October 23 & 24

COMBURA NVV 2024

Book of Abstracts

NVV
Nederlandse Vereniging
voor Vlamonderzoek

THE COMBUSTION INSTITUTE 1954

Combura 2024

October 23 & 24, 2023

Domusdela, Eindhoven, The Netherlands

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Combura 2024

October 23 & 24,

Domusdela, Kanaalstraat 4, 5611 CT Eindhoven, The Netherlands

Program outline, version of October 17, 2024

GENERAL INFORMATION

The COMBURA symposium stands as a pivotal annual event fostering the exchange of insights within combustion research and its tangible applications in the Netherlands. It is an initiative of the Nederlandse Vereniging voor Vlamonderzoek NVV (Netherlands Association for Flame Research).

This year, the general theme of the symposium is
Focus on numerical and experimental developments to aid with the energy transition.
Participants from universities, research institutes, and industrial companies in the Netherlands and surrounding countries are cordially invited.

Information on all aspects of the symposium is available on the Combura website (www.combura.nl).

The COMBURA event will start in the late afternoon of October 23rd with a poster session held in parallel with the NVV Members Meeting, followed by the conference dinner. The dinner is open to all participants provided a registration is made. The program on October 24th consists of invited lectures, oral and poster presentations and a workshop on industrial combustion.

CONTACT

For questions regarding the program contact Anna Felden at a.m.j.felden@tudelft.nl
For any other questions, contact Marjan Beekmans at m.beekmans@tue.nl

Program Committee

- Francesca De Domenico, Delft University of Technology
- Anna Felden, Delft University of Technology
- Domenico Lahaye, Delft University of Technology
- Jeroen van Oijen, Eindhoven University of Technology
- Dirk Roekaerts, Delft University of Technology

Organizing Committee

- Marjan Beekmans, Eindhoven University of Technology
- Domenico Lahaye, Delft University of Technology

PROGRAM OUTLINE

(Location of poster session and plenary sessions: De Kapel)

October 23 2024

16:30-19:00 *Poster session*
17:00-19:00 *NVV Members Meeting*
19:30-21:00 *Conference dinner*

October 24 2024

9:00 *Symposium opening*
9:15-10:45 *Keynote Lectures*

Nicolas Noiray

CAPS Laboratory, Mechanical and Process Engineering Department, ETH Zürich (Switzerland)

Combustion Dynamics in Hydrogen-fueled Aeroengines and Power Gas Turbines

Vincent Moureau

CNRS research fellow, CORIA Rouen (France)

Scale adaptive methods and acceleration techniques for LES of turbulent flames and interfaces

10:45-11:00 *Coffee break*
11:00-12:15 *Poster Session*
12:15-13:00 *Lunch*
13:00-13:50 *Plenary session*

Industrial combustion problems

The session on industrial combustion problems wishes to promote the dialogue between industry and academia and targets the challenges faced in computational investigations. In the plenary part, three short presentations with specific problem description and current approaches are given, followed by discussions with the audience. In the second part (parallel session) the focus will be on a dialogue to come to next steps in tool development and use via fruitful collaboration between academia and industry.

Presenters:
Josue Melguizo Gavilanes (Shell) on: ***Safety Concerns in Storing and Transporting Hydrogen***. The talk discusses the use of open-source CFD tools for the improved understanding of industrial hazards (accidental releases, dispersion, fire, explosions, etc.) with special attention to the case of hydrogen and ammonia.

Rudy Sadi (Almadouie-deRijke) on:
Building the Hydrogen Storage Infrastructure in the Arabian Gulf Region using Metal-Organic Frameworks.

Third presenter: to be confirmed

13:50-14:00 *Break*
14:00-16:20 *Parallel sessions*

Oral presentations of the selected contributed papers will be taking place in two parallel sessions. In a third session, the discussion related to industrial combustion problems will continue in a workshop format.

