Agenda for the thematic workshop COMBUSTION AND MACHINE LEARNING

Of the French section of the Combustion Institute (GFC)

Wednesday 27th March at IFP Energies Nouvelles, Rueil-Malmaison
and broadcast online

Organizers : Cédric MEHL (IFPEN), Roda BOUNACEUR (LRGP), Corentin LAPEYRE (Nvidia)

8:30 Welcome

9:00 Opening words, **Luc Vervisch**, president of the scientific council at IFPEN

9:10 Invited plenary, **Alessandro PARENTE** (ULB)
An overview of data-driven methods to accelerate, improve and encode the simulations of turbulent reacting flows

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10:00 Turbulent combustion of lean hydrogen premixed flames: from physical assessment to data-driven modeling
Victor COULON, Corentin LAPEYRE, Thierry POINSOT (IMFT/CERFACS)

10:20 Gaussian Process Regression-based reduced-order model for data-driven forecast of reacting dynamical systems
Alberto PROCACCI[1], **Salvatore IAVARONE[2]**, Axel COUSSEMENT[1], Alessandro PARENTE[1]
[1] Aero-Thermo-Mechanics Laboratory, Université Libre de Bruxelles
[2] EM2C Laboratory, CNRS-CentraleSupelec, Université Paris-Saclay

10:40-11:10 Coffee break

11:10 A performance comparison of optimization algorithms applied to kinetic mechanism optimization
Luu TAN-PHONG, Nasser DARABIHA, Benoît FIORINA
EM2C Laboratory, CNRS-CentraleSupelec, Université Paris-Saclay

11:30 Deep Learning Dynamical Latencies for the Analysis and Reduction of Combustion Chemistry Kinetics
Luisa CASTELLANOS[1,2], R. S. M. FREITAS[2], Alessandro PARENTE[2], Francesco CONTINO[1]
[1] *Université Catholique de Louvain, Ecole polytechnique de Louvain, Institute of Mechanics, Materials and Civil Engineering*
[2] *Aero-Thermo-Mechanics Laboratory, Université Libre de Bruxelles*

11:50 Bayesian calibration of a global chemical scheme and uncertainty propagation to flame-vortex interactions
Juan ARMENGOL[1], Olivier Le Maître[2], **Ronan VICQUELIN**[1]
[1] *EM2C Laboratory, CNRS-CentraleSupelec, Université Paris-Saclay*
[2] *CMAP Laboratory, Ecole Polytechnique*

12:10-14:00 Lunch

14:00 Invited plenary, **Elie HACHEM** (CEMEF)
Coupling Computational Fluid Dynamics and Machine Learning for Optimization and Design

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14:50 Criteria to switch from chemistry tabulation to neural networks in computational combustion and application of ANN-CNN to detailed chemistry in sooting flames
Zakaria NIKOLAOU, Andrea SELTZ, Pascale DOMINGO, **Luc VERVISCH**
CNRS CORIA Laboratory, INSA Rouen Normandie

15:10 On-the-fly accuracy evaluation of Artificial Neural Networks and hybrid method to improve the robustness of neural network accelerated chemistry solving
Cédric MEHL, Damien AUBAGNAC-KARKAR
IFPEN

15:30-16:00 Coffee break

16:00 Acceleration of flash computations using a machine learning enhanced solver,
Thibault FANEY, Jingang QU, Paul MCGINN
IFPEN

16:20 Advanced Post-Processing Simulation of Nitrogen Oxides in a Testing Furnace for Steel Reheating Furnaces via Integrated Machine Learning-CFD Approach
Minh Duy LE, Hassan MOHANNA, Sébastien CAILLAT
Fives Stein

16:40 Deep-Learning model based on a QSPR approach for the estimation of RON, MOM and Cetane Number, for any C, H, O, N hydrocarbons
Roda BOUNACEUR
LRGP Laboratory, Université de Lorraine

17 :00 End of day

ABSTRACTS

PLENARY TALKS

Alessandro PARENTE (ULB)
An overview of data-driven methods to accelerate, improve and encode the simulations of turbulent reacting flows

Elie HACHEM (CEMEF)
The challenges of modeling turbulent combustion with the introduction of hydrogen into reactive systems

CONTRIBUTED TALKS

Turbulent combustion of lean hydrogen premixed flames: from physical assessment to data-driven modeling
Victor COULON, Corentin LAPEYRE, Thierry POINSOT (IMFT/CERFACS)
Hydrogen, with its rising prominence in combustion applications, presents distinctive challenges in combustion modeling. This is largely because the conventional flamelet assumption often falls short for hydrogen. Moreover, the stretch response of hydrogen flames significantly alters its structure, leading to pronounced local consumption rates, especially under turbulent and lean conditions. In light of these challenges, there is growing momentum in the research community to develop dependable turbulent models that can accurately depict hydrogen flame dynamics. Our study contributes to this effort by harnessing high-fidelity Direct Numerical Simulation data to explore potential modeling pathways. Specifically, we employ a Convolutional Neural Network to model turbulent hydrogen flames in lean conditions, crafting an efficiency function grounded in hydrogen reaction rates within the Thickened Flame Large Eddy Simulation paradigm. The efficacy of this data-driven modeling approach is then assessed through both offline and online calculations.

