

# ABSTRACTS INDEX

1st General Meeting  
of the CYPHER COST Action



Ljubljana, April 10<sup>th</sup> – 12<sup>th</sup>, 2024



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## Table of Contents

<b>EVENT OVERVIEW .....</b>	<b>6</b>
<b>ORGANIZING COMMITTEE.....</b>	<b>6</b>
<b>PROGRAM OF THE EVENT.....</b>	<b>7</b>
<b>WORKING GROUP 1: RENEWABLE SYNTHETIC FUELS (RSF) COMBUSTION.....</b>	<b>9</b>
<hr/>	
<b>    Keynote Lecture: On the Virtual Development of Renewable Fuels for Real or Virtual Powertrains .....</b>	<b>9</b>
<b>    List of Abstracts.....</b>	<b>10</b>
Oxidation of NH <sub>3</sub> -DEE mixtures .....	10
Tabulation of Autoignition and Laminar Flame Speed of Ammonia / Methane Mixtures for the ECFM Simulation .....	10
Experimental study of the combustion of phenol and cresol isomers.....	10
Exploring plasma-assisted ammonia combustion in the MILD regime.....	10
Towards An Ab initio Based Isomer Specific Cresol Sub-Mechanism .....	11
Preliminary numerical study of the influence in the production of OH radicals in a jet stirred reactor fuelled with ammonia and addition of methanol .....	11
Small-Scale CHP Downdraft Biomass Gasification Technology Integrated with an Internal Combustion Engine.....	11
A Comparative Study on the Hydrogen Storage Capacities of Microporous and Mesoporous Materials .....	11
Numerical investigation of oxy-methane and oxy-methanol combustion for stationary engines .....	12
Ammonia and ammonia/hydrogen combustion: Comprehensive quantitative evaluation and further improvement of kinetic models.....	12
Robust design of a stagnation-point reverse-flow staged combustor for NH <sub>3</sub> oxidation with low NO <sub>x</sub> emissions .....	12
Experimental study of the effect of hydrogen addition on a natural gas and oxygen burner ...	12
Decarbonization effects of using renewable synthetic fuels for energy-intensive industries .	13
Experimental Wood Chips Biomass Co-Firing in Large Combustion Plants – EPBiH Case Study .....	13
Intermediate pyrolysis of wood in a continuous feed retort reactor for designing a fluidized bed pyrolyser .....	13
Application and Perspective of Geothermal Utilization in Albania for Contribution Low Carbon Strategy .....	13
The analysis of operating parameters for synthetic natural gas production from green hydrogen utilisation.....	13
Combustion air sensitization by NO and its multiplication effect on NO <sub>x</sub> emissions .....	14
Machine Learning and HSQC NMR Spectroscopy for the Pre-screening of Sustainable Aviation Fuel Certification Properties .....	14
Plasma-assisted combustion of ammonia/biogas mixtures .....	14



Emission control strategy for glycerol combustion under MILD conditions .....	14
Influence of NO addition on the co-oxidation of NH <sub>3</sub> and CH <sub>4</sub> : sensitizing effect and DeNO <sub>x</sub> reactions .....	14
Particle formation in counter diffusion laminar flame burning OME3 and Ethanol at different strain rates .....	15
Methane/Hydrogen MILD combustion: Process stability and NO <sub>x</sub> emissions .....	15
An overview of hydrogen-based synthetic fuels for energy-intensive industries .....	15
Decarbonising energy-intensive industries with plasma-assisted combustion .....	15
Performance Investigation of Recent Detailed Combustion Mechanisms on a Large Amount of Ammonia/Air Laminar Burning Velocity Measurements .....	15
Local biomass potential for syngas production and further conversion into synthetic fuel ...	16
Optimized Hydrogen Peroxide-Mediated Synthesis of Molybdenum Carbide for Improved Hydrogen Evolution Reaction.....	16
Synthesis and Electrochemical Characterisation of Tungsten Carbide for Efficient Hydrogen Evolution .....	16
<b>WORKING GROUP 2: HIGH-FIDELITY COMBUSTION SIMULATIONS AND DATA ANALYTICS.....</b>	<b>17</b>
<b>Keynote Lecture: Are we there yet? Towards foundational ML models for combustion through accessible community-involved big databases .....</b>	<b>17</b>
<b>List of Abstracts.....</b>	<b>18</b>
Preliminary Experimental and Computational Investigation of a Laboratory Gas Turbine Combustor .....	18
Experimental and modeling high-pressure study of ammonia/dimethyl-ether conversion in a flow reactor .....	18
Analysis of flame propagation in spray flames of aviation fuels.....	18
Advanced methods for kinetic parameter optimization .....	18
The burning features of NH <sub>3</sub> /DME/air Bunsen flames: a modelling study .....	19
Kinetic modelling data for co-combustion process to accelerate energy transition in large power plants.....	19
Mechanism reduction-assisted optimization of the ethylene chemistry in the AramcoMech 2.0 combustion mechanism .....	19
Recent advancements in the reaction kinetics branch of the ReSpecTh Information System	20
Experimental-numerical workflow for high-temperature decomposition process of sewage sludge aimed towards P extraction. ....	20
Numerical analysis of flameless combustion in a thermal oxidation chamber.....	20
<b>WORKING GROUP 3: HYBRID PHYSICS-BASED DATA-DRIVEN MODELS.....</b>	<b>21</b>
<b>Keynote Lecture: Opportunities for machine learning assisted design of energy conversion machines.....</b>	<b>21</b>
<b>List of Abstracts.....</b>	<b>22</b>
Combustion Modelling and Dimensionality Reduction in Turbulent Non- Premixed Sooting Flames with Convolutional Neural Networks .....	22
Kernel method for reactive flows.....	22