16:20-16:30 *Coffee break*
16:30-17:00 *Plenary session*

Results and recommendations of the industrial combustion workshop will be reported.
Then, the winner of the NVV Combustion Award 2024 will be announced. This award is given to the young expert with the best MSc thesis (obtained from a University in the Netherlands) in the field of combustion technology. The evaluation is done by a jury composed by the board of NVV.
Finally, the three best posters presented at the symposium will receive an award from the Dutch Section of the Combustion Institute (DSCI). The evaluation will be done by a jury composed by the board of DSCI.

17:00 *Symposium closing*

ABSTRACTS OF KEYNOTE LECTURES

Keynote lecture 1

By **Nicolas Noiray,**
CAPS Laboratory, Mechanical and Process Engineering Department, ETH Zürich (Switzerland)

Combustion Dynamics in Hydrogen-fueled Aeroengines and Power Gas Turbines

To decarbonize civil air transport and electric power generation, there is an urgent need for new technologies enabling clean combustion of sustainably-produced hydrogen. More specifically, the difficulty of achieving low nitrogen oxide emissions, while eliminating the risks of flashback and thermoacoustic instabilities calls for radically different burner designs when using hydrogen compared to kerosene and natural gas, because of its higher reactivity. In this context, a significant research effort is necessary for the development of these hydrogen-based combustion technologies. This presentation deals with the combustion dynamics and the emissions of hydrogen-air flames in different combustor concepts for aeronautic and power gas turbines: array of small premixed turbulent jet flames, premixed and non-premixed swirled flames, autoignition-stabilized premixed flames and lean azimuthal flames. Hydrodynamic and thermoacoustic stability of these flames are investigated with experiments and large eddy simulations. This presentation will highlight the diversity of scientific problems to tackle for achieving these combustion engineering challenges.

CV

Nicolas Noiray is Associate Professor at ETH Zürich, where he established the laboratory of Combustion, Acoustics & Flow Physics (CAPS) in 2014. He obtained his Ph.D. from the Ecole Centrale Paris in 2007, and then worked in the Gas Turbine Research Division of Alstom until his appointment at ETH. His theoretical, experimental and computational research activities in the fields of Combustion, Acoustics and Fluid Mechanics address fundamental and applied problems. He has received the Silver Medal and the Hiroshi Tsuji Early Career Researcher Award of the International Combustion Institute, and he was awarded a Consolidator Grant and a Synergy Grant by the European Research Council. A key theme of the research performed by his group is the modeling and control of instabilities at various time and length scales.

Keynote lecture 2

By **Vincent Moureau,**
CNRS research fellow, CORIA Rouen (France)

Scale adaptive methods and acceleration techniques for LES of turbulent flames and interfaces

Over the last decades, Large-Eddy Simulation (LES) has proven to be a valuable tool for the 3D unsteady simulation of a wide variety of flows. It is based on a scale separation, obtained by filtering the Navier-Stokes equations, in which the large scales are resolved while the impact of the small scales on the large scales is modeled. With the constant growth of computational power, the targetable scale range in LES continues to increase and motivates the development of scale adaptive methods such as Adaptive Mesh Refinement. Recent advances in numerical methods for tetrahedron-based meshes and parallel mesh adaptation strategies raise the attractiveness of unstructured grids. The use of tetrahedra has two advantages for practical configurations: complex geometries are easily meshed and the mesh is locally more isotropic than Cartesian grids. Combining this scale adaptivity to acceleration techniques such as i) Dynamic Cell Clustering based on Principal Component Analysis, ii) dynamic scheduling of chemistry stiff integration and iii) load balancing of Lagrangian droplets, substantial gains are obtained and enable the high-fidelity simulation of spray flames. The presentation will detail these recent algorithmic advances and illustrate their performances on different applications such as the CORIA Rouen Spray Burner (CRSB).

CV

Vincent Moureau is a CNRS (French National Center for Scientific Research) senior researcher at CORIA (Complexe de Recherche Interprofessionnel en Aérothermochimie). His research is focused on turbulent combustion and spray modelling, and on the development of the YALES2 solver for Large-Eddy Simulation and Direct Numerical Simulation of turbulent flows in complex geometries using massively parallel computers. This flow solver is now used by a large community of researchers and engineers for various applications such as aeronautics and space, renewable energies, bio-mechanics, process engineering. He received the Yves Chauvin award for his PhD thesis in 2005, the 3rd prize of the Bull Joseph Fourier award for the promotion of numerical simulation in 2010, an IBM faculty award in 2011, and the aeronautical and aerospace science award of the French Academy of Science in 2018.

