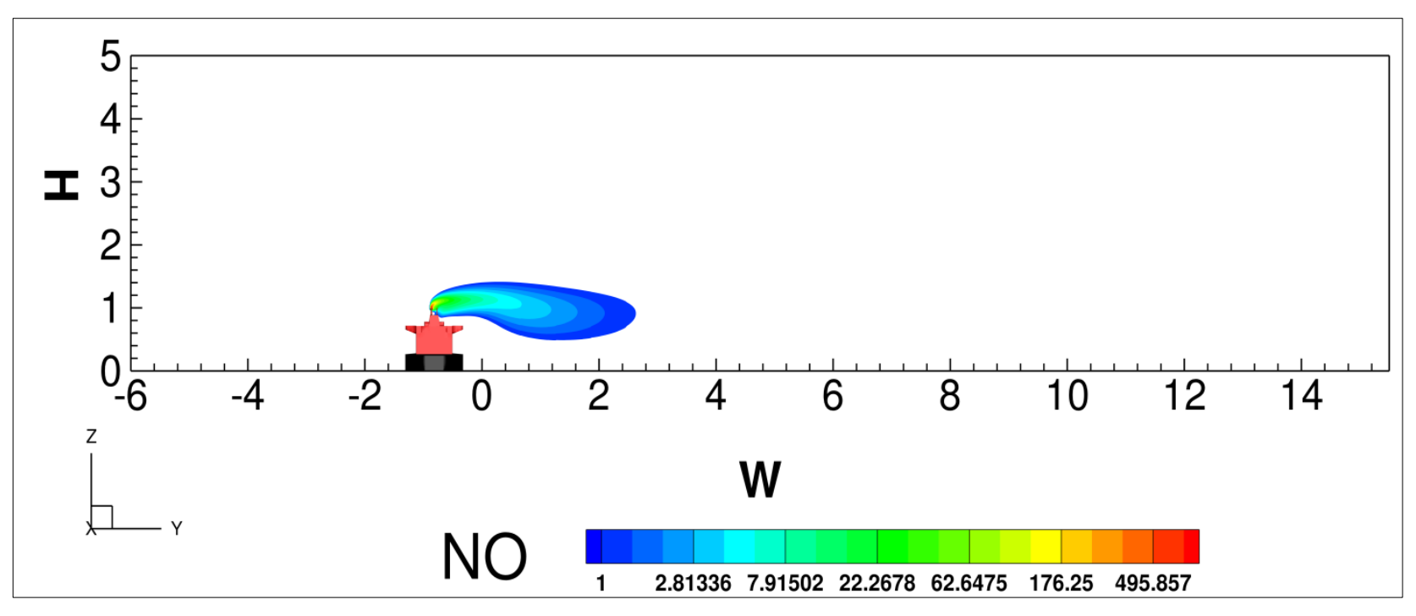
Detailed photochemistry using CBM IV Mechanism [1]

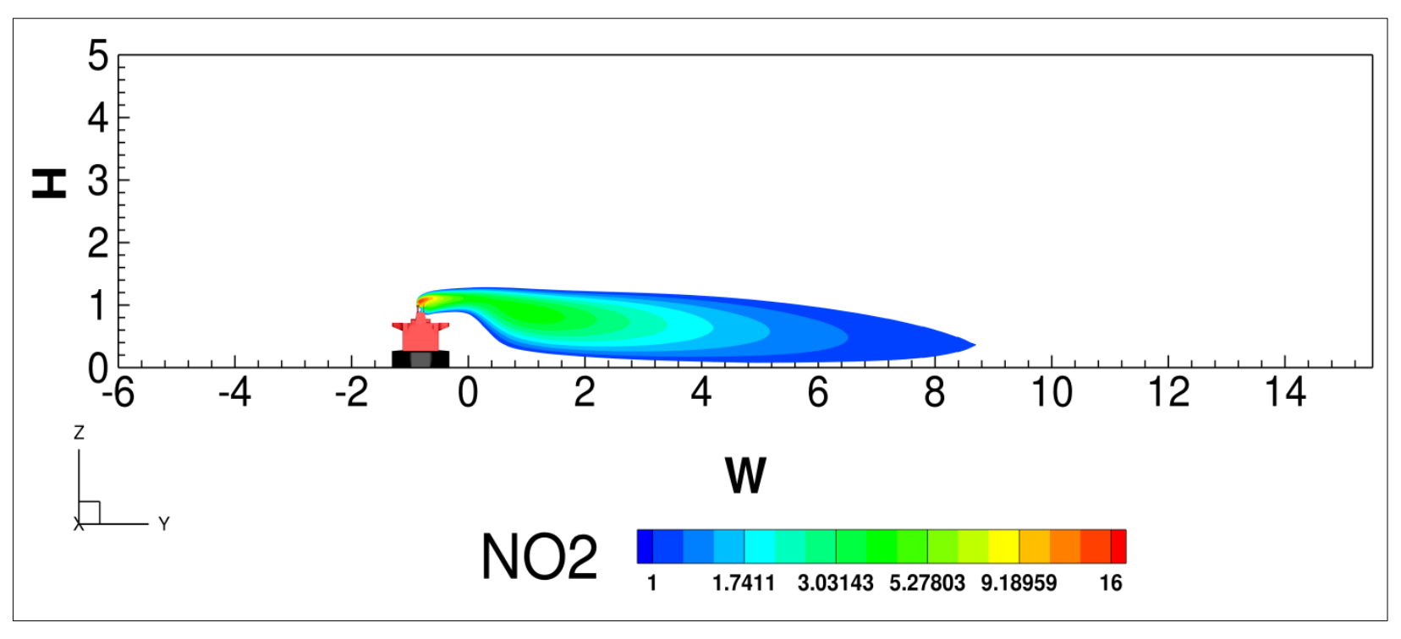
- 28 species with fast & slow chemistry
- good for urban problems
- NOx (e.g., NO + hν → NO_2 +O)
- VOC (e.g., FORM + NO_3 → HNO_3+HO_2+CO)

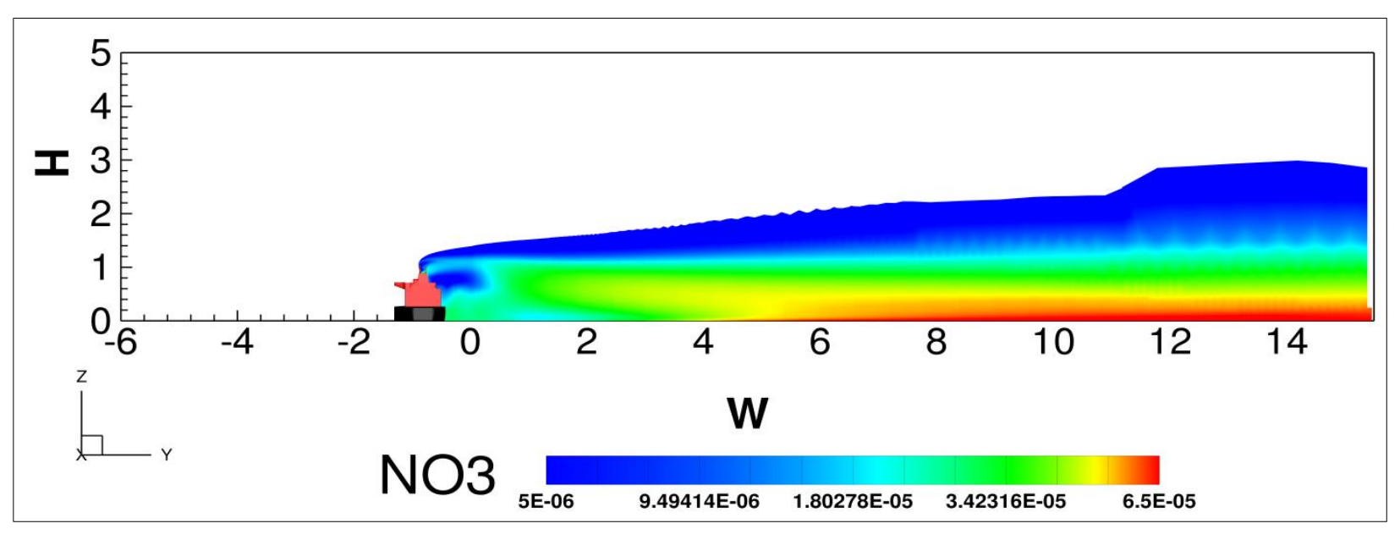
Distribution of PAN after ISRN Calculations along y = 0 plane