Hybrid modelling of sorptive capture of carbon dioxide from flue gases in presence of competing phenomena .....	22
Dynamical Characterization for the Convergence Enhancement and Dimensionality Reduction of Combustion Chemical Kinetics .....	22
Reduced modelling, Convergence enhancement, Dimensionality reduction A Co-kurtosis Principal Component Analysis and Modularity-based Clustering for Flashback Precursor Identification .....	23
Machine Learned Compact Kinetic Model for Liquid Fuel Combustion.....	23
Combining data-driven and physics-based methods for stiffness reduction in combustion systems.....	23
Perturbation; Stiffness; Machine Learning Combustion Model for Coupling with a Cement Kiln CFD Digital Twin Model: Coal and Extension to an Alternative Fuel .....	23
A neural network and low cost SVD based hybrid model for forecasting of reactive flows. ...	24
A data-driven approach to correct the cell reacting fraction in the partially stirred reactor closure for LES of premixed flames .....	24
Feature identification for optimal Chemical Reactor Networks for Combustion Systems....	24
Towards physics-based digital twins of combustion systems: a sparse sensing and Chemical Reactor Network approach.....	24
Detailed Kinetic Mechanisms Investigation in Parameters Space .....	25
Probabilistic and data-efficient machine learning framework for chemical source term integration .....	25
Hydrogen and hydrogen/ammonia scale-resolving simulation activities at Aalto University using DLBFoam.....	25
<b>WORKING GROUP 4: DIGITAL TWINS .....</b>	<b>26</b>
<b>Keynote Lecture: Reinforcement Twinning: from digital twins to model-based reinforcement learning .....</b>	<b>26</b>
<b>List of Abstracts.....</b>	<b>27</b>
Digital twins based on real-time flame monitoring. Still an elusive objective?.....	27
Green and digital transformation of the industry by employing digital twin in the learning factories .....	27
JThermodynamicsCloud: A Case study in FAIR data practices, data traceability and data-lineage promotion.....	27
Digital twin simulation and data-driven model for automotive injector spray characteristics prediction .....	27
A Probabilistic Framework for Data Assimilation of Reacting Dynamical Systems using a Gaussian Process Regression-based Reduced-Order Model and Sparse Measurements....	27
Digital Twin of a Membrane Electrode Assembly Reactor for Electrochemical Reduction of CO <sub>2</sub> to E-Fuels.....	28
Real-time monitoring of pollutant emission by photoacoustic technique for turbulent combustion .....	28
Digital twin of a stagnation-point reverse-flow combustor for the oxidation of NH <sub>3</sub> /H <sub>2</sub> blends .....	28
Multi-Fidelity Surrogate Framework for Digital Twin Development in Flameless Combustion Systems Using Heterogeneous Data .....	29



A Probabilistic Framework for Data Assimilation of Reacting Dynamical Systems using a Gaussian Process Regression-based Reduced-Order Model and Sparse Measurements.....	29
Numerical-Experimental Analysis of the Thermomechanical State of Fire-Tube Boiler Structure under Transient Operational Regime .....	29
Exploratory analysis for soft sensing strategies under MILD conditions using validated kinetic mechanism for ammonia-hydrogen combustion .....	29
<b>WORKING GROUP 5: COMMUNICATION, DISSEMINATION, PARTNERING.....</b>	<b>30</b>
<b>Keynote Lecture: The twin transitions .....</b>	<b>30</b>



## Event Overview

The CYPHER COST Action First General Meeting was a key event aimed at fostering collaborative research and knowledge exchange in the field of Renewable Synthetic Fuel (RSF) Combustion. This meeting brought together a diverse network of researchers, entrepreneurs, policymakers, and industry partners with the common goal of advancing innovative solutions for the decarbonization of Energy-Intensive Industries (EIs) in Europe and beyond.

The meeting discussed the current developments in the working groups of the Action, focusing on the combustion characteristics of Renewable Synthetic Fuels (WG1), advanced simulations and data-driven insights for combustion processes (WG2), hybrid physics-based data-driven models for reacting flows (WG3), and digital twins (WG4). Targeted discussions focusing on data and software sharing, including returns on experience and best practices, were specifically organized for young researchers and innovators joining the event.

## Organizing Committee

- **Host:** Dr. Tine Seljak, Chair of Power Engineering at the Laboratory for Internal Combustion Engines and Electromobility, LICeM, Faculty of Mechanical Engineering, University of Ljubljana.
- Prof. Alessandro Parente, from the Aero-Thermo-Mechanics Department., École Polytechnique de Bruxelles, Université Libre de Bruxelles and Chair of CYPHER CA22151 COST Action.
- Dr. Giancarlo Sorrentino, research fellow at the Institute of Sciences and Technologies for Sustainable Energy and Mobility (STEMS) of the Italian National Research Council (CNR) in Napoli and Vice-Chair of CYPHER CA22151 COST Action.
- Dr. Patricia Domingo Alvarez, from the Aero-Thermo-Mechanics Department., École Polytechnique de Bruxelles, Université Libre de Bruxelles and Grant Holder Manager of CYPHER CA22151 COST Action.



## Program of the event

Wednesday 10/4/24	
8:00	Registration / Sign attendance list
08:45 - 09:00	Welcome with Tine Seljak (Local Organiser, University of Ljubljana) and Alessandro Parente (Chair, ULB)
09:00 - 13:00	<b>WORKSHOP:</b> <b>Digitalization for the Decarbonization of energy-intensive industries</b> <i>Chair: Giancarlo Sorrentino (CNR - STEMS)</i>
09:00 - 09:15	Maria Georgiadou (EU) - <i>Online</i>
09:15 - 09:30	Sebastiano Fumero (EU) - <i>Online</i>
09:30 - 09:45	<b>Introduction WG5:</b> Gokçe Nur Yilmaz (TED University)
09:45 - 10:30	<b>Keynote Speaker:</b> Elena Verdolini (Università degli Studi di Brescia) - <i>Online</i>
10:30- 11:00	Break
	<u>ROUND TABLE with:</u>
11:00 - 13:00	Miriam Rabaçal Federico Di Pierro Zakaria Nait Mohamed - <i>Online</i> Nina Meglic Tilen Sever Anes Kazagic
13:00 - 14:00	Break
14:00 - 14:15	<b>Introduction to CYPHER:</b> Alessandro Parente (Chair, ULB)
14:15 - 14:30	<b>Introduction WG1:</b> Pino Sabia (CNR - STEMS)
14:30 - 15:15	<b>Keynote Lecture WG1:</b> Fabian Mauss (BTU Cottbus-Senftenberg)
15:15 - 16:00	Poster Session WG1
16:00 - 16:30	Break
16:30 - 17:30	Poster Session WG1
17:30 - 19:00	<b>Management Committee</b>



Thursday 11/4/24	
8:30	Registration / Sign attendance list
09:00 - 09:15	<b>Introduction WG2:</b> Antonio Attili (The University of Edinburgh)
09:15 - 10:00	<b>Keynote Speaker:</b> Matthias Ihme (Stanford University)
10:00- 10:30	Break
10:30 - 11:30	Poster Session WG2
11:30 - 11:45	<b>Introduction WG3:</b> Anh Khoa Doan (TU Delft)
11:45 - 12:30	<b>Keynote Speaker:</b> Paola Cinnella (Sorbonne Université)
12:30 - 14:00	Break
14:00 - 15:00	Poster Session WG3
15:00 - 15:15	<b>Introduction WG4:</b> Alessandro Parente (ULB)
15:15 - 16:00	<b>Keynote Lecture WG4:</b> Miguel Alfonso Mendez (Von Karman Institute)
16:00 - 16:30	Break
16:30 - 17:30	Poster Session WG4
19:00	Dinner
Friday 12/4/24	
8:30	Registration / Sign attendance list
ROUND TABLE: <b>Database and Benchmark cases in the CYPHER project</b> <i>Chairs: Pasquale Lapenna (Sapienza Università di Roma)</i>	
09:00 - 09:05	Introduction by Alessandro Parente (Chair) and Pasquale Lapenna (Database and benchmark Cases Coordinator)
09:00 - 09:25	Classification and gathering of the datasets
09:25 - 10:05	Sharing the data with: Antonio Attili (The University of Edinburgh) Matthias Ihme (Stanford University) Tamás Turányi (Eötvös Loránd University Budapest)
10:05 - 10:25	Benchmarks for ML, AI, and other tools with Paola Cinnella (Sorbonne Université, Database and benchmark Cases Coordinator)
10:25 - 10:30	Summary and closing
10:30- 11:00	Break
Workshop: <b>Software Demonstrators</b> <i>Chairs: Daniel Mira (Barcelona Supercomputing Center) and Alberto Cuoci (Politecnico di Milano)</i>	
11:00 - 11:30	Jupyter-CoEC with Mathis Bode (Jülich Supercomputing Centre)
11:30 - 12:00	SciExpm: Scientific Experiments and Models with Alberto Cuoci (Polimi and Software and HPC enabling technologies Coordinator)
12:00 - 13:00	<b>Young Researchers and Innovators Mixer</b>
13:00	Farewell