COMBURA 2024: PROGRAM OF CONTRIBUTED PRESENTATIONS

ORAL PRESENTATIONS

October 24	SESSION I August	SESSION II De Kapel (main room)	SESSION III Louis
14:00-14:20	Stijn **Schepers**	Louisa **Castellanos**	WORKSHOP ON INDUSTRIAL COMBUSTION PROBLEMS
14:20-14:40	Alessandro **Ballatore**	Mihnea **Floris**	
14:40-15:00	Thijs **Bouten**	Boyan **Xu**	
15:00-15:20	**BREAK**	**BREAK**	**BREAK**
15:20-1540	Berksu **Erkal**	Wenjiang **Tian**	WORKSHOP ON INDUSTRIAL COMBUSTION PROBLEMS
15:40-16:00	Dario **Passato**	Mohamad **Fathi**	
16:00-16:20	Pablo **Rouco Pousada**	Jesse **Hofsteenge**	

Parallel Session I

FGM Modeling of Hydrogen Boundary Layer Flashback in a Turbulent Channel
Stijn Schepers, Jeroen van Oijen
Eindhoven University of Technology

Large-eddy simulation of high-pressure direct injections of hydrogen in argon-oxygen environment with tabulated chemistry
Alessandro Ballatore, Jeroen van Oijen
Eindhoven University of Technology

H2Flex: The Development of a Hydrogen Turbine Burner Prototype
Thijs Bouten*, Teja Donepudi**, Rene Pecnik**, Jurriaan Peeters**, Sikke Klein**, Lars-Uno Axelsson*
*Destinus Energy, **Delft University of Technology

THERMOACOUSTIC INSTABILITIES IN HYDROGEN-METHANE COMBUSTION: ANALYSIS OF SELF-EXCITED DYNAMICS IN A CYCLONE BURNER SYSTEM
Berksu Erkal, Jim Kok
University of Twente

THERMOACOUSTIC ANALYSIS OF A LABORATORY-SCALE COMBUSTOR
Dario Passato, Danilo Beli, Ines Lopez Arteaga
Eindhoven University of Technology

Investigation of kerosene-hydrogen mixtures: spray modelization and emissions analysis
Pablo Rouco Pousada, Kaushal Dave, Arvind Gangoli Rao, Ivan Langella
Delft University of Technology

Parallel Session II

Deep Learning Dynamical Latencies for the Representation of Complex Chemical Kinetics
Luisa Castellanos*,***, Rodolfo S. M. Freitas**, Alessandro Parente***, Francesco Contino*
*Université de Louvain, **Queen Mary University London, ***Université Libre de Bruxelles

Data-driven prediction and water injection-based prevention of flashback in a lean hydrogen reheat combustor
Mihnea Floris, Nguyen Anh Khoa Doan, Ivan Langella, Konduri Aditya
Delft University of Technology

Numerical simulation for the effect of hydrogen differential diffusion on premixed NH3/H2/N2 flame extinction
Boyan Xu, Rob Bastiaans
Eindhoven University of Technology

Experimental study on the combustion characteristics of millimeter-sized iron particles
Wenjiang Tian, XiaoCheng Mi, Yuriy Shoshin, Viktor Kornilov, Philip de Goey
Eindhoven University of Technology

Turbulence Effects On The NOx Suppression by Straining Lean Premixed Hydrogen Flames
Mohamad Fathi, Stefan Hickel, Anh Khoa Doan, Ivan Langella
Delft University of Technology

Combustion Dynamics of two Hot Blast stove designs: Flame Transfer Function analysis
Jesse Hofsteenge, Jim Kok
University of Twente

POSTER PRESENTATIONS
Poster sessions place and time
De Kapel, October 23, 16:30-19:00 and October 24, 11:00-12:15