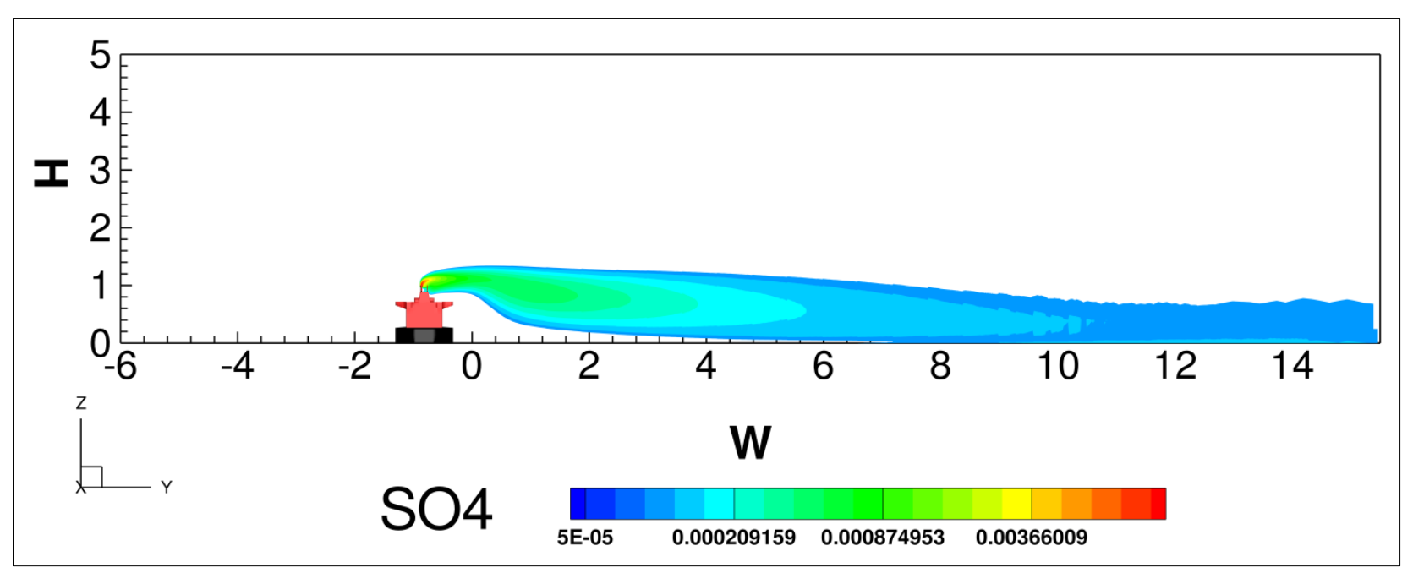


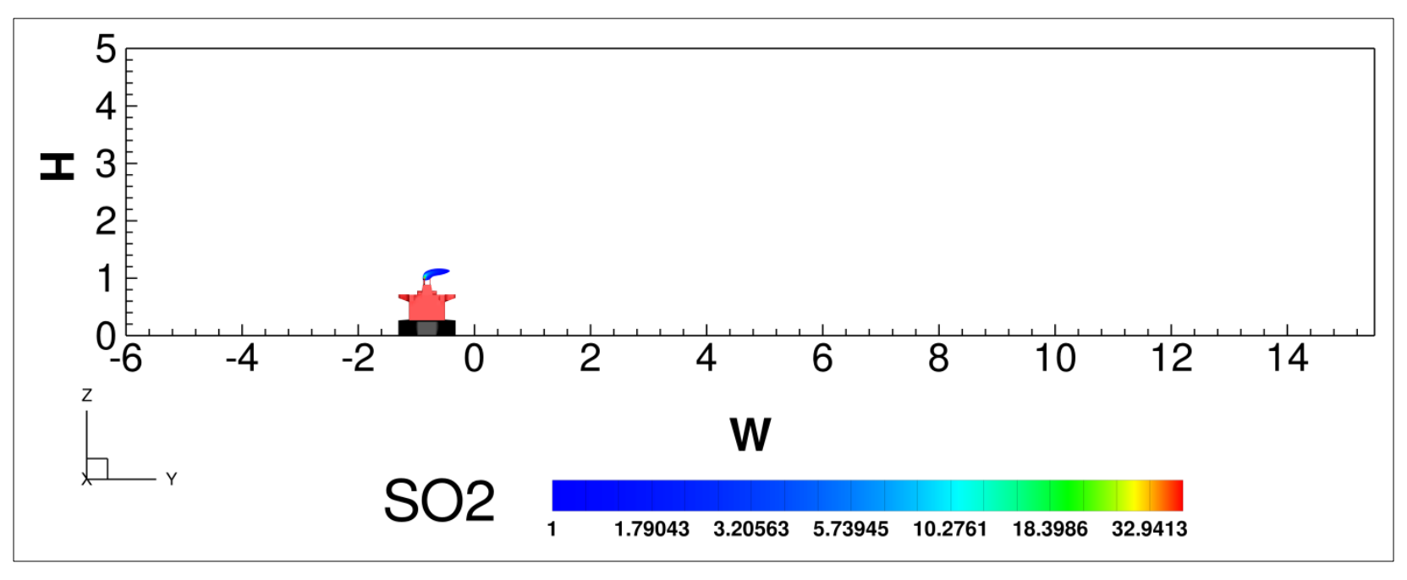
Un-Conditional Nox and Sox Species at CFD Resolution











Conclusions

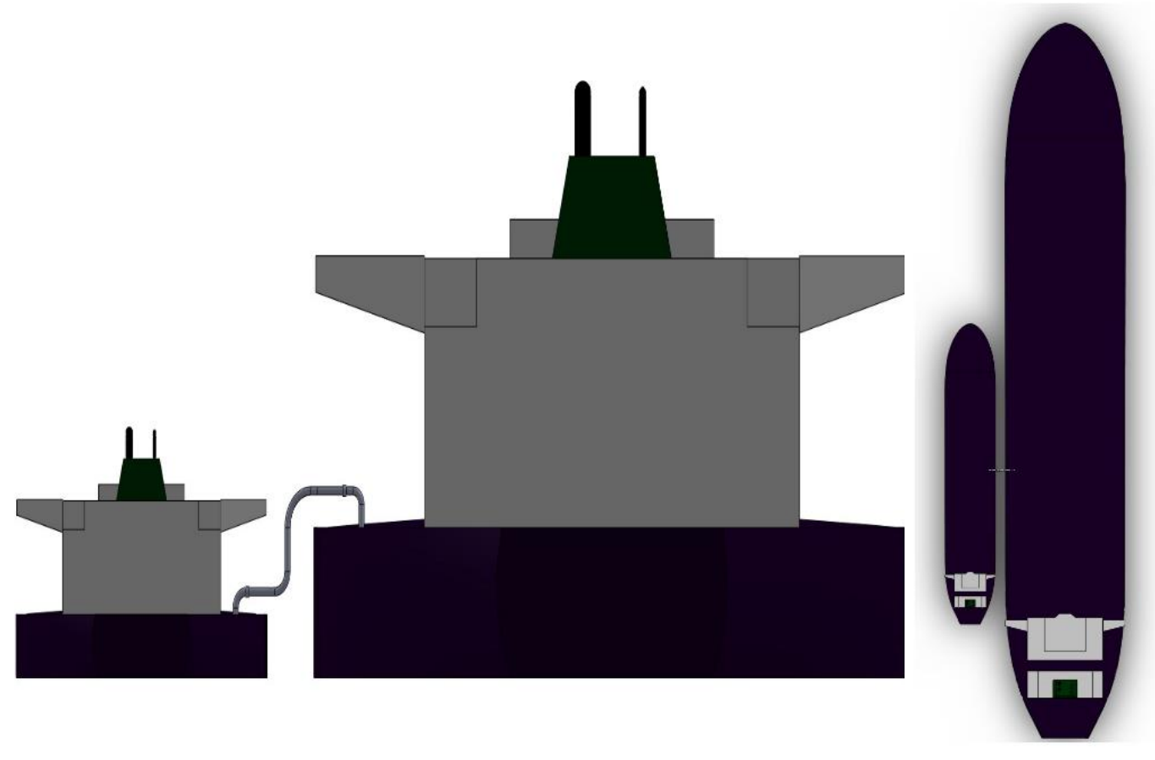
- Micro-mixing and inhomogeneity effects appear to be significant in the near-field.
- With the availability of CFD solutions, ISRN allows for a broader range of analyses involving more chemistry.
- The level of importance of micro-mixing in this context remains uncertain.

Future work

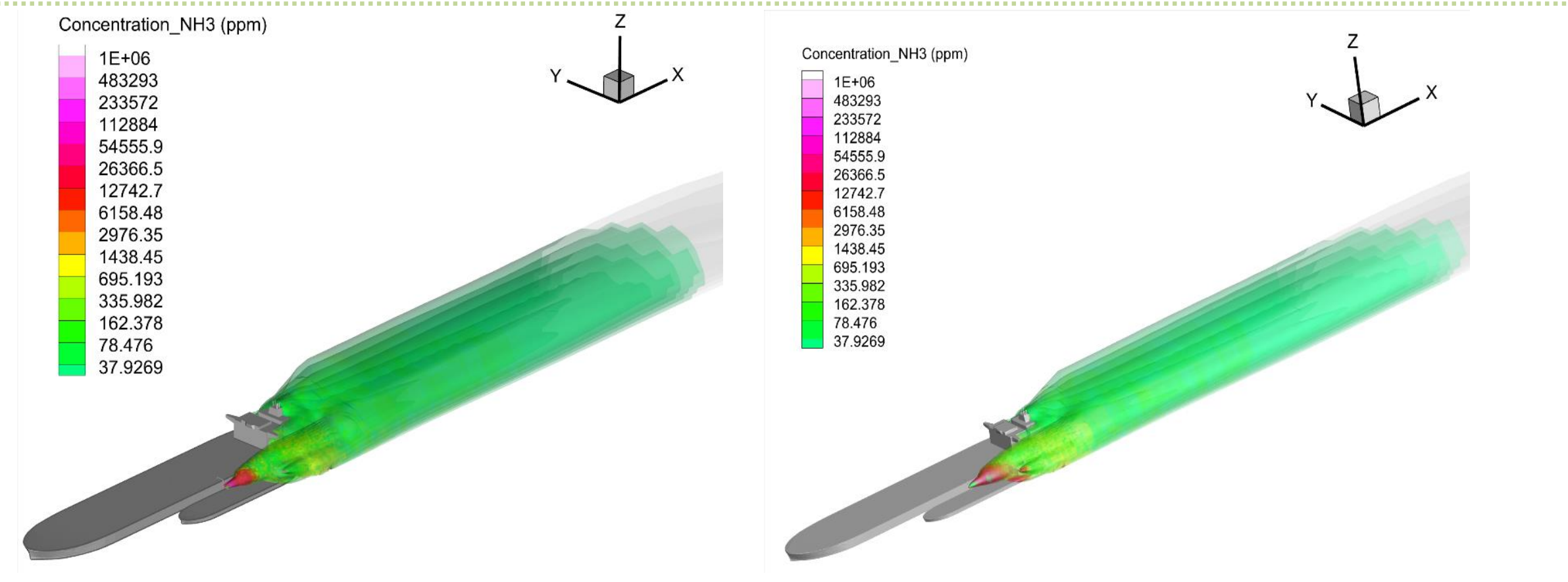
- Sensitivity analysis for ISRN: Cd, background, ISR spacing.
- Comparative analysis with simplified models.
- Assessment of pollutant absorption at sea level.
- Evaluation of particulate matter models: BC, OC, sulphates, and methods such as moment or sectional approaches.

Ammonia Leakage & Dispersion During Ship-to-ship Bunkering

Example for ship-to-ship bunkering operation [2].



Schematic diagram for ship-to-ship ammonia bunkering operation.



3D view of horizontal (left) and vertical (right) leakage scenarios: exposure regions of ammonia concentration > 30 ppm.

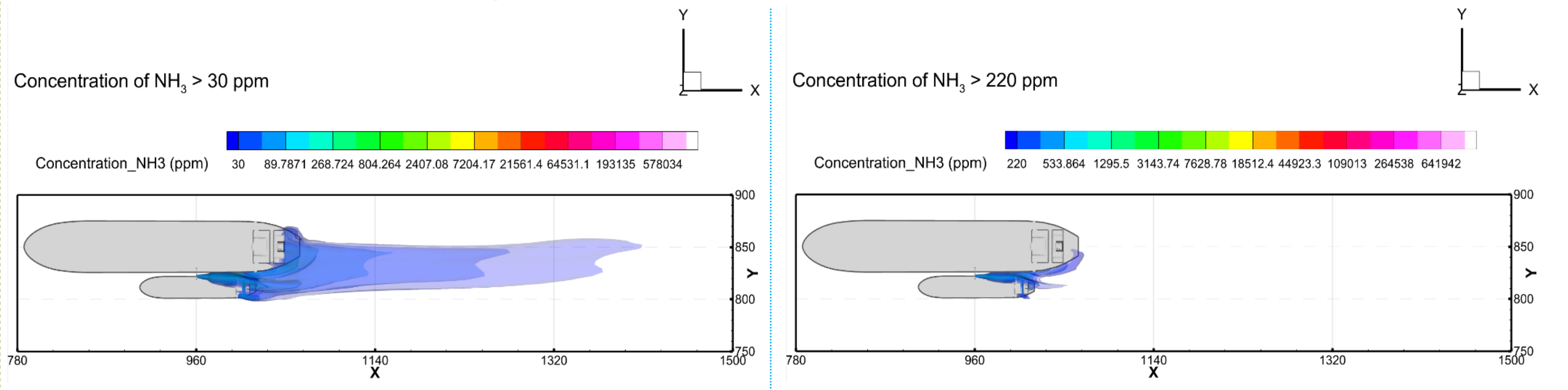
- ✓ *Effects of superstructures on-board vessels on the dispersion of released ammonia in the near field. (vs. Gaussian plume models)*

Future work
- ☐ *Effects of leakage position, atmospheric conditions, etc.*

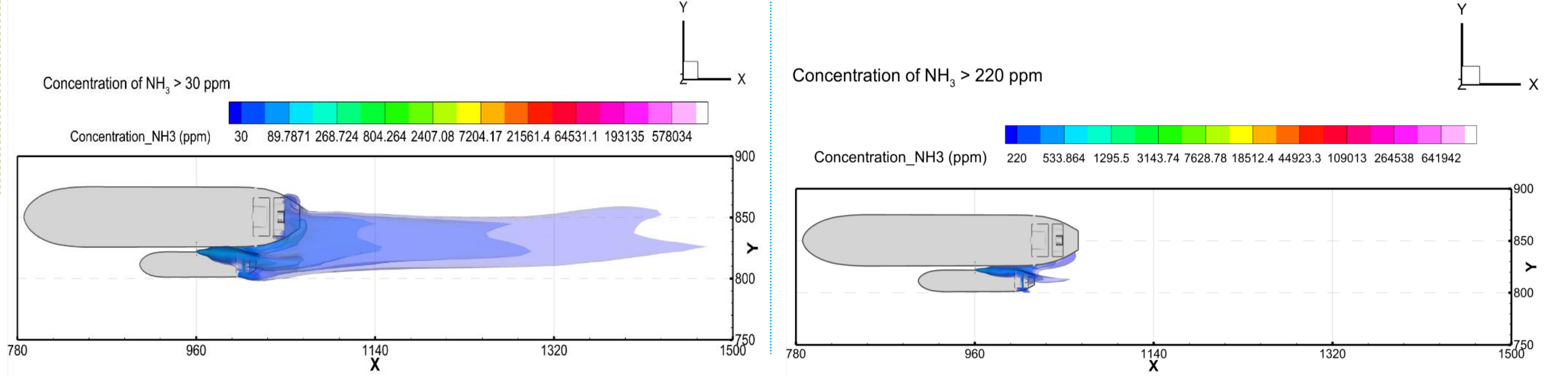
- ➢ *Risk assessment.*
- ➢ *Effective operational and mitigation control measures for ammonia bunkering operations.*

Horizontal Leakage.