# Working Group 1: Renewable Synthetic Fuels (RSF) Combustion

**Keynote Lecture: On the Virtual Development of Renewable Fuels for Real or Virtual Powertrains**

**Prof. Dr.-Ing. Fabian Mauss**

*Thermodynamics and Thermal Process Engineering, Brandenburg University of Technology*

The need to use renewable fuels for future energy converters opens many research opportunities. Compared to conventional fuels, many renewable fuels are polar, which affects the evaporation process. The lack of experimental data for possible candidates for blends of renewable fuels leads to challenges in kinetic modeling. Renewables can be designed for high-octane numbers or low-decane numbers. They may be subject to machine-integrated fuel reforming to improve the efficiency of the energy converter.

The virtual simulation of energy converters enables the joint optimization of fuel and engine. The virtual simulation of a powertrain enables the virtual development of optimized control strategies to maximize energy efficiency and minimize emissions from real driving cycles. The presentation will introduce examples of the virtual fuel development of future energy converters and their application in the real world. In each development step, the usage of detailed reaction kinetic information is proposed. Particular attention will be paid to the use of artificial intelligence to increase the speed of development.





## List of Abstracts

### Oxidation of NH<sub>3</sub>-DEE mixtures

**A. Ruiz-Gutierrez\*, A. Bello and M.U. Alzueta**

Presenter: María Uxue Alzueta

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**Keywords:** Ammonia, combustion, kinetics, carbon-free fuel.

### Tabulation of Autoignition and Laminar Flame Speed of Ammonia / Methane Mixtures for the ECFM Simulation

**Filip Jurić<sup>1</sup>, Marko Ban<sup>2</sup>, Jakov Baleta<sup>\*3</sup>, Hrvoje Mikulčić<sup>1</sup>, Milan Vujanović<sup>1</sup>**

Presenter: Jakov Baleta

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**Keywords:** Ammonia, methane, laminar flame speed, autoignition, tabulation.

### Experimental study of the combustion of phenol and cresol isomers

**Frédérique Battin-Leclerc<sup>1</sup>, Nicolas Delort<sup>1</sup>, Ismahane Meziane<sup>1</sup>, Olivier Herbinet<sup>1</sup>, Roda Bounaceur<sup>1</sup> and Hans-Heinrich Carstensen<sup>3</sup>**

Presenter: Frédérique Battin-Leclerc

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**Keywords:** Phenol, Cresol isomers, Laminar burning velocity, Jet-stirred reactor, Detailed kinetic model.

### Exploring plasma-assisted ammonia combustion in the MILD regime

**Georgios Rekkas-Ventiris<sup>1,2</sup>, Pino Sabia<sup>3</sup>, Giancarlo Sorrentino<sup>3</sup>, and Aurélie Bellemans<sup>\*1,2</sup>**

Presenter: Aurélie Bellemans

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<sup>2</sup> Brussels Institute for Thermal-fluid Systems and Clean Energy (BRITE), Vrije Universiteit Brussel (VUB) and Université Libre de Bruxelles (ULB), Brussels, Belgium

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**Keywords:** Plasma-assisted combustion, ammonia, MILD, nanosecond pulsed discharges.



**Towards An Ab initio Based Isomer Specific Cresol Sub-Mechanism****Hans-Heinrich Carstensen<sup>\*1</sup>, Nicolas Delort<sup>2</sup>, Olivier Herbinet<sup>3</sup>, and Frédérique Battin-Leclerc<sup>4</sup>****Presenter:** Hans-Heinrich Carstensen<sup>1</sup>Fundación Agencia Aragonesa para la Investigación y el Desarrollo (ARAID), Zaragoza, SpainE-mail: [hcarsten@posteo.de](mailto:hcarsten@posteo.de)<sup>2,3,4</sup>Université de Lorraine, CNRS, LRGP, F-54000 Nancy, FranceE-mail: [nicolas.delort@univ-lorraine.fr](mailto:nicolas.delort@univ-lorraine.fr), [olivier.herbinet@univ-lorraine.fr](mailto:olivier.herbinet@univ-lorraine.fr), [frederique.battin-leclerc@univ-lorraine.fr](mailto:frederique.battin-leclerc@univ-lorraine.fr)**Keywords:** Phenol, Cresol isomers, Detailed kinetic model development.**Preliminary numerical study of the influence in the production of OH radicals in a jet stirred reactor fuelled with ammonia and addition of methanol****V. Castro<sup>\*1,2</sup>, P. Sabia<sup>1</sup>, R. Ragucci<sup>1</sup> and M. de Joannon<sup>1</sup>****Presenter:** Vicente Castro<sup>1</sup>Istituto di Scienze e Tecnologie per l'Energia e la Mobilità sostenibili, Consiglio Nazionale delle Ricerche, Napoli, ItalyE-mail: [pino.sabia@stems.cnr.it](mailto:pino.sabia@stems.cnr.it), [raffaele.ragucci@stems.cnr.it](mailto:raffaele.ragucci@stems.cnr.it), [mara.dejoannon@stems.cnr.it](mailto:mara.dejoannon@stems.cnr.it)<sup>2</sup>Dipartimento di Ingegneria Chimica, dei Materiali e della Produzione Industriale, Università degli studi di Napoli Federico II, Napoli, ItalyE-mail: [vicente.castro@stems.cnr.it](mailto:vicente.castro@stems.cnr.it)**Keywords:** Mild Combustion, Jet stirred reactor, ammonia-methanol, OH\* radical.**Small-Scale CHP Downdraft Biomass Gasification Technology Integrated with an Internal Combustion Engine****I. Čeković<sup>\*1</sup>, D. Stojiljković<sup>2</sup> and N. Manić<sup>3</sup>****Presenter:** Ivana Čeković<sup>1</sup>Department of Mechanical and Technological Engineering, Western Serbia Academy of Applied Studies, SerbiaE-mail: [ivanacekovic@yahoo.com](mailto:ivanacekovic@yahoo.com)<sup>2,3</sup>Fuel and Combustion Lab, University of Belgrade, Faculty of Mechanical Engineering, SerbiaE-mail: [dstoiljkovic@mas.bg.ac.rs](mailto:dstoiljkovic@mas.bg.ac.rs), [nmanic@mas.bg.ac.rs](mailto:nmanic@mas.bg.ac.rs)**Keywords:** Biomass, CHP, ICE, Aspen Plus.**A Comparative Study on the Hydrogen Storage Capacities of Microporous and Mesoporous Materials****Fatma Oguz Erdogan<sup>1</sup>, Cenk Çelik<sup>\*2</sup>****Presenter:** Cenk Çelik<sup>1</sup>Department of Chemistry and Chemical Processing Technologies, Kocaeli Vocational School, Kocaeli University, KocaeliE-mail: [foerdogan@gmail.com](mailto:foerdogan@gmail.com)<sup>2</sup>Department of Mechanical Engineering, Kocaeli University, KocaeliE-mail: [cenkcelik@kocaeli.edu.tr](mailto:cenkcelik@kocaeli.edu.tr)**Keywords:** Hydrogen storage, graphene, palladium, carbon, composite.