Posters listed alphabetically on first author's name

Effect of coflow temperature on iron particle ignition.
Muhammed Abdallah, Giulia finotello, Yuriy Shoshin, Philip De Goey
Eindhoven University of Technology

Hydrogen combustion simulation using FGM
Lisa Bachmann*,**, Evert Bunschoten***, Nijso Beishuizen*
*Bosch Thermotechnology, **University of Stuttgart, ***Delft University of Technology

Thermoacoustic Analysis of Highly Strained Hydrogen Flames
Emre Böncü
Delft University of Technology

Hybrid CFD-CRN model for a micro gas turbine's combustor for emission prediction
Farshid Y. Farrokhi*,** , Alessandro Piscopo**,*, Alessandro Parente**, Ward De Paepe*
*Université de Mons, **Université Libre de Bruxelles

Predictive Models and Experimental Insights for NOx Emissions in Multi-Fuel Combustion Systems
Alam Uziel Garciduenas Correa, Kaushal Dave, Francesca de Domenico, Arvind Gangoli Rao
Delft University of Technology

A computational framework for plasma assisted process intensification
Duarte Gonçalves*, Anna Felden**, Margherita Altin*, Paola Diomede*
*Maastricht University, **Delft University of Technology

Preferential Concentration in Iron Powder Combustion - Analysis of Timescales
Shyam Sundar Hemamalini*, Benedicte Cuenot**, XiaoCheng Mi*
*Eindhoven University of Technology, **CERFACS

Numerical Investigations of a Trapped Vortex Hydrogen Burner
Tarun Hegde, Anna Felden, Sikke Klein
Delft University of Technology

STRATEGIES TO USE AMMONIA AS FUEL FOR RECIPROCATING INTERNAL COMBUSTION ENGINES
Isabelle Jacobs, Peter de Vos
Delft University of Technology

Numerical Analysis of Quenching Distance in Laminar Premixed Hydrogen and Methane Flames
Tahsin Berk Kiymaz*, Jeroen van Oijen*, Nijso Beishuizen**,*
*Eindhoven University of Technology, **Bosch Thermotechnology

Experimental study of autoignition behavior of methanol/syngas
MohammadReza Kohansal*, Anatoli Mokhov**, Sander Gersen***, Rob Bastiaans*
Eindhoven University of Technology, University of Groningen, DNV Company

Quenching Distance of Premixed Hydrogen-Air Flames
Dongliang Liu*, Jeroen van Oijen*, Yuriy Shoshyn*, Nijso Beishuizen*,**
*Eindhoven University of Technology, **Bosch Thermotechnology

Controlling Hydrogen Flames Through Magnetic Conditioning
Vaibhav Mysore Natesh
Delft University of Technology

What happens when the combustion is cooled by argon or xenon at 60 bar?
Sylwia Oles, Artur Pozarlik
University of Twente

Experimental Investigation of Flame Flashback in Hydrogen-Air Mixtures
Rafael Pichler, Mark Tummers, Sikke Klein
Delft University of Technology

Assessing turbulent transport and its modeling in hydrogen-argon and argon-argon mixing layers by means of direct, large eddy, and Reynold's-averaged Navier-Stokes numerical simulations
Diego Quan*, Nick Diepstraten*, Alessandro Ballatore*, Dirk Roekaerts**, Jeroen van Oijen*
*Eindhoven University of Technology, **Delft University of Technology

Direct numerical simulations of hydrogen-argon and argon-argon mixing layers.
Understanding the effect of the Lewis number in turbulent transport.
Diego Quan*, Dirk Roekaerts**, Jeroen van Oijen*
*Eindhoven University of Technology, **Delft University of Technology

Where does ignition happen? Direct numerical simulations of non-premixed hydrogen combustion at Reynolds numbers 5,000, 10,000 and 20,000
Diego Quan*, Dirk Roekaerts**, Jeroen van Oijen*
*Eindhoven University of Technology, **Delft University of Technology

Modelling woody biomass combustion in an industrial furnace
Anne Rikhof*, Jing Fu*, Pieter Koster*, Amir Mahmoudi*, Huub Ratering**, Artur Pozarlik*
*University of Twente, **HoSt