X-Y plane view: exposure regions of ammonia.



Vertical Leakage.



- ✓ *Higher and further ammonia dispersion for vertical leakage.*

- ❖ *People aboard may be exposed to a larger dangerous area.*

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[1] Gery et al., Journal of Geophysical Research, 94(D10):12925, 1989

[2] https://www.marineinsight.com/guidelines/bunkering-is-dangerous-procedure-for-bunkering-operation-on-a-ship/.

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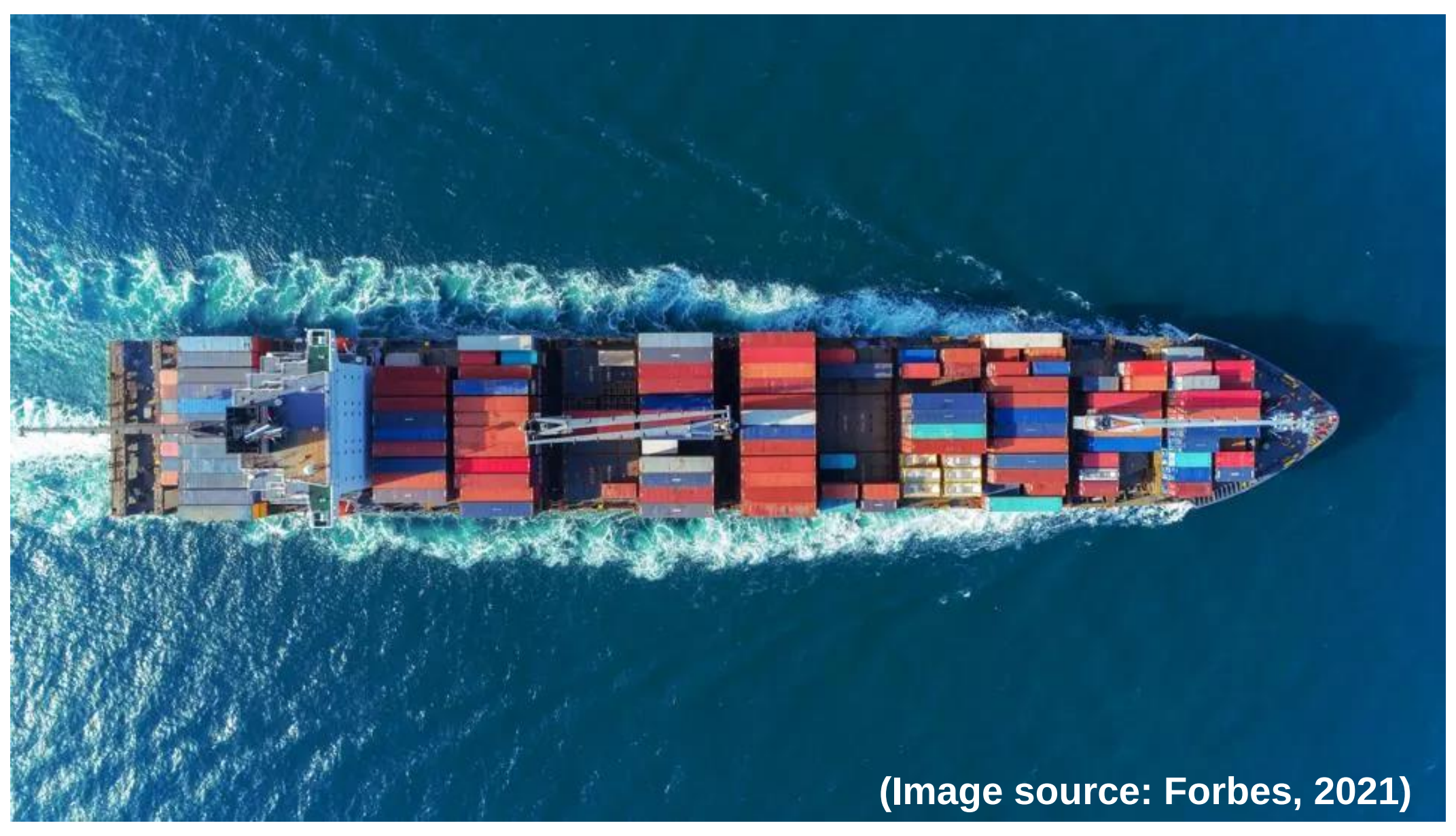
UNDERSTANDING SOOT FORMATION OF BIOFUELS FOR CLEAN COMBUSTION

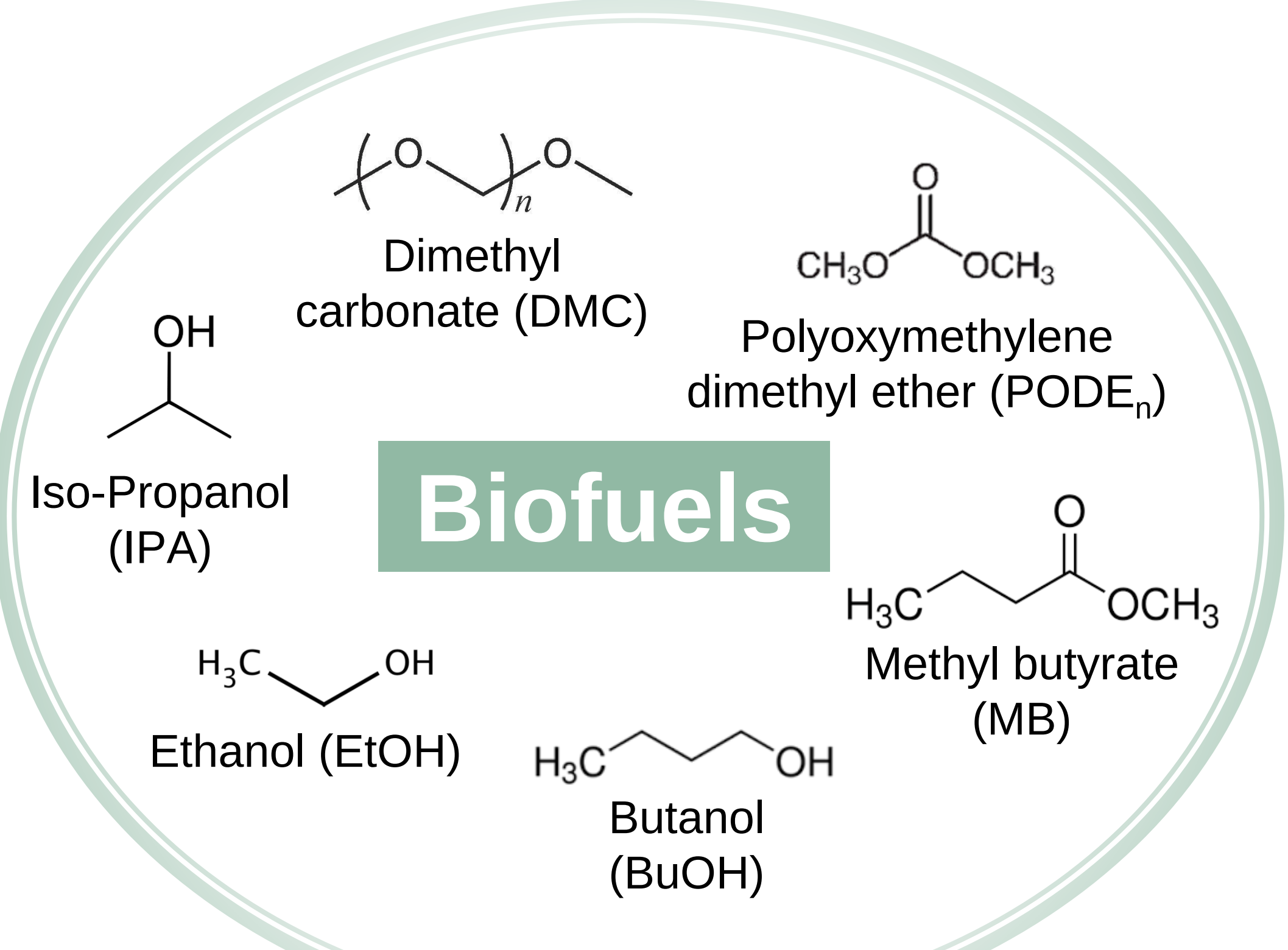
Yong Ren TAN[1,2,3], Maurin SALAMANCA[4], Yichen ZONG[2,3], Jethro AKROYD[1,3], Markus KRAFT[1,3,5,6]

Introduction

Liquid fuels remained the prominent means to power the heavy transport sector despite efforts of electrification. Hence, the usage of biofuels is promising in reducing the carbon footprint of the industry. This research aims to understand the soot formation from the combustion of different biofuels using different experimental techniques to have an environmental assessment of the usage of different biofuels.

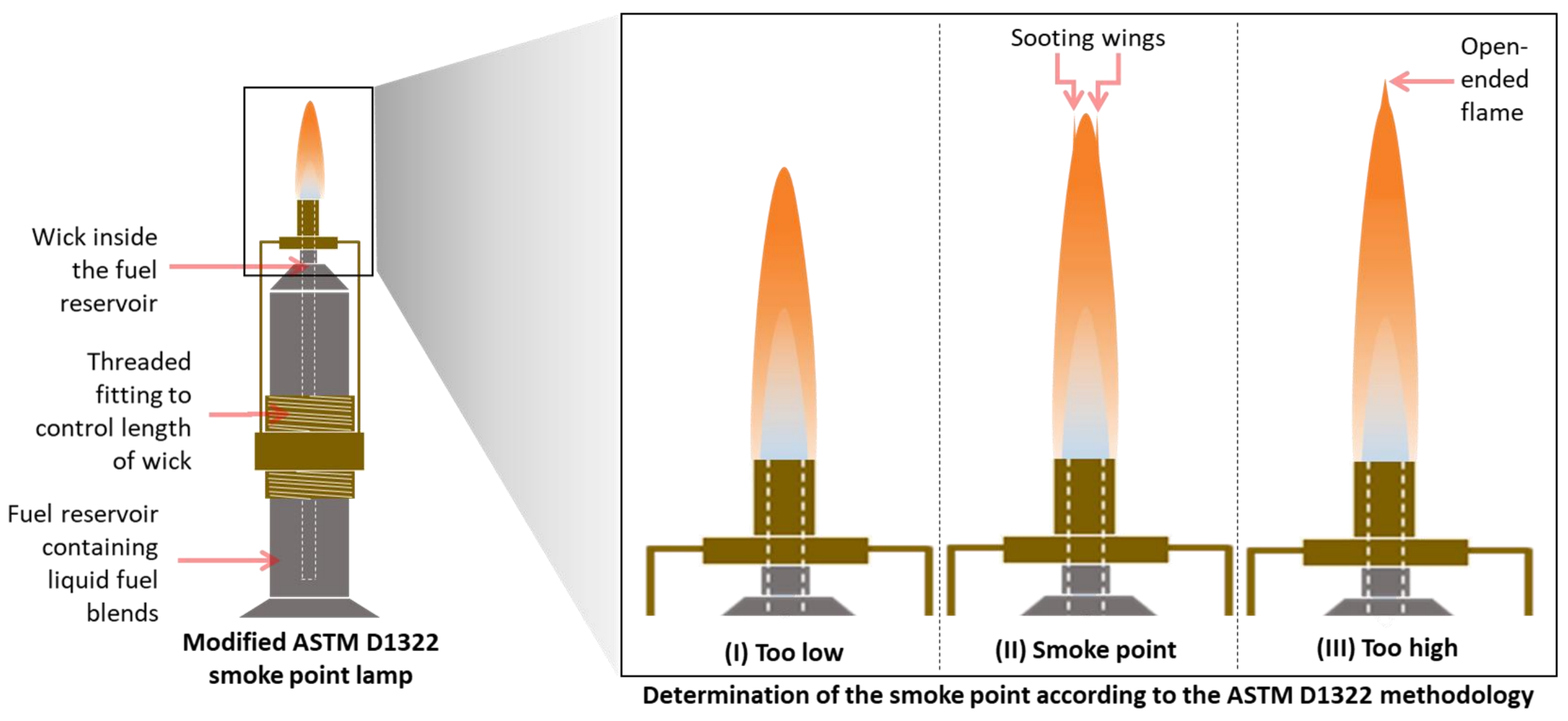


(Image source: Forbes, 2021)