## Numerical investigation of oxy-methane and oxy-methanol combustion for stationary engines

**Tim Franken<sup>\*1</sup>, Fabian Rachow<sup>2</sup>, Evgenia Charlafti<sup>2</sup>, Jan Ingo Flege<sup>2</sup>, Rakhi<sup>1</sup>, Vivien Günther<sup>3</sup> and Fabian Mauß<sup>1</sup>**

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**Keywords:** Methane, Methanol, Oxyfuel, Detailed Chemistry, Computational Fluid Dynamics

## Ammonia and ammonia/hydrogen combustion: Comprehensive quantitative evaluation and further improvement of kinetic models

**Sanket Girhe<sup>\*1</sup>, Heinz Pitsch<sup>2</sup>**

Presenter: Sanket Girhe

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**Keywords:** Ammonia, Hydrogen, Carbon-free fuel, Chemical kinetic models, Quantitative model assessment

## Robust design of a stagnation-point reverse-flow staged combustor for NH<sub>3</sub> oxidation with low NO<sub>x</sub> emissions

**L. Giuntini<sup>1,2</sup>, C. Novelli<sup>1,2</sup>, M. Jamshidiha<sup>1,2</sup>, A. Piscopo<sup>1,2,3</sup>, M. Remacle<sup>1,2</sup>, A. Coussement<sup>1,2</sup>, A. Parente<sup>1,2</sup>**

Presenter: Lorenzo Giuntini

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**Keywords:** Ammonia, Low-NO<sub>x</sub> emissions, Stagnation-Point Reverse-Flow combustor, Staged combustion

## Experimental study of the effect of hydrogen addition on a natural gas and oxygen burner

**A. Hasche<sup>1,\*</sup>, S. Eckart<sup>2</sup> and H. Krause<sup>3</sup>**

Presenter: Anna Hasche

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**Keywords:** oxyfuel flame, hydrogen admixture, temperature measurement, optical investigation, exhaust gas analyse.





## Decarbonization effects of using renewable synthetic fuels for energy-intensive industries

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**Keywords:** Renewable synthetic fuels, decarbonization, greenhouse gas emissions, energy-intensive industry.

## Experimental Wood Chips Biomass Co-Firing in Large Combustion Plants – EPBiH Case Study

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Presenter: Anes Kazagic

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**Keywords:** Biomass, Co-firing, Ash, Deposits, Emissions.

## Intermediate pyrolysis of wood in a continuous feed retort reactor for designing a fluidized bed pyrolyser

**Alar Konist<sup>\*1</sup>, Mais Baqain<sup>2</sup>, Alejandro Lyons Ceron<sup>3</sup> and Mari-Liis Ummik<sup>4</sup>**

Presenter: Alar Konist

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**Keywords:** Intermediate pyrolysis , Retort reactor , Wood dust, RSF, EII.

## Application and Perspective of Geothermal Utilization in Albania for Contribution Low Carbon Strategy

**N. Kodhelaj<sup>\*1</sup> and A.Leskoviku<sup>2</sup>**

Presenter: Artan Leskoviku

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**Keywords:** Geothermal, utilization, springs, wells, scheme.

## The analysis of operating parameters for synthetic natural gas production from green hydrogen utilisation

**Nebojša Manić<sup>\*1</sup>, Ivana Čeković<sup>2</sup>, Dragoslava Stojiljković<sup>3</sup>**

Presenter: Nebojša Manić

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**Keywords:** synthetic natural gas, green hydrogen, operating parameters, methanation, waste heat.





## Combustion air sensitization by NO and its multiplication effect on NOx emissions

**N. Müller<sup>1</sup>, D. Kazangas<sup>2</sup>, V. Marojević<sup>1</sup>, G. Skevis<sup>3</sup>, L. Kaiktsis<sup>2</sup>, U. Žvar Bašković<sup>1</sup>, T. Katrašnik<sup>1</sup> and T. Seljak<sup>\*1</sup>**

Presenter: Neza Müller

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**Keywords:** Combustion kinetics; Emissions of pollutants; Nitric oxides; Combustion Analysis; NO doping

## Machine Learning and HSQC NMR Spectroscopy for the Pre-screening of Sustainable Aviation Fuel Certification Properties

**Tiarnán Watson-Murphy<sup>\*1</sup>, Robert Parker<sup>1</sup>, Mark Kelly<sup>1</sup>, Andrew Ure<sup>1</sup> and Stephen Dooley<sup>1</sup>**

Presenter: Tiarnán Watson-Murphy

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**Keywords:** Synthetic Aviation Fuel, Machine Learning, Nuclear Magnetic Resonance, Pre-screening.

## Plasma-assisted combustion of ammonia/biogas mixtures

**R.Paulauskas<sup>\*1</sup>, E.Bykov<sup>2</sup> and K.Zakarauskas<sup>3</sup>**

Presenter: Rolandas Paulauskas

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**Keywords:** non-thermal plasma, ammonia, flame emission spectroscopy, infrared, ICCD.

## Emission control strategy for glycerol combustion under MILD conditions

**Žiga Rosec<sup>1</sup>, Tomaž Katrašnik<sup>1</sup> and Tine Seljak<sup>\*1</sup>**

Presenter: Žiga Rosec

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**Keywords:** Glycerol, MILD, Emissions, Combustion, Exhaust gas recirculation

## Influence of NO addition on the co-oxidation of NH<sub>3</sub> and CH<sub>4</sub>: sensitizing effect and DeNO<sub>x</sub> reactions

**Maria Virginia Manna<sup>\*1</sup>, Pino Sabia<sup>1</sup>, Raffaele Ragucci<sup>1</sup> and Mara de Joannon<sup>1</sup>**

Presenter: Pino Sabia

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**Keywords:** Ammonia-Methane oxidation; NOx emissions; DeNOx chemistry; NO-sensitizing effect.





## Particle formation in counter diffusion laminar flame burning OME3 and Ethanol at different strain rates

**V. Esposito<sup>1</sup>, M. Sirignano<sup>\*1</sup>**

Presenter: Mariano Sirignano

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**Keywords:** Nanoparticles, renewable synthetic fuels, e-fuels, OME3, diffusion flames.