Combustion Optimization of Renewable DME and LPG Blends
Saket Sahu, Mohammad Mehrali, Artur Pozarlik, Jan Withag
University of Twente

Comparison of methods for thermoacoustic stability analysis of a hydrogen-fueled condensing boiler
Marc Shair Ali, Jesse Hofsteenge, Jim Kok
University of Twente

Exploring the Influence of Temperature on OH PLIF Absorption Spectra
André Silva Correia, Francesca de domenico, Arvind Gangoli Rao, Leonardo Castellanos, Francesco Mazza
Delft University of Technology

Design of Experiments Optimized Combustion and Emissions for OMEx-Diesel Blends on a Heavy-Duty Engine
Zhongcheng Sun, Harold van Beers, Michel Cuijpers, Bart Somers, Noud Maes
Eindhoven University of Technology

Fuel spray ignition simulations using a two-stage Lagrangian model with detailed chemistry
Yu Wang, Hesheng Bao, Bart Somers, Jeroen van Oijen, Noud Maes
Eindhoven University of Technology

Auto-igniting hydrogen injections in high-pressure nitrogen and argon environments
Giliam van der Wielen, Max Peters, Noud Maes, Nico Dam, Jeroen van Oijen
Eindhoven University of Technology

D. ABSTRACTS

(Alphabetical order according first author's name)

Large-eddy simulation of high-pressure direct injections of hydrogen in argon-oxygen environment with tabulated chemistry

A. Ballatore*, J. van Oijen
*a.ballatore@tue.nl
Department of Mechanical Engineering, Power & Flow, Eindhoven University of Technology., Groene Loper 5, 5612 AE, Eindhoven, The Netherlands

Abstract

Within the context of a global de-carbonization, hydrogen plays a significant role in the transition to low-carbon activities. In particular, the Argon Power Cycle (APC) is a revolutionary engine concept that circulates argon in a closed-loop configuration, burning only hydrogen and oxygen and thus rendering a zero-emissions system. The work at hand aims at providing a first step towards accurate and affordable modelling of such an engine in the high-pressure direct-injection (HPDI-H2) configuration. Leveraging on the large eddy simulation (LES) technique, coupled with a novel tabulated chemistry approach (HR-FGM), several injections of hydrogen at high pressure in an argon-oxygen atmosphere are performed. More in detail, parametric studies on the injection pressure, ambient temperature and ambient oxygen level are carried out and analysed in terms of ignition delay, flame dynamics and heat release rate. The corresponding results represent valuable insights towards the modelling of the APC.

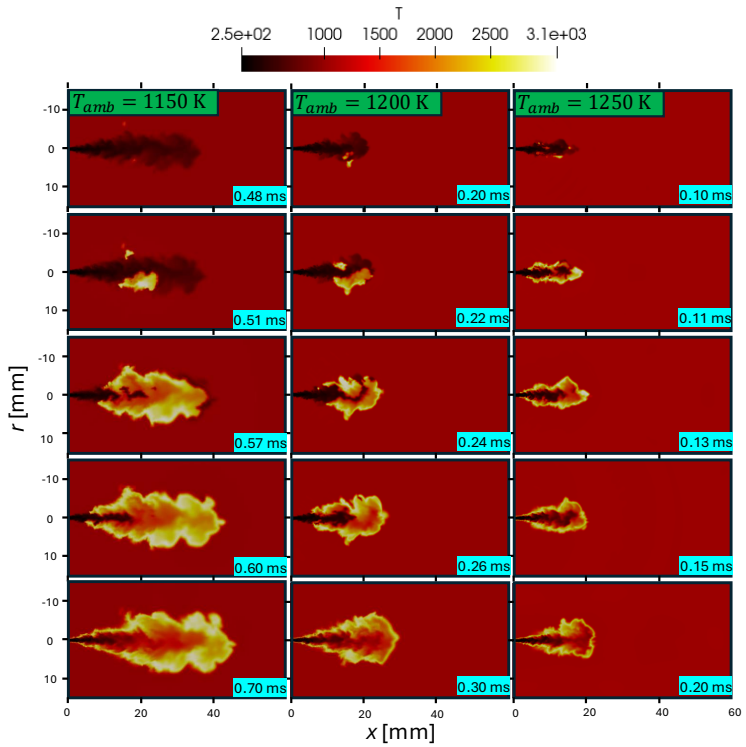


Figure 1: mid-plane contours of temperature [K] for three hydrogen injections with increasing ambient temperature.