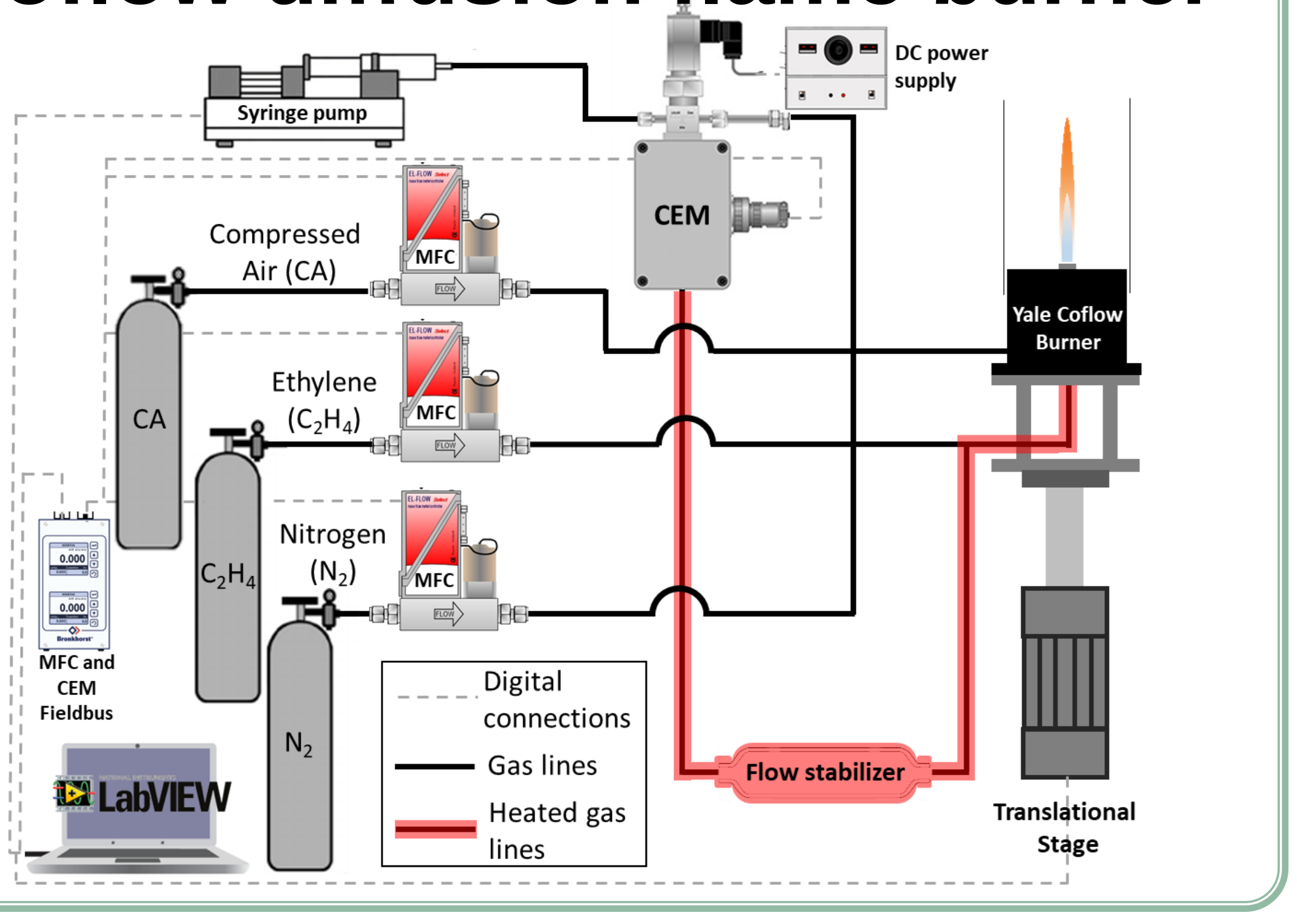
Methods

ASTM D1322 Smoke Point lamp



Determination of the smoke point according to the ASTM D1322 methodology

Coflow diffusion flame burner



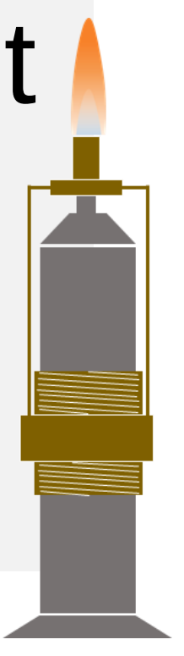
Results

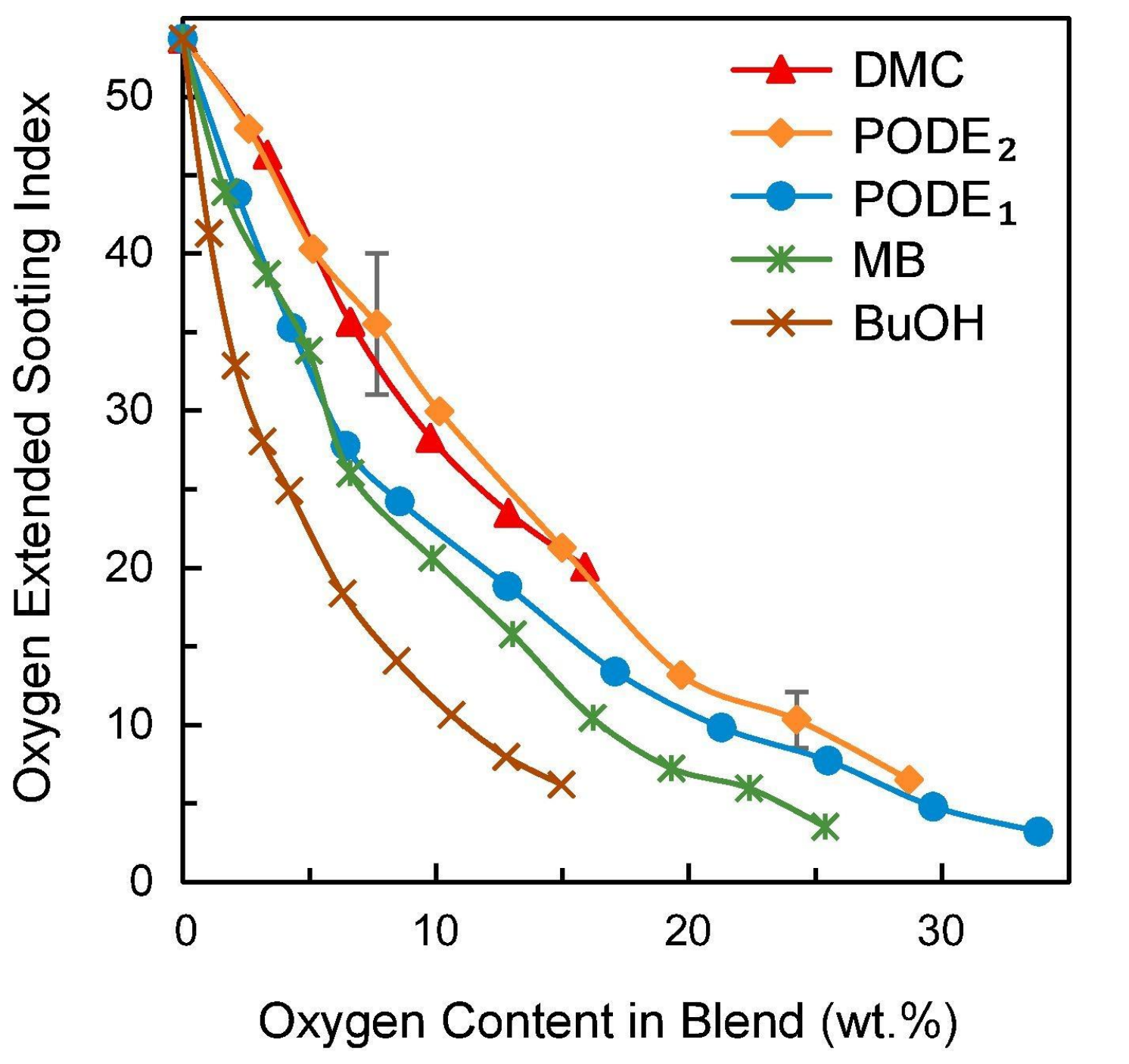
Oxygen Extended Sooting Index (OESI),

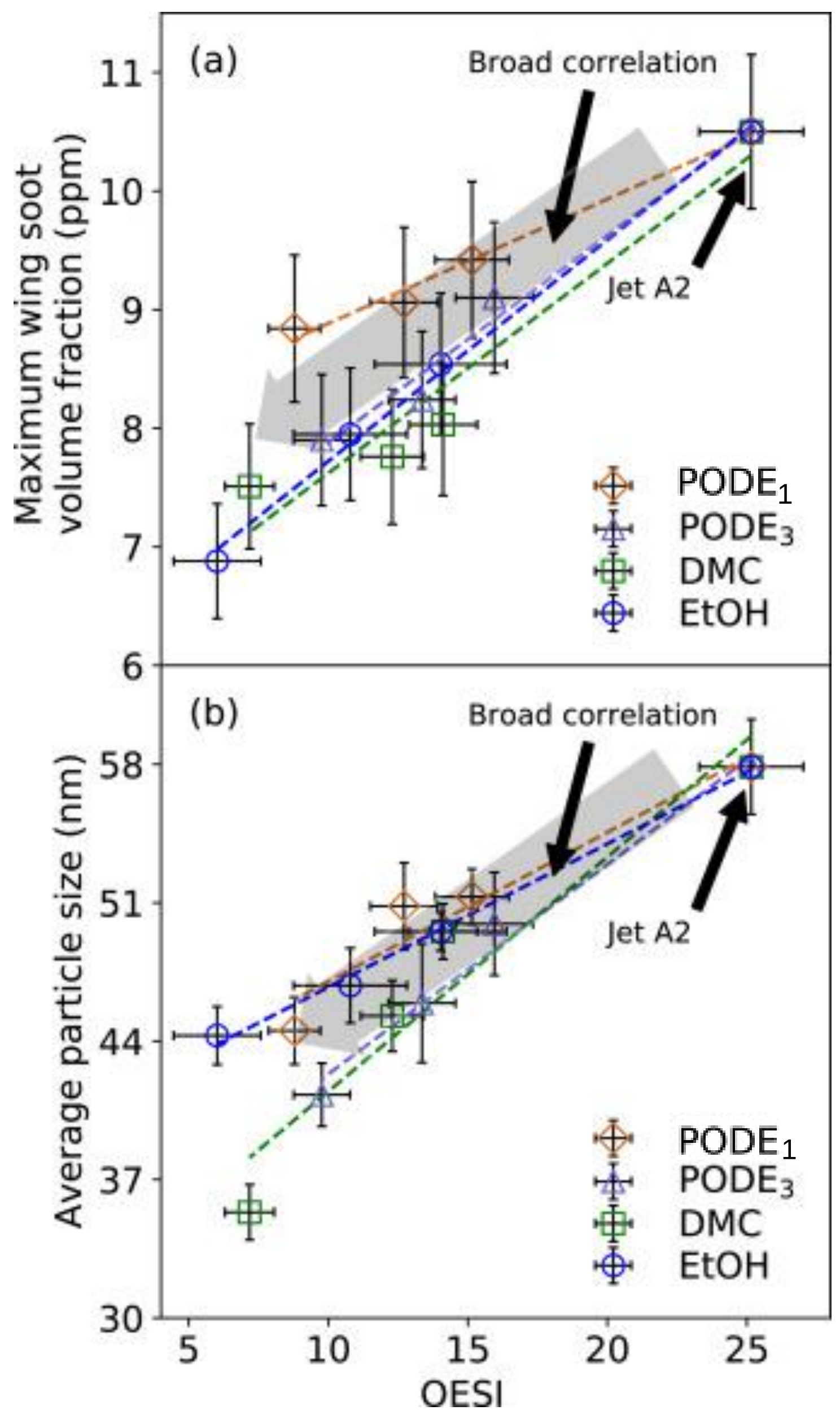
$$OESI = a_{OESI}\left(\frac{n+\frac{m}{4}-\frac{p}{2}}{Smoke\ Point}\right) + b_{OESI}$$

where n, m and p are $C_nH_mO_p$.