## Methane/Hydrogen MILD combustion: Process stability and NOx emissions

**G.B. Ariemma<sup>1</sup>, G. Sorrentino<sup>1</sup>, P. Sabia<sup>1</sup>, M. de Joannon<sup>1</sup>, R. Ragucci<sup>1</sup>**

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**Keywords:** Methane-hydrogen oxidation; Process stability; MILD combustion; Pollutants reduction.

## An overview of hydrogen-based synthetic fuels for energy-intensive industries

**Z Kahraman<sup>1</sup>, M Hacı<sup>2</sup> and H S Soyhan<sup>\*3</sup>**

Presenter: Hakan Serhad Soyhan

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**Keywords:** Hydrogen, synthetic fuels, greenhouse gas (GHG) emissions, energy-intensive industries (EIs).

## Decarbonising energy-intensive industries with plasma-assisted combustion

**N. Striūgas<sup>\*1</sup> and A. Tamošiūnas<sup>2</sup>**

Presenter: Nerijus Striūgas

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**Keywords:** Plasma, combustion, hydrogen, methane, glass industry.

## Performance Investigation of Recent Detailed Combustion Mechanisms on a Large Amount of Ammonia/Air Laminar Burning Velocity Measurements

**András Gy. Szanthoffer<sup>\*1</sup>, Máté Papp<sup>2</sup>, István Gy. Zsély<sup>3</sup> and Tamás Turányi<sup>4</sup>**

Presenter: András Gy. Szanthoffer

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**Keywords:** ammonia, carbon-free, renewable, combustion, mechanisms





## Local biomass potential for syngas production and further conversion into synthetic fuel

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Presenter: Monika Uler Zefikj

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**Keywords:** biomass, gasification, syngas, synthetic fuel

## Optimized Hydrogen Peroxide-Mediated Synthesis of Molybdenum Carbide for Improved Hydrogen Evolution Reaction

**Sreedhanya Pallilavalappil<sup>1</sup>, Shaista Jabeen<sup>1</sup>, Maida A costa de Oliveira<sup>2</sup>, Paula E. Colavita<sup>2</sup> and Suresh C Pillai<sup>1\*</sup>**

Presenter: Saritha Unnikrishnan

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**Keywords:** Molybdenum carbide, Hydrogen evolution reaction, water-splitting, H<sub>2</sub>O<sub>2</sub> assisted

## Synthesis and Electrochemical Characterisation of Tungsten Carbide for Efficient Hydrogen Evolution

**Shaista Jabeen<sup>\*1</sup>, Sreedhanya Pallilavalappil<sup>2</sup>, Maida A. C. Oliveira<sup>3</sup>, Paula E. Colavita<sup>4</sup>, Suresh Pillai<sup>5</sup>**

Presenter: Saritha Unnikrishnan

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**Keywords:** Hydrogen evolution reaction, Tungsten carbide, Electrochemistry, stable electrocatalyst





# Working Group 2: High-Fidelity Combustion Simulations and Data Analytics

**Keynote Lecture: Are we there yet? Towards foundational ML models for combustion through accessible community-involved big databases**

**Prof. Matthias Ihme**

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Department of Photon Sciences, SLAC National Accelerator Laboratory  
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Recent advances in data-driven methods and machine-learning techniques rely on large datasets and massive deep learning models to predict quantities of interest. Within the field of combustion, large amounts of data exist in the form of high-fidelity simulation data and detailed measurements that have been accumulating. Yet, this data remains distributed and can be difficult to access. To make this data available, this presentation presents a realistic and feasible framework which combines (i) community involvement, (ii) public data repositories, and (iii) lossy compression algorithms for enabling broad access to high-fidelity data via a network-of-datasets approach. This Bearable Large Accessible Scientific Training Network-of- Datasets (BLASTNet) is consolidated on a community-hosted web-platform (at <https://blastnet.github.io/>), and is targeted towards improving accessibility to diverse scientific data for deep learning algorithms. We discuss procedures for community to contribute and utilize this database and present illustrative examples on how this database has contributed towards the development of new ML models in the context of turbulent subgrid-scale modeling.



## List of Abstracts

### Preliminary Experimental and Computational Investigation of a Laboratory Gas Turbine Combustor

**Gonçalo P. Pacheco, Afonso Santoalha, Bruno M. Pinto, Miguel A. A. Mendes and Pedro J. Coelho**

Presenter: Pedro J. Coelho

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**Keywords:** Gas turbine combustor, Eddy dissipation concept. Flamelet model, Emissions

### Experimental and modeling high-pressure study of ammonia/dimethyl-ether conversion in a flow reactor

**P. García-Ruiz, P. Ferrando, M. U. Alzueta**

Presenter: Pedro García-Ruiz

*Aragón Institute of Engineering Research (I3A), Department of Chemical and Environmental Engineering,*

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**Keywords:** Ammonia, Dimethyl Ether, High-pressure, Kinetic modeling, N<sub>2</sub>O.

### Analysis of flame propagation in spray flames of aviation fuels

**Giuseppe Indelicato<sup>\*1</sup>, Daniel Mira<sup>1</sup>**

Presenter: Giuseppe Indelicato

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**Keywords:** liquid fuels, multi-component, premixed flames, evaporation.

### Advanced methods for kinetic parameter optimization

**T. Nagy<sup>\*1</sup>, M. Papp<sup>2,3</sup>, M. Kovács<sup>2</sup>, L. Horváth<sup>1,2</sup>, P. Wang<sup>3</sup>, H. J. Curran<sup>3</sup>, T. Turányi<sup>2</sup>**

Presenter: Tibor Nagy

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**Keywords:** Optima++, active parameter selection, uncertainty scaled local sensitivity matrix, model reduction assisted parameter optimization, rate rule optimization