Acknowledgements
This publication is part of the Argon Power Cycle project (project number 17868) financed by the Dutch Research Council (NWO).

THERMOACOUSTIC INSTABILITIES IN HYDROGEN-METHANE COMBUSTION: ANALYSIS OF SELF-EXCITED DYNAMICS IN A CYCLONE BURNER SYSTEM

Berksu Erkal* and Jim Kok**
e-mail of principal author
*b.erkal@utwente.nl
**j.b.w.kok@utwente.nl

Abstract

In today's world, the need to meet energy demands through cleaner and more sustainable methods has become essential across all sectors, including industrial furnaces and boilers. In this context, transitioning from methane, one of the most widely used fuels in industrial energy production, to hydrogen is a key goal in reducing carbon emissions. However, the adaptation and maintenance of existing industrial systems and subsystems for hydrogen combustion remain areas of ongoing research. One of the most critical challenges is ensuring that these furnaces can combust without experiencing thermoacoustic instability, using existing burners or with minimal modifications. As part of the DYNAF project, a combustor equipped with a cyclone burner capable of burning hydrogen and methane blends, with a capacity of 50 kW, has been designed to simulate current conditions. Additionally, an adjustable-length upstream tube has been integrated into the system to investigate the acoustic characteristics and combustion instabilities. This study examines the contributions of hydrogen addition to self-excited thermoacoustic activities in detail.

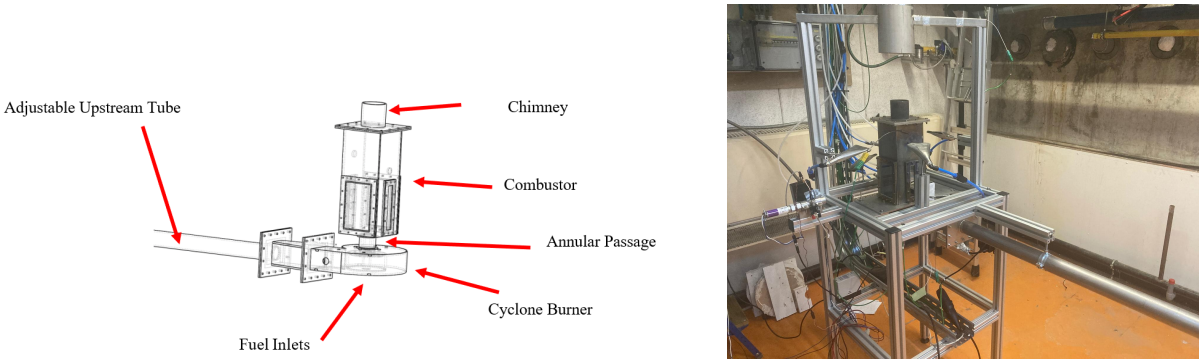
Introduction

Industrial furnaces can experience structural vibrations due to various reasons, which may lead to failures. Since changes in fuel composition directly affect combustion characteristics, a lab-scale combustor was developed to investigate low-frequency combustion dynamics that may occur during this energy transition. As shown in Figure 1, the self-excitation characteristics of the airflow were modified using an adjustable-length tube. The airflow then enters a cyclone burner to gain a swirling motion and combines with the fuel in the annular passage. The fuel is supplied through 12 holes with a diameter of 2 mm, positioned perpendicular to the flow.

In the annular passage, the airflow, now premixed with the fuel due to the swirling motion, burns in the combustor and exits through a chimney that narrows to one-quarter of its original area. During the experiment, pressure measurements are taken from four different points. One of these points is located at the inlet of the cyclone burner, while the others