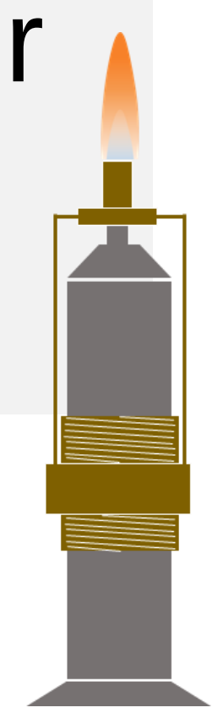
Sooting propensity varies according to the chemical structure, not just the oxygen content of fuel blend



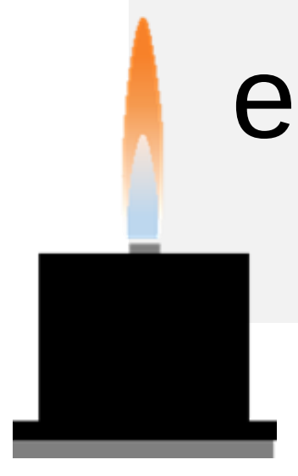


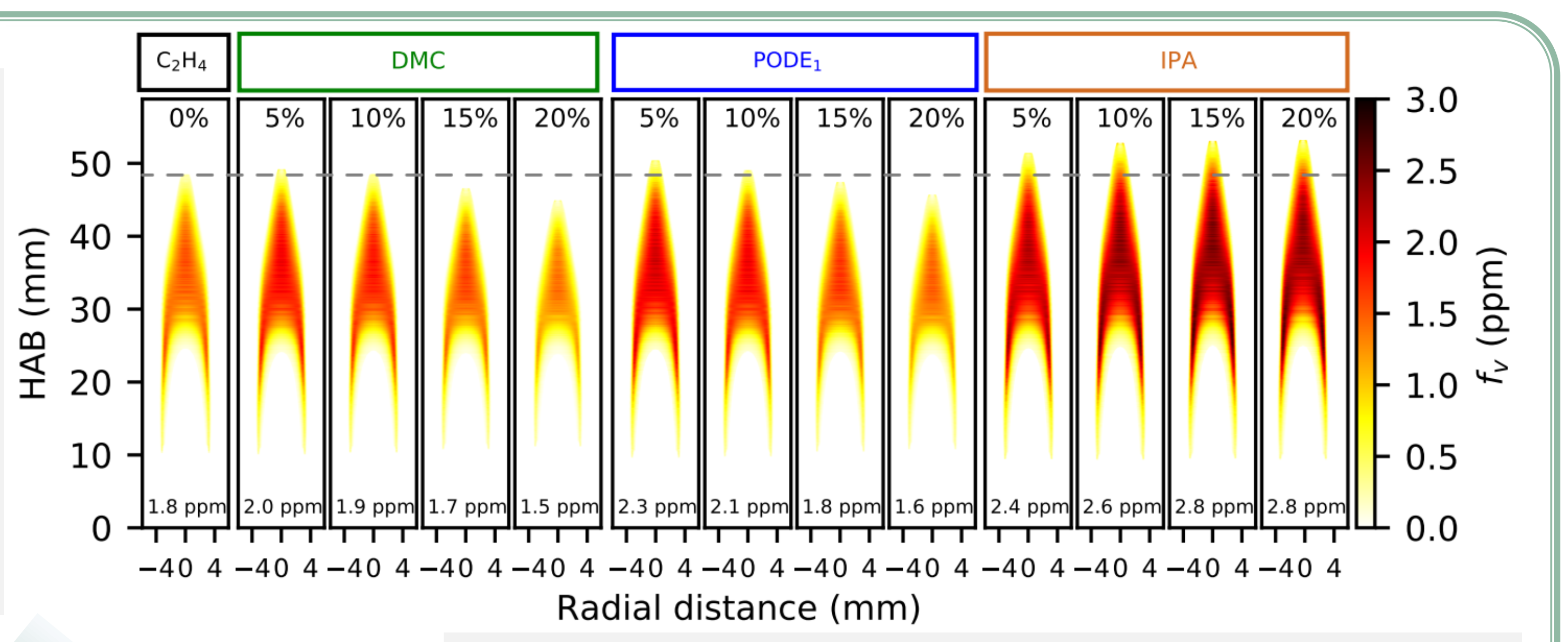


Impact:
Could be used to support the evaluation of the capability of new Sustainable Aviation Fuel blends to meet the particulate matter standards in the aviation sector

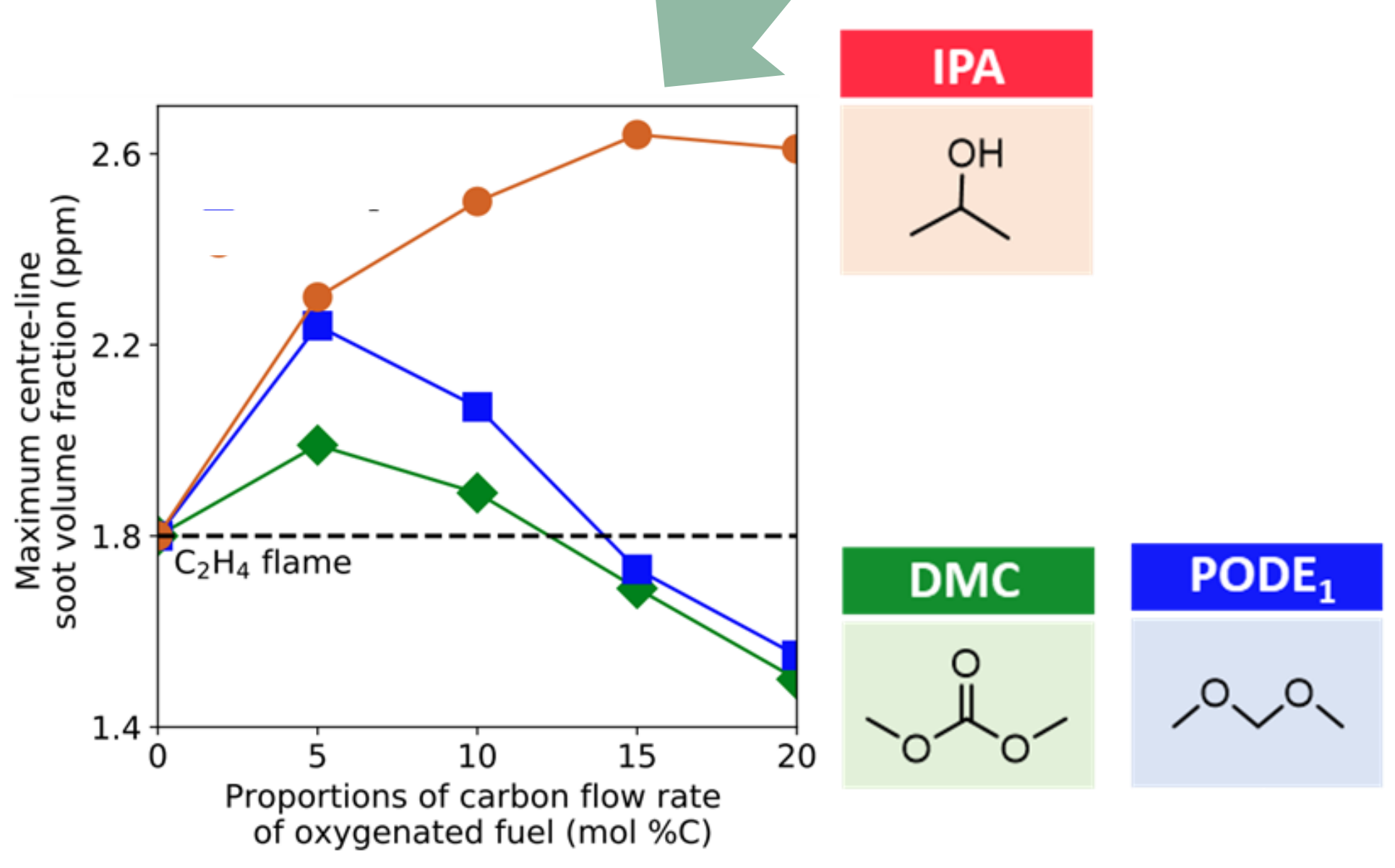


Soot volume fraction shows different degree of synergistic effect in soot formation