Gaussian Process Regression-based reduced-order model for data-driven forecast of reacting dynamical systems
Alberto PROCACCI[1], **Salvatore IAVARONE[2]**, Axel COUSSEMENT[1], Alessandro PARENTE[1]
[1] *Aero-Thermo-Mechanics Laboratory, Université Libre de Bruxelles*
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In the current energy transition scenario, developing cost-effective simulation approaches is highly desirable to accelerate the required innovations in combustion science and technologies. An appealing solution is the use of Reduced-Order Models (ROMs) that feature lower dimensionality and limited loss of accuracy, allowing for predicting and controlling the behavior of combustion systems in real time. This work proposes a ROM based on

dimensionality reduction and Gaussian Process Regression for a reacting dynamical system. The ROM is constructed and tested on a Computational Fluid Dynamics (CFD) simulation database of an axisymmetric time-varying non-premixed co-flow nitrogen-diluted methane flame. GPR simultaneously enables the reconstruction of the CFD fields in time and, more importantly, the estimation of local uncertainty due to local interpolation error and truncation of the high-dimensional state space.

A performance comparison of optimization algorithms applied to kinetic mechanism optimization

Luu TAN-PHONG, Nasser DARABIHA, Benoît FIORINA

EM2C Laboratory, CNRS-CentraleSupelec, Université Paris-Saclay

Simplified chemistry models are needed to predict major chemical effects at a low CPU cost in practical applications. Among such approaches, the virtual chemistry method aims to reproduce selected flame properties of interest by building a simplified reaction mechanism from scratch using virtual species and reactions whose thermochemical properties are optimized. From a theoretical point of view, the error can still be further reduced and depends notably on the reliability of the optimization process, which has been observed to fail as the number of optimized variables increases. In this work, a representative optimization problem based on retrieving the parameters of a known kinetic mechanism is defined and the performance of different optimization algorithms is compared.

Deep Learning Dynamical Latencies for the Analysis and Reduction of Combustion Chemistry Kinetics

Luisa CASTELLANOS[1,2], R. S. M. FREITAS[2], Alessandro PARENTE[2], Francesco CONTINO[1]

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The curse of dimensionality is the main issue when it comes to the modeling of combustion's chemical kinetics. Currently, many Machine Learning (ML) dimensionality reduction techniques have been applied to the problem of chemistry kinetics. In this work, time-lag autoencoders (TAE) temporal characteristics are exploited for the analysis of latencies, allowing for the identification of key chemical species that describes the statistical variance of the mechanism. Such chemical species provide hints of the main chemical reactions that represent the chemistry kinetics. The application of TAE is presented as a technique that could help in the development and analysis of reduced mechanisms. A test case for hydrogen is presented (9 variables), as well as a detailed mechanism for methane combustion (491 variables).

Bayesian calibration of a global chemical scheme and uncertainty propagation to flame-vortex interactions

Juan ARMENGOL[1], Olivier Le Maître[2], **Ronan VICQUELIN**[1]

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Simplified chemistry models are commonly used in reactive computational fluid dynamics (CFD) simulations to alleviate the computational cost. Uncertainties associated with the calibration of such simplified models have been characterized in some works, but there is a

lack of studies analyzing the subsequent propagation through CFD simulation of combustion processes. This work propagates the uncertainties - arising in the calibration of a global chemistry model through direct numerical simulations (DNS) of flame-vortex interactions. Calibration uncertainties are derived by inferring (MCMC method) the parameters of a two-step reaction mechanism for methane. The inference is assisted by surrogate models of laminar flame computations taking advantage of Principal Component Analysis (PCA) and Polynomial Chaos (PC) expansion.

Criteria to switch from chemistry tabulation to neural networks in computational combustion and application of ANN-CNN to detailed chemistry in sooting flames

Zakaria NIKOLAOU, Andrea SELTZ, Pascale DOMINGO, **Luc VERVISCH**
CNRS CORIA Laboratory, INSA Rouen Normandie

Analytical expressions will be presented for the computational cost of tabulation and of neural networks including the effect of network structure. The scaling laws are validated using both model test-data but also data based on a canonical problem which involves inferring laminar flame speeds of methane/hydrogen mixtures at off-training conditions. The proposed scaling laws lead naturally to a framework for effective decision-making between adopting look-up tables or neural networks. A combination of trained ANN and CNN is then applied to the prediction of particle size distribution in sooting flames, a canonical laminar flame and a representative aeronautical combustion chamber are simulated.