**The burning features of NH<sub>3</sub>/DME/air Bunsen flames: a modelling study****Luca Granata<sup>1</sup>, Federica Ferraro<sup>2</sup>, Francesco Roman Artoli<sup>1</sup>, Alessandro Stagni<sup>\*1</sup>****Presenter:** Alessandro Stagni<sup>1</sup>*Department of Chemistry, Materials, and Chemical Engineering “G. Natta”, Politecnico di Milano, Italy**E-mail: [luca.granata@mail.polimi.it](mailto:luca.granata@mail.polimi.it), [alessandro.stagni@polimi.it](mailto:alessandro.stagni@polimi.it), [francescoroman.artoli@polimi.it](mailto:francescoroman.artoli@polimi.it)*<sup>2</sup>*Institute of Jet Propulsion and Turbomachinery, Technische Universität Braunschweig, Germany**E-mail: [federica.ferraro@tu-braunschweig.de](mailto:federica.ferraro@tu-braunschweig.de)***Keywords:** Ammonia, Dimethyl ether, Hydrogen carriers, Nitrogen Oxides, Bunsen burner.**Kinetic modelling data for co-combustion process to accelerate energy transition in large power plants****Dragoslava Stojiljković<sup>\*1</sup>, Nebojša Manić<sup>2</sup>, Miloš Radojević<sup>3</sup>, Bojan Janković<sup>4</sup>, Anes Kazagić<sup>5</sup>, Nihad Hodžić<sup>6</sup>, Kenan Kadić<sup>7</sup>****Presenter:** Dragoslava Stojiljković<sup>1,2,3</sup>*University of Belgrade, Faculty of Mechanical Engineering, Fuel and Combustion Laboratory, Belgrade, Serbia**E-mail: [nmanic@mas.bg.ac.rs](mailto:nmanic@mas.bg.ac.rs), [dstojiljkovic@mas.bg.ac.rs](mailto:dstojiljkovic@mas.bg.ac.rs), [mradojevic@mas.bg.ac.rs](mailto:mradojevic@mas.bg.ac.rs)*<sup>4</sup>*University of Belgrade, Vinča Institute of Nuclear Sciences - National Institute of the RS, Belgrade, Serbia**E-mail: [bojan.jankovic@vinca.rs](mailto:bojan.jankovic@vinca.rs)*<sup>5</sup>*JP Elektroprivreda BiH d.d. – Sarajevo Power Utility, Sarajevo, Bosnia and Herzegovina**E-mail: [a.kazagic@epbih.ba](mailto:a.kazagic@epbih.ba)*<sup>6</sup>*Faculty of Mechanical Engineering, University of Sarajevo, Sarajevo, Bosnia and Herzegovina**E-mail: [hodzic@mef.unsa.ba](mailto:hodzic@mef.unsa.ba)*<sup>7</sup>*JP Elektroprivreda BiH d.d. – Sarajevo Power Utilit, Kakanj Power Station, Bosnia and Herzegovina**E-mail: [k.kadic@epbih.ba](mailto:k.kadic@epbih.ba)***Keywords:** kinetic modelling, model-based, low rank coal, biomass, co-combustion.**Mechanism reduction-assisted optimization of the ethylene chemistry in the AramcoMech 2.0 combustion mechanism****Boyang Su<sup>1</sup>, Tibor Nagy<sup>2,\*</sup>, Máté Papp<sup>1,3</sup>, István Gy. Zsély<sup>1</sup>, Tamás Turányi<sup>1,\*</sup>****Presenter:** Tamás Turányi<sup>1</sup>*Institute of Chemistry, ELTE Eötvös Loránd University, Budapest, Hungary**E-mails: [boyang@student.elte.hu](mailto:boyang@student.elte.hu), [mate.papp@ttk.elte.hu](mailto:mate.papp@ttk.elte.hu), [istvan.zsely@ttk.elte.hu](mailto:istvan.zsely@ttk.elte.hu), [tamas.turanyi@ttk.elte.hu](mailto:tamas.turanyi@ttk.elte.hu)*<sup>2</sup>*Institute of Materials and Environmental Chemistry, HUN-REN Research Centre for Natural Sciences, Budapest, Hungary**E-mail: [nagy.tibor@ttk.hu](mailto:nagy.tibor@ttk.hu)*<sup>3</sup>*HUN-REN-ELTE Research Group on Complex Chemical Systems, Budapest, Hungary***Keywords:** ethylene, combustion mechanism, mechanism reduction, mechanism optimization



## Recent advancements in the reaction kinetics branch of the ReSpecTh Information System

**Á. Veres-Ravai<sup>\*1</sup>, M. Kovács<sup>1</sup>, A. Gy. Szanthoffer<sup>1</sup>, É. Valkó<sup>1,2</sup>, P. Zhang<sup>1,3,4</sup>, M. Papp<sup>1,5</sup>, B. Su<sup>1</sup>, T. Nagy<sup>6</sup>, I. Gy. Zsély<sup>1</sup>, T. Turányi<sup>1</sup>**

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**Keywords:** ReSpecTh Information System, RKD format, detailed combustion kinetic mechanisms, experimental data collection, searchable database

## Experimental-numerical workflow for high-temperature decomposition process of sewage sludge aimed towards P extraction.

**A. Žnidarčič<sup>1</sup> and T. Seljak<sup>1</sup>**

Presenter: Anton Žnidarčič

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**Keywords:** Surrogate fuel, sewage sludge, thermal treatment, combustion modelling, 3D CFD.

## Numerical analysis of flameless combustion in a thermal oxidation chamber

**Vid Zuljan<sup>1</sup>, Tine Seljak<sup>\*1</sup>**

Presenter: Vid Zuljan

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**Keywords:** CFD, TOC, distributed combustion, EDC, emissions





# Working Group 3: Hybrid physics-based data-driven models

**Keynote Lecture: Opportunities for machine learning assisted design of energy conversion machines**

**Prof. Paola Cinnella**

*Sorbonne University in Paris and member of the Jean Le Rond D'Alembert Institute of Theoretical and Applied Mechanics*

In the last decade or less, applications of data science, and more specifically of so-called machine learning (ML), in physical sciences have been growing exponentially. ML-assisted Computational Fluid Dynamics (CFD) models with magnified predictive capabilities and computational efficiency can play a game changing role in carbon-intensive industries. However, several criticalities must be addressed for ML-enhanced CFD scaling-up to large problems of Engineering interest, including the need for suitable high-fidelity databases, the lack of generalization to out-of-sample environments, and the need for quantifying prediction uncertainties. In my talk, I will adopt the point of view of Bayesian machine learning. Such a framework is well-suited for scarce/noisy data, it enables simultaneous model selection and inference, and it provides estimates of uncertainty in the predicted model outputs, a critical information in view of the robust design of energy conversion machines.



## List of Abstracts

### Combustion Modelling and Dimensionality Reduction in Turbulent Non-Premixed Sooting Flames with Convolutional Neural Networks

**Geveen Arumapperuma<sup>\*1</sup>, Oliver Bladék<sup>1</sup> and Antonio Attili<sup>1</sup>**

Presenter: Antonio Attili

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**Keywords:** Turbulent flames, non-premixed combustion, Direct Numerical Simulation, Convolutional Neural Networks.