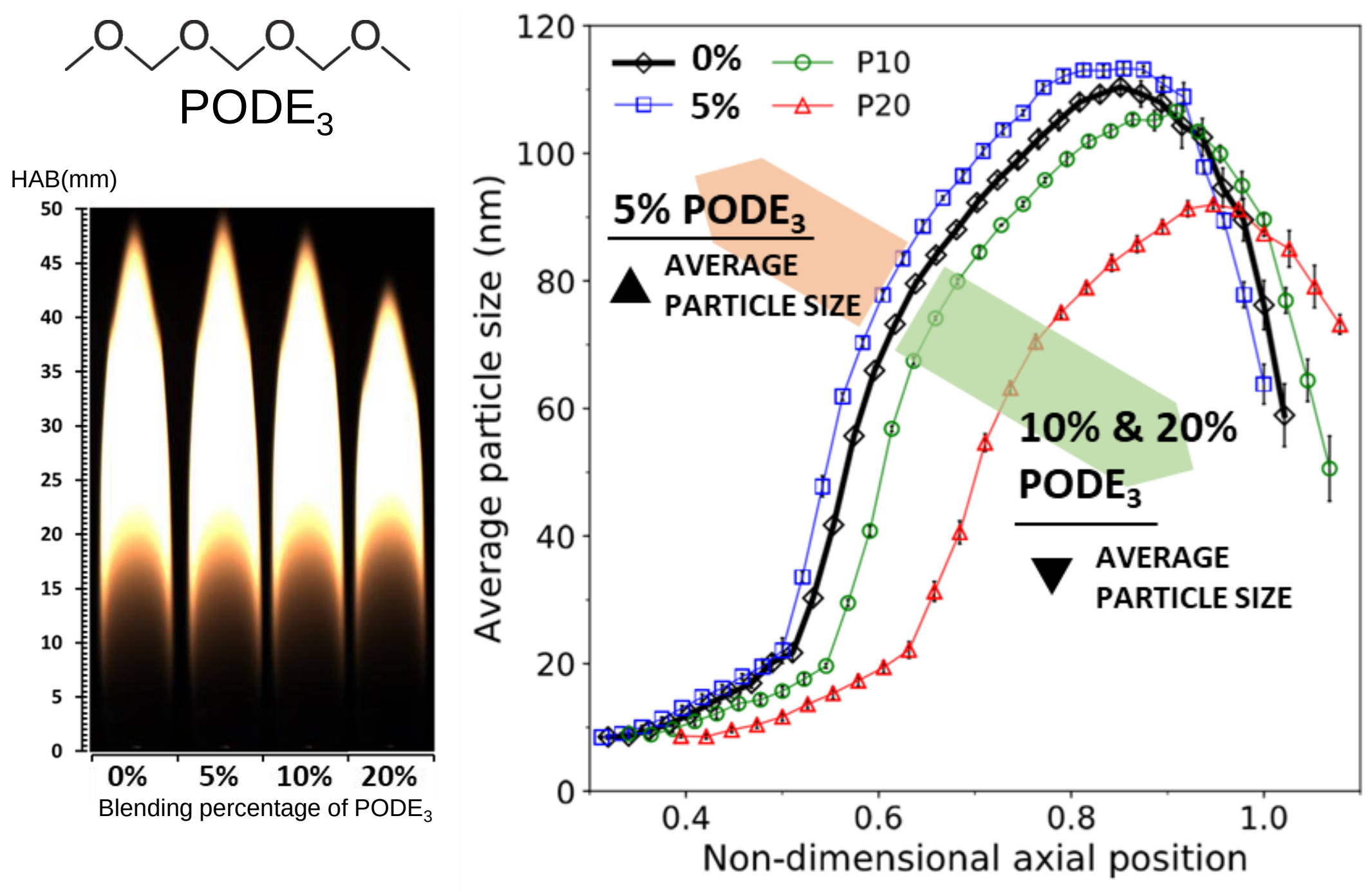


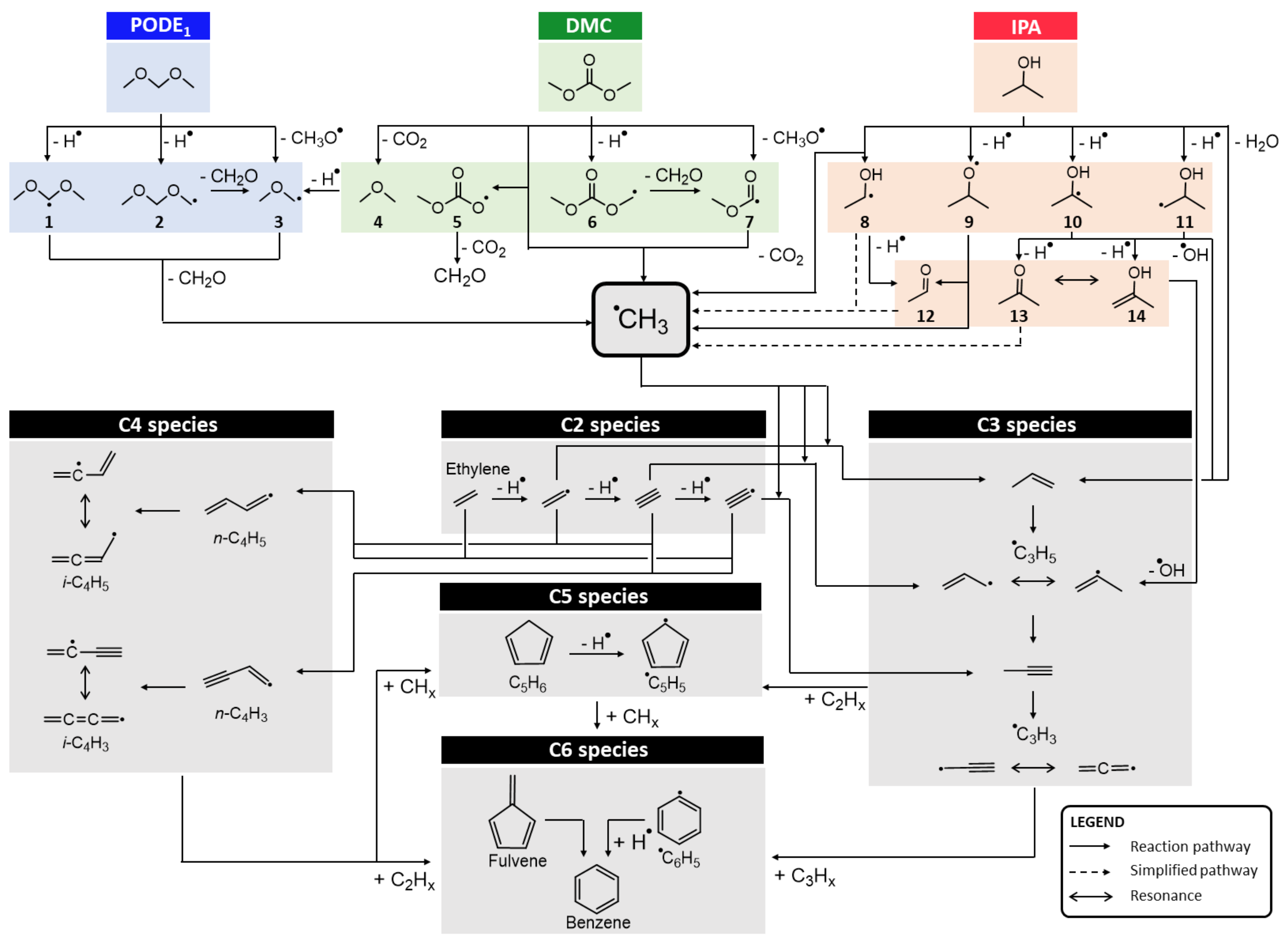


Max. soot volume fraction



Blending effect of $PODE_3$ in average particle size





Despite having the same number of carbon, the differences in soot formation can be understood via mechanistic understanding of the biofuel pyrolysis

References

Y. R. Tan et al., Fuel, 2021, 283:118769
Y. R. Tan et al., Combust. Flame, 2021, 232:111512
Y. R. Tan et al., Combust. Flame, 2022, 243:111849
Y. R. Tan et al., Fuel, 2018, 224:499-506

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UNDERSTANDING SOOT NUCLEATION FOR A GREENER FUTURE

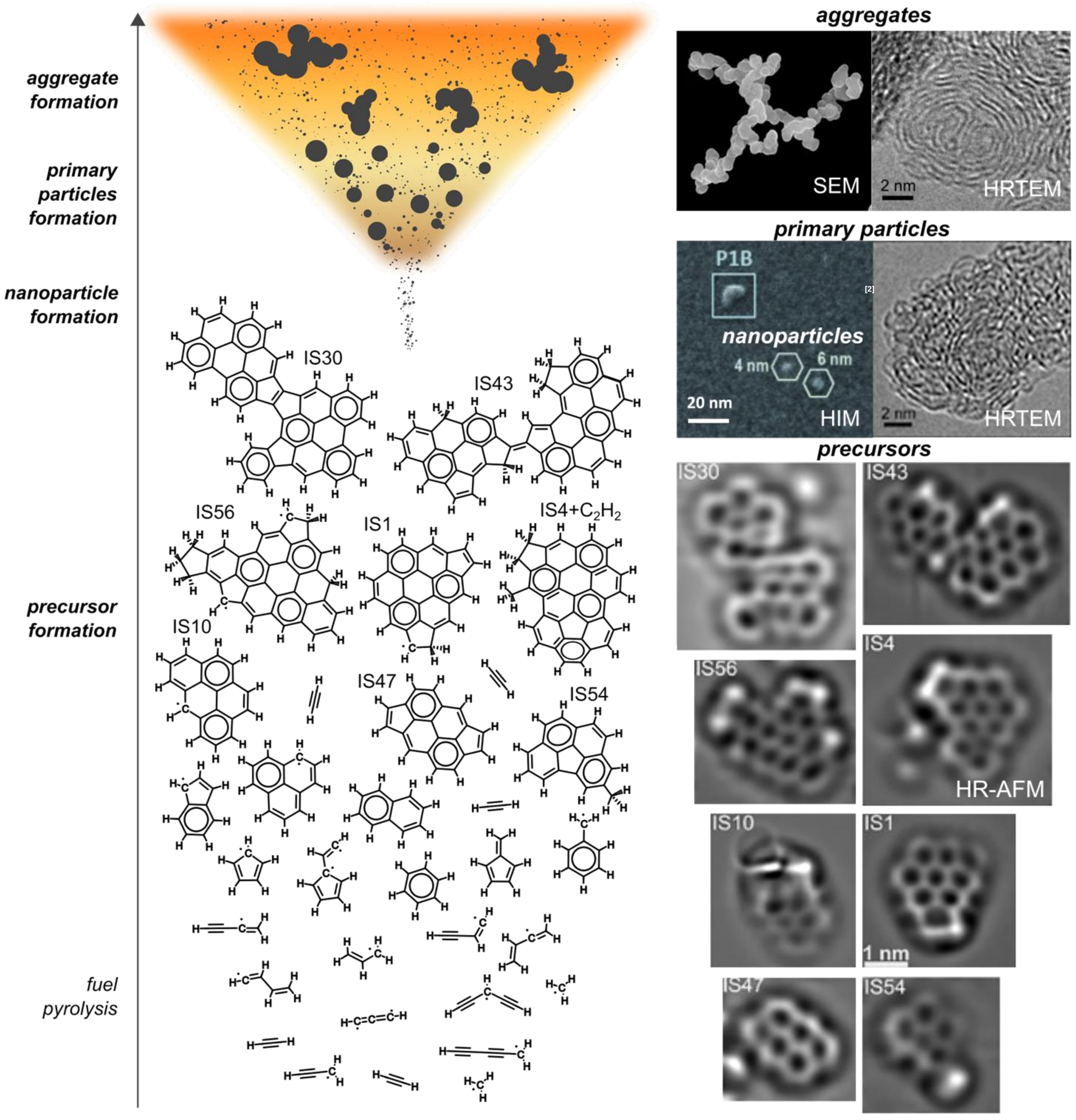
Laura PASCAZIO[1], Jacob W. MARTIN[1,2], Angiras MENON[1,2], Kimberly BOWAL[2], Gustavo L. CAZARES[1],
Maria BOTERO[2], Maurin SALAMANCA[2], Jethro AKROYD[1,2,3], Markus KRAFT[1,2,3,4,5]

Introduction

Soot contributes to climate change and causes an estimated 7 million premature deaths per year. By understanding the formation of soot we aim to eliminate its production in engines. Soot nucleation is the least understood of particle formation process.

This work presents the advances we have made on modeling and understanding soot nucleation.