On-the-fly accuracy evaluation of Artificial Neural Networks and hybrid method to improve the robustness of neural network accelerated chemistry solving

Cédric MEHL, Damien AUBAGNAC-KARKAR
IFPEN

A chemistry acceleration strategy based on the coupling of Artificial Neural Networks (ANNs) and Direct Integration (DI) is proposed and evaluated in the context of turbulent combustion. The main novelty of this study is its focus on ANNs robustness assessment. A hybrid DI/ANN strategy is proposed, which allows for a direct control of the prediction errors. This control is achieved by evaluating the ANN prediction error after each inference. To this end, a simple yet novel criterion based on mass conservation is proposed and compared to a criterion based on the distance between the inferred state and the training database, as done previously in the literature in the context of on-the-fly learning. A two-dimensional turbulent premixed hydrogen ignition case is used to assess the performance of the strategy and challenge the two criteria. An a priori study demonstrates that the state-space based criterion cannot correctly describe the ANN error, while the mass conservation based one provides a good match with the ANN error. An a posteriori evaluation, involving actual simulations of the turbulent case, show the ability of the hybrid DI/ANN model based on mass conservation error to improve the quality of the predictions and thus the robustness of ANNs. The increase of computational cost due to the hybrid model is acceptable as the DI is only applied in very localized regions in space and in time.

Acceleration of flash computations using a machine learning enhanced solver

Thibault FANEY, Jingang QU, Paul MCGINN
IFPEN

Phase equilibrium calculations are an essential part of numerical simulations of combustion processes and can account for a large share of the total computational time, effectively limiting the number of species that can be modeled. Data-driven approaches have been developed to alleviate this issue, however they also have limitations: tabulation approaches are limited by memory to a small number of species, while “black-box” machine learning approaches don’t offer sufficient guarantees on the result. In this work, we present a hybrid approach that carefully ties the numerical simulator and deep learning algorithms in order to accelerate convergence while guaranteeing the end result. We illustrate the results on a combustion test case where the hybrid solver is embedded in the CFD solver CONVERGE.

Advanced Post-Processing Simulation of Nitrogen Oxides in a Testing Furnace for Steel Reheating Furnaces via Integrated Machine Learning-CFD Approach

Minh Duy LE, Hassan MOHANNA, Sébastien CAILLAT
Fives Stein

As a leading player in the metallurgy industry, Fives Stein focuses on optimizing reheating furnaces, critical components in the steel production process. Burners used in these furnaces must not only meet heat transfer requirements (including power, safety, and temperature homogeneity) but also comply with stringent environmental regulations, notably for reducing nitrogen oxides (NOx). Computational Fluid Dynamics (CFD) modeling is a conventional method for analyzing flame structures. Commercial software like Ansys Fluent can yield NOx predictions based on a post-processing method. However, the numerical results often diverge from empirical data. To bridge this gap, we have pioneered an integrated post-processing approach that combines CFD calculations with machine learning algorithms. This innovation enhances predictive accuracy, aligning NOx predictions more closely with real-world observations from our in-house testing furnace. The integrated approach shows promise in improving modelling accuracy without requiring extensive computational resources.

Deep-Learning model based on a QSPR approach for the estimation of RON, MOM and Cetane Number, for any C, H, O, N hydrocarbons

Roda BOUNACEUR
LRGP Laboratory, Université de Lorraine

With the increasing demand in alternative fuels and the use of biomass as the feedstock for the production of fuel commodities, a wider range of oxygenated hydrocarbons as fuel additives needs to be considered. Consequently, the development of robust method for the prediction of criterium as Research Octane Number (RON), Motor Octone Number (MOM) and Cetane Number (CN), will play a crucial role in the characterization of novel fuels. In this study we proposed a robust deep-learning model based on a Quantitative Structure−Property Relationship (QSPR) approach for the estimation of RON, MOM and CN of any C, H, O, N molecules. We develop a multimodal learning model from a combination of two types of data and based on an Artificial Neural Network. The Mordred algorithm has been used in order the

determine 457 descriptors to characterize any hydrocarbons. These numerical values represent the first type of data considered in the present study. To consider the effect of mesomerism or chirality of molecules the InChiKey notation has been used. This notation, composed by 27 letters, represent the second type of data and are considered as text data. To encode textual variables into numeric data, we have used a Word Embedding method. The final model has been tested with success on a large set of experimental data and compared with three recent learning models: GNN, ANN and GPR. The methodology of GNN (Graph Neural Networks) model is based on the architecture of the molecule, that of the ANN (Artificial Neural Networks) is based on a limited number of chemical groups, whereas the GPR model is mainly based on Joback groups. The full comparison and the several tests show a very robust and predictive ability of our newly proposed multimodal learning model.