### Kernel method for reactive flows

**Davide Baroli<sup>\*1</sup>**

Presenter: Davide Baroli

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**Keywords:** surrogate model, manifold learning

### Hybrid modelling of sorptive capture of carbon dioxide from flue gases in presence of competing phenomena

**Katarzyna Bizon<sup>\*1</sup>, Enrico A. Cutillo<sup>2</sup> and Gaetano Continillo<sup>3</sup>**

Presenter: Katarzyna Bizon

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**Keywords:** CO<sub>2</sub> capture, multicomponent adsorption, artificial neural network, Kriging interpolation

### Dynamical Characterization for the Convergence Enhancement and Dimensionality Reduction of Combustion Chemical Kinetics

**L. Castellanos<sup>1,2</sup>, R. S. M. Freitas<sup>3</sup>, A. Parente<sup>2</sup>, F. Contino<sup>1</sup>**

Presenter: Luisa Castellanos

<sup>1</sup>Thermodynamics and Fluid Mechanics, Institute of Mechanics, Materials and Civil Engineering, École Polytechnique de Louvain, Université Catholique de Louvain, Ottignies-Louvain-la-Neuve, Belgium

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**Keywords:** Combustion chemistry kinetics, Dynamical system, Time-derivatives behavior,





## Reduced modelling, Convergence enhancement, Dimensionality reduction A Co-kurtosis Principal Component Analysis and Modularity-based Clustering for Flashback Precursor Identification

**M. Floris<sup>1</sup>, D. Nayak<sup>2</sup>, T. S. Sai<sup>2</sup>, I. Langella<sup>1</sup>, K. Aditya<sup>2</sup> and N. A. K. Doan<sup>\*1</sup>**

Presenter: Anh Khoa Doan

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**Keywords:** Hydrogen combustion, Flashback, Precursor identification, Featurization, Clustering

## Machine Learned Compact Kinetic Model for Liquid Fuel Combustion

**Mark Kelly<sup>\*1</sup>, Gilles Bourque<sup>2</sup>, Matthias Hase<sup>3</sup>, Stephen Dooley<sup>1</sup>**

Presenter: Mark Kelly

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<sup>3</sup>*Siemens Energy Global GmbH & Co. KG, Mülheim an der Ruhr, Germany*

**Keywords:** Compact Models, Mechanism Optimization, Machine Learning, Liquid Fuels, Gas-Turbine Physics.

## Combining data-driven and physics-based methods for stiffness reduction in combustion systems

**Riccardo Malpica Galassi<sup>\*1</sup>, M. Rafi Malik<sup>2</sup>, Hong G. Im<sup>2</sup>, and Mauro Valorani<sup>1</sup>**

Presenter: Riccardo Malpica Galassi

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<sup>2</sup>*CCRC, King Abdullah University of Science and Technology (KAUST), Thuwal, 23955-6900, Kingdom of Saudi Arabia*

**Keywords:** Model reduction; Principal Component Analysis; Computational Singular

## Perturbation; Stiffness; Machine Learning Combustion Model for Coupling with a Cement Kiln CFD Digital Twin Model: Coal and Extension to an Alternative Fuel

**M. Mouratidis<sup>\*1</sup>, E. Gkagkari<sup>2</sup>, C. Pagkoura<sup>3</sup>, V. Zacharopoulou<sup>4</sup>, G. Karagiannakis<sup>5</sup> and A. Asimakopoulou<sup>6</sup>**

Presenter: Michalis Mouratidis

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**Keywords:** Coal, Combustion, Devolatilization, CFD, Cement





## A neural network and low cost SVD based hybrid model for forecasting of reactive flows.

**Prajith Pillai<sup>1</sup>, R. Abadía-Heredia<sup>1</sup>, Ashton Hetherington<sup>1</sup>, A. Corrochano<sup>1</sup>, Laura Saavedra<sup>1</sup> and Soledad Le Clainche<sup>1</sup>**

**Presenter:** Prajith Pillai

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**Keywords:** Combustion, Reactive flows, Renewable synthetic fuels, Reduced order modelling, Singular value decomposition, Low-cost singular value decomposition.

## A data-driven approach to correct the cell reacting fraction in the partially stirred reactor closure for LES of premixed flames

**Lorenzo Piu<sup>1,2</sup>, Arthur Péquin<sup>1,2</sup>, Rodolfo Freitas<sup>3</sup>, Salvatore Iavarone<sup>1,2</sup>, Heinz Pitsch<sup>4</sup>, Alessandro Parente<sup>1,2</sup>**

**Presenter:** Lorenzo Piu

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<sup>3</sup>School of Engineering and Materials Science, Queen Mary University of London, Mile End Road, London, UK

<sup>4</sup>Institut für Technische Verbrennung, RWTH Aachen University, Germany

**Keywords:** Combustion, Neural Networks, Partially Stirred Reactor, LES, Premixed Flames.

## Feature identification for optimal Chemical Reactor Networks for Combustion Systems

**A. Remiddi<sup>\*1,2</sup>, M. Savarese<sup>1,2</sup> and A. Parente<sup>1,2</sup>**

**Presenter:** Arianna Remiddi

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**Keywords:** Reduced-order modelling, Chemical Reactor Network, Digital Twin

## Towards physics-based digital twins of combustion systems: a sparse sensing and Chemical Reactor Network approach

**M. Savarese<sup>\*1,2,3</sup>, A. Procacci<sup>1,3</sup>, S. Iavarone<sup>1,3</sup>, L. Giuntini<sup>1,3</sup>, W. De Paepe<sup>2</sup> and A. Parente<sup>3</sup>**

**Presenter:** Matteo Savarese

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**Keywords:** Reduced-order modelling, Chemical Reactor Network, Sparse sensing, Digital twin, Ammonia combustion.





## Detailed Kinetic Mechanisms Investigation in Parameters Space

**Francesco Saverio Marra<sup>1</sup>, Luigi Acampora<sup>2</sup>**

Presenter: Francesco Saverio Marra

<sup>1</sup>*Istituto di Scienze e Tecnologie per l'Energia e la Mobilità Sostenibili, CNR, Italy*

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**Keywords:** Bifurcation, Continuation analysis, Community analysis, Detailed mechanisms.

## Probabilistic and data-efficient machine learning framework for chemical source term integration

**Cihat Emre Ustun\* and Amin Paykani**

Presenter: Cihat Emre Ustun

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**Keywords:** Probabilistic machine learning; Gaussian Processes; Hydrogen combustion; Uncertainty quantification

## Hydrogen and hydrogen/ammonia scale-resolving simulation activities at Aalto University using DLBFoam

**Ville Vuorinen, Parsa Tamadonfar, Aleksi Rintanen, Zin Shahin, Ali Haider, Ilya Morev, Ossi Kaario, Mahmoud Gadalla, Ali Shahanaghi, Shervin Karimkashi**

Presenter: Ville Vuorinen

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**Keywords:** Direct chemistry, DLBFoam, hydrogen/ammonia combustion, combustion phenomena





## Working Group 4: Digital Twins

**Keynote Lecture: Reinforcement Twinning: from digital twins to model-based reinforcement learning**

**Miguel Alfonso Mendez**

*Associate Professor at the von Karman Institute for Fluid Dynamics (VKI)*

The concept of digital twins promises to revolutionize engineering by offering new avenues for optimization, control, and predictive maintenance. Digital twins seek to virtually replicate systems using models that continuously "learn" from data, automatizing data collection, validation and refinement to achieve the "self-learning" status. This talk presents a new framework for combining ideas from reinforcement learning and data assimilation to simultaneously train the digital twin of an engineering system and a control law to maintain its optimal performance.

We refer to this framework as Reinforcement Twinning (RT).