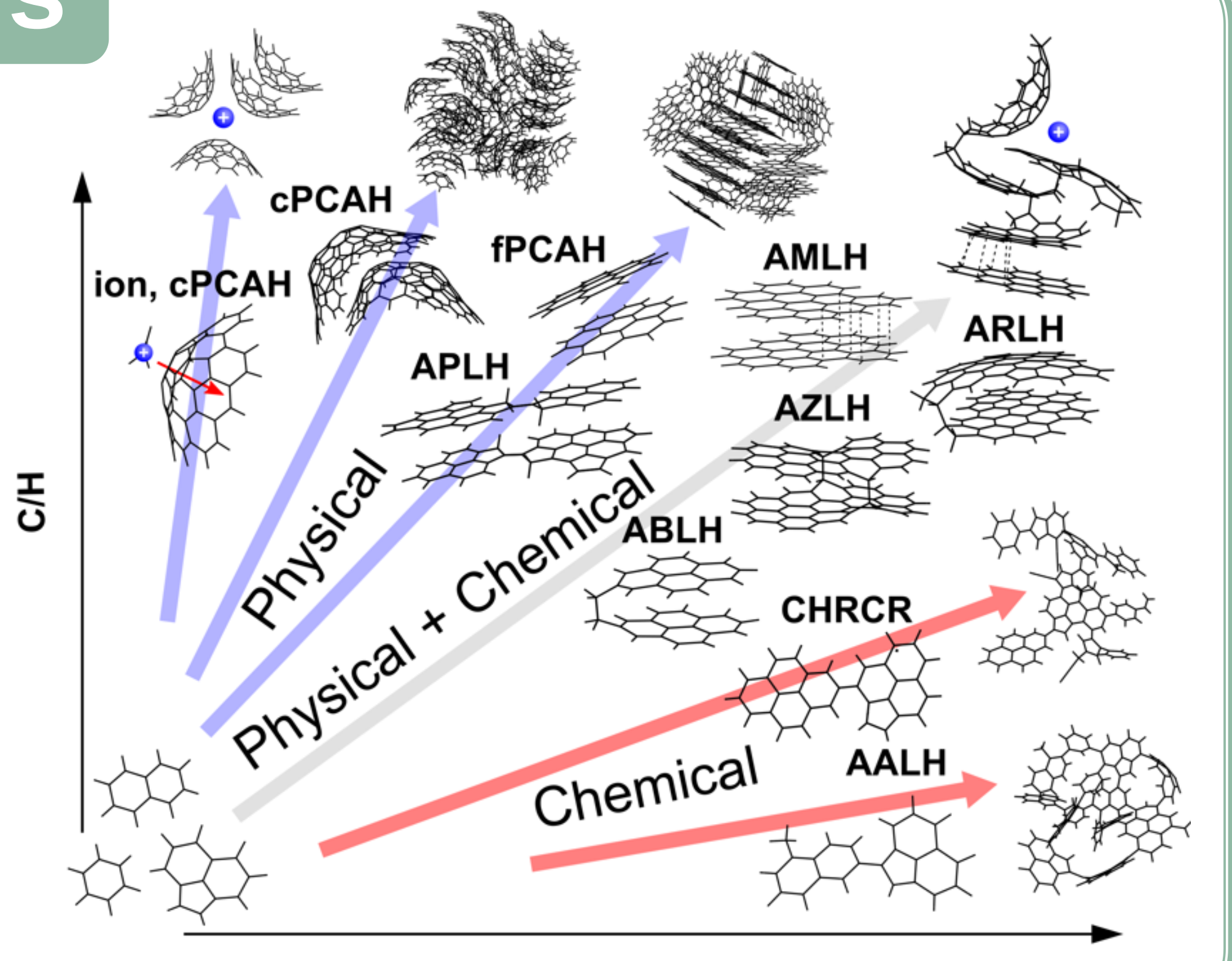
WHAT ALLOWS THE MOLECULAR SOOT PRECURSORS TO CLUSTER INTO NANOPARTICLES IN THE FLAME?



Nucleation pathways

Different pathways have been hypothesised for soot nucleation:

- PHYSICAL PATHWAY
- CHEMICAL PATHWAY
- PHYSICALLY STABILISED CHEMICAL PATHWAY

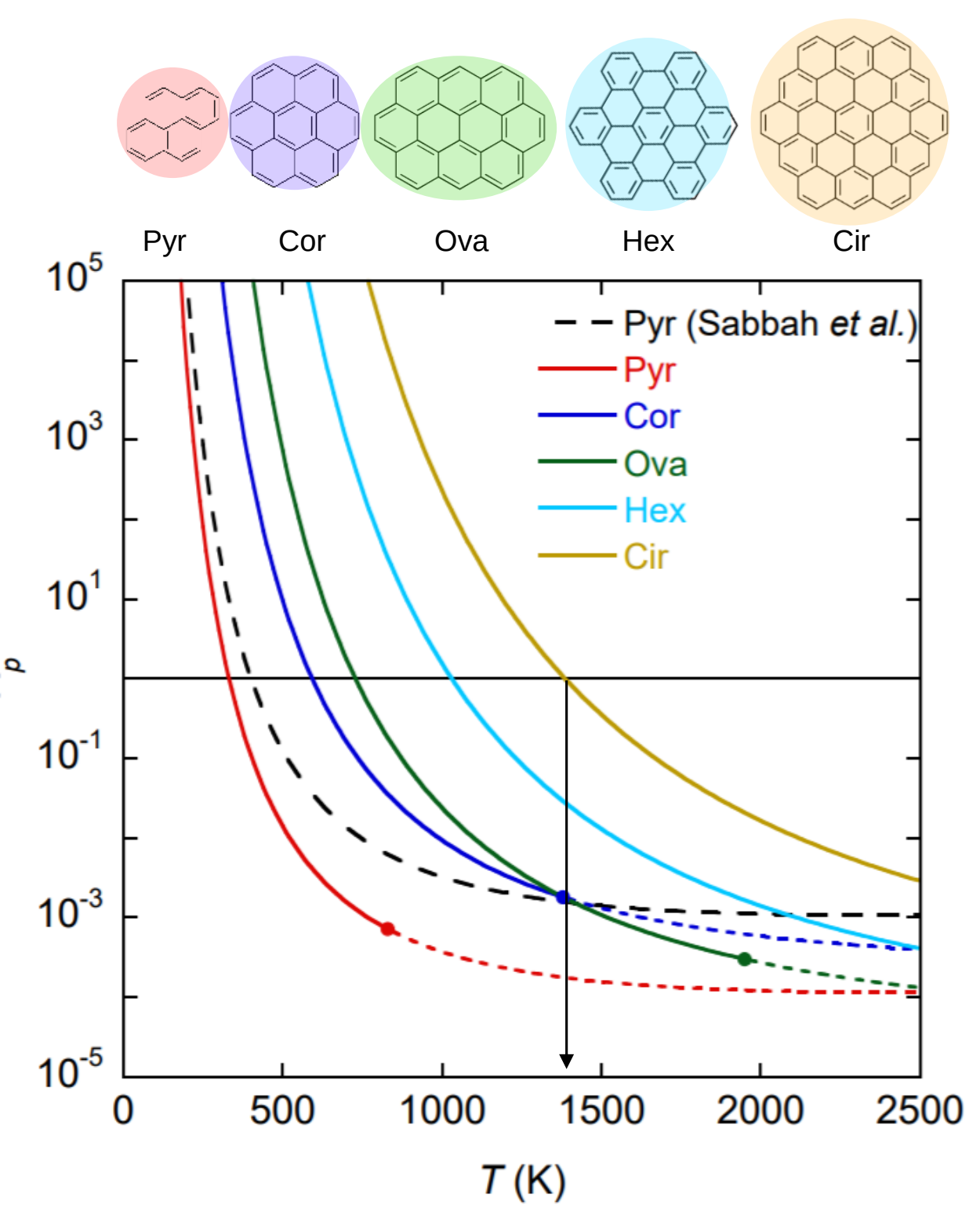


Our contributions

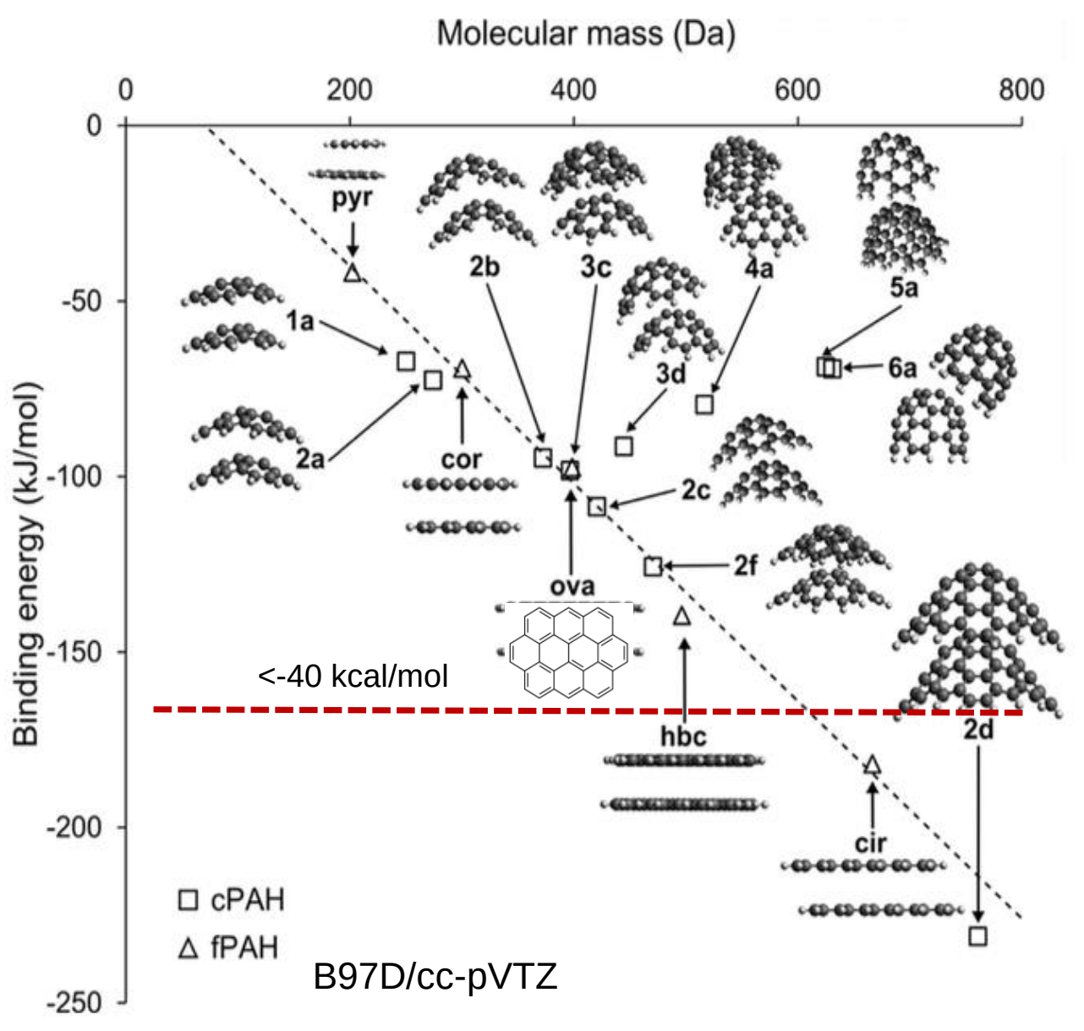
PHYSICAL PATHWAY

Binding energies greater in magnitude than 40 kcal/mol required. Small flat and curved polycyclic aromatic hydrocarbons (PAHs) do not have enough energy to nucleate into droplets.

Totton et al. (2012)
Martin et al. (2019a)



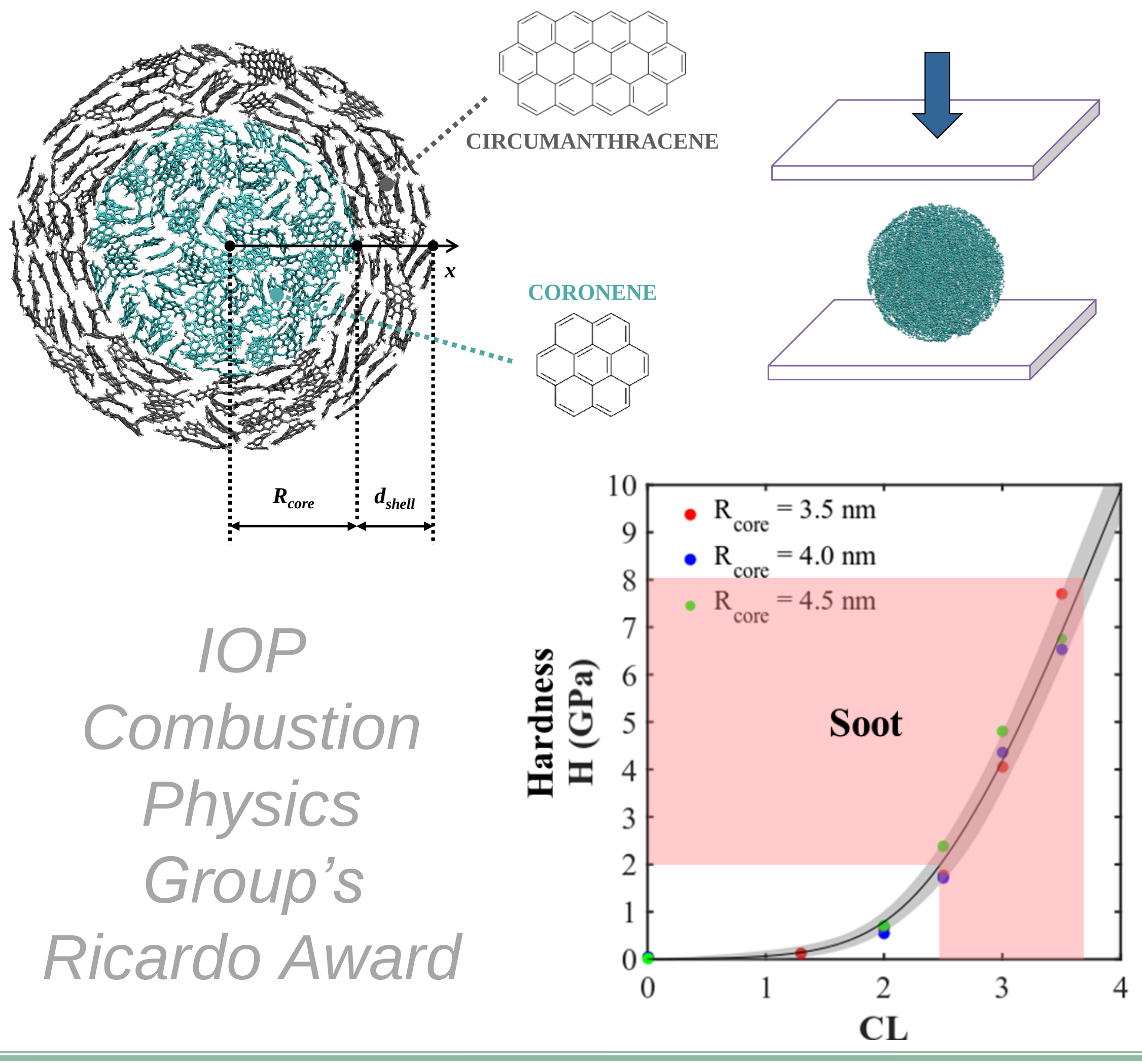
Gaydon Award



CHEMICAL PATHWAY

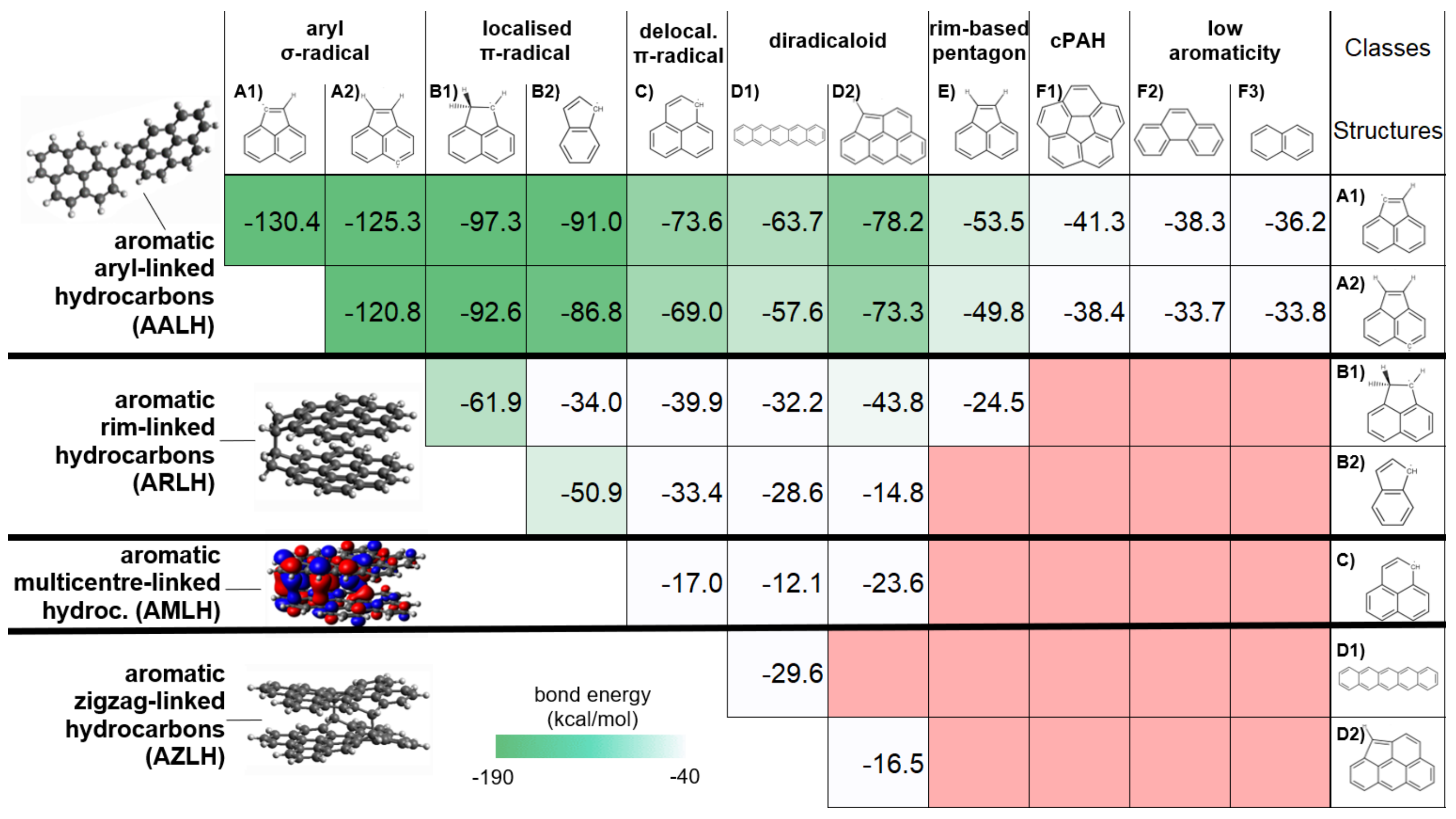
Simulated nanoindentation study finds that mature soot particles are expected to present crosslinks between their aromatic constituents to have a comparable value of the hardness found experimentally (2 - 8 GPa).

Pascazio et al. (2021)



IOP Combustion Physics Group's Ricardo Award

PHYSICAL + CHEMICAL PATHWAY



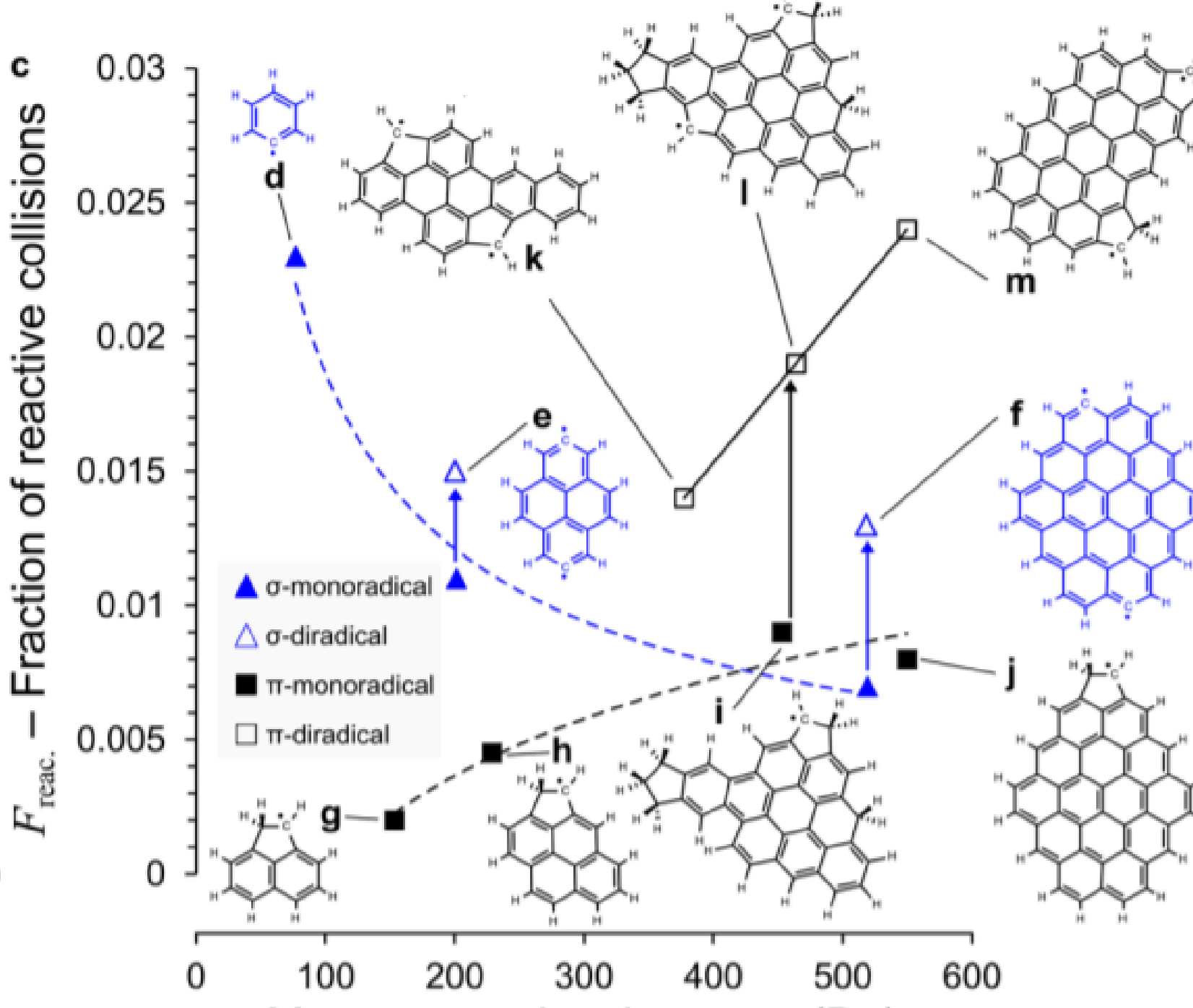
		aryl σ-radical A1)	aryl σ-radical A2)	localised π-radical B1)	localised π-radical B2)	delocal. π-radical C)	diradicaloid D1)	diradicaloid D2)	rim-based pentagon E)	cPAH F1)	low aromaticity F2)	low aromaticity F3)	Classes Structures
aromatic aryl-linked hydrocarbons (AALH)	A1)	-130.4	-125.3	-97.3	-91.0	-73.6	-63.7	-78.2	-53.5	-41.3	-38.3	-36.2	A1)
	A2)		-120.8	-92.6	-86.8	-69.0	-57.6	-73.3	-49.8	-38.4	-33.7	-33.8	A2)
aromatic rim-linked hydrocarbons (ARLH)	B1)			-61.9	-34.0	-39.9	-32.2	-43.8	-24.5				B1)
	B2)				-50.9	-33.4	-28.6	-14.8					B2)
aromatic multicentre-linked hydroc. (AMLH)	C)					-17.0	-12.1	-23.6					C)
aromatic zigzag-linked hydrocarbons (AZLH)	D1)						-29.6						D1)
	D2)							-16.5					D2)

bond energy (kcal/mol)
-190 -40

Localised π-radicals are of particular interest.

- They have been detected in high-resolution transmission electron microscopy (HRTEM).
- They can form rim bonds where physical interactions are combined with thermally stable bonds.

Martin et al. (2019b)
Martin et al. (2021)



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Martin et al. (2019b) The Journal of Physical Chemistry C, 123(43), 26673-26682.
Martin et al. (2021) Journal of the American Chemical Society, 143(31), 12212-12219.

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[4] School of Chemical and Biomedical Engineering, Nanyang Technological University
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