The training of the digital twin combines methods from adjoint-based data assimilation and system identification, while the training of the control agent combines model-based optimal control and model-free reinforcement learning. The main underlying idea is to deploy "learning feedback" to allow the digital twin to learn from the control agent and the control agent to learn from the digital twin. In this talk, we mainly explore the second path, allowing the control agent to use the virtual environment as a playground for confrontation and indirect interaction by imitation: once the predictive performances of the twin are successful, a model-based controller acts as an "expert demonstrator".

The talk explores three vastly different engineering systems and control tasks, namely (1) the control of a wind turbine subject to time-varying wind speed, (2) the trajectory control of flapping-wing micro air vehicles (FWMAVs) subject to wind gusts, and (3) the mitigation of thermal loads in the management of cryogenic storage tanks. The test cases are implemented using simplified models for which the ground truth on the closure law is available. The results show that the adjoint-based training of the digital twin is remarkably sample-efficient and completed within a few iterations. Concerning the control agent training, the results show that the model-based and the model-free control training benefit from the learning experience and the complementary learning approach of each other. The encouraging results open the path towards implementing the RT framework on lab-scale prototypes, which is currently being explored.





## List of Abstracts

### Digital twins based on real-time flame monitoring. Still an elusive objective?

**Javier Ballester\***, Álvaro Muelas and Álvaro Sobrino

Presenter: Javier Ballester

*Laboratory of Fluids Engineering and Energy (LIFEn), I3A/Univ. Zaragoza, Spain*

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**Keywords:** Flame monitoring, radiation sensors, hydrogen combustion, AI, digital twin.

### Green and digital transformation of the industry by employing digital twin in the learning factories

**Aleksandar Argilovski<sup>\*1</sup>**

Presenter: Aleksandar Argilovski

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**Keywords:** digital twin, learning factory, twin transition, digital transformation, green transformation.

### JThermodynamicsCloud: A Case study in FAIR data practices, data traceability and data-lineage promotion.

**Edward S. Blurock<sup>\*1</sup>**

Presenter: Edward S. Blurock

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**Keywords:** Thermodynamics, database management. data lineage, database.

### Digital twin simulation and data-driven model for automotive injector spray characteristics prediction

**Charalambos A. Chasos<sup>\*1</sup>**

Presenter: Charalambos A. Chasos

*<sup>1</sup>Mechanical Engineering Department, Frederick University, Cyprus*

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**Keywords:** Automotive injector, digital twin, CFD simulation, data-driven model, spray penetration

### A Probabilistic Framework for Data Assimilation of Reacting Dynamical Systems using a Gaussian Process Regression-based Reduced-Order Model and Sparse Measurements

**L. Donato<sup>1,2,3</sup>, M. M. Kamal<sup>1,2</sup>, A. Procacci<sup>1,2</sup>, M. Cafiero<sup>1,2</sup>, S. Sharma<sup>1,2</sup>, C. Galletti<sup>3</sup>, A. Coussement<sup>1,2</sup> and A. Parente<sup>1,2</sup>**

Presenter: Laura Donato

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*<sup>3</sup>Department of Civil and Industrial Engineering, University of Pisa, L.go Lucio Lazzarino, 56122, Pisa, Italy*

**Keywords:** Reduced-order model, Gaussian Process Regression, Proper Orthogonal Decomposition, Data Assimilation, Kalman Filter.





## Digital Twin of a Membrane Electrode Assembly Reactor for Electrochemical Reduction of CO<sub>2</sub> to E-Fuels

**Harry Dunne<sup>1</sup>, Weiming Liu<sup>1</sup>, Bernardo Ballotta<sup>1</sup>, Mohammad R. Ghaani<sup>2</sup>, Kim McKelvey<sup>3</sup>, Stephen Dooley<sup>1</sup>**

**Presenter:** Stephen Dooley

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**Keywords:** CO<sub>2</sub> electrolysis, Membrane Electrode Assembly, Anion Exchange Membrane, 1-D simulation.

## Real-time monitoring of pollutant emission by photoacoustic technique for turbulent combustion

**Viktor Józsa<sup>\*1</sup>, Réka A. Kardos<sup>1</sup>, Diána Kiss<sup>2,3</sup>, Gergely Kiss-Albert<sup>2</sup> and Zoltán Bozóki<sup>2,4</sup>**

**Presenter:** Viktor Józsa

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**Keywords:** NO<sub>x</sub>, NO, NO<sub>2</sub>, emission, burner.

## Digital twin of a stagnation-point reverse-flow combustor for the oxidation of NH<sub>3</sub>/H<sub>2</sub> blends

**Chiara Novelli<sup>1,2</sup>, Lorenzo Giuntini<sup>1,2</sup>, Matteo Savarese<sup>1,2</sup>, Axel Coussement<sup>1,2</sup> and Alessandro Parente<sup>1,2</sup>**

**Presenter:** Chiara Novelli

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**Keywords:** Reduced-order modelling, digital twin, ammonia, combustion.





## Multi-Fidelity Surrogate Framework for Digital Twin Development in Flameless Combustion Systems Using Heterogeneous Data

**A. Özden<sup>\*1,2,3</sup>, A. Procacci<sup>1,2</sup>, R. Malpica Galassi<sup>4</sup>, A. Coussement<sup>1,2</sup> and A. Parente<sup>1,2</sup>**

Presenter: Aysu Özden

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**Keywords:** Multi-Fidelity ROM, Digital Twin, Proper Orthogonal Decomposition, Manifold Alignment, Co-Kriging

## A Probabilistic Framework for Data Assimilation of Reacting Dynamical Systems using a Gaussian Process Regression-based Reduced-Order Model and Sparse Measurements

**A. Procacci<sup>\*1,2</sup>, S. Iavarone<sup>1,2</sup>, L. Donato<sup>1,2</sup>, A. Coussement<sup>1,2</sup> and A. Parente<sup>1,2</sup>**

Presenter: Alberto Procacci

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**Keywords:** Reduced-order model, Gaussian Process Regression, Proper Orthogonal Decomposition, Bayesian Inference, Dynamical Systems.

## Numerical-Experimental Analysis of the Thermomechanical State of Fire-Tube Boiler Structure under Transient Operational Regime

**Milena N. Rajic<sup>\*1</sup>, Dragoljub S. Zivkovic<sup>2</sup> and Milan Banic<sup>3</sup>**

Presenter: Milena N. Rajic

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**Keywords:** fire-tube hot water boiler, thermomechanical analysis, transient operational regime, numerical simulation, experimental analysis

## Exploratory analysis for soft sensing strategies under MILD conditions using validated kinetic mechanism for ammonia-hydrogen combustion

**Vincenzo Rosati<sup>\*1,2</sup>, Giancarlo Sorrentino<sup>1</sup>, Raffaele Ragucci<sup>1</sup> and Mara de Joannon<sup>1</sup>**

Presenter: Vincenzo Rosati

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**Keywords:** MILD combustion, Perfectly Stirred Reactor, Soft Sensor, Ammonia-hydrogen oxidation.





# Working Group 5: Communication, Dissemination, Partnering

**Keynote Lecture: The twin transitions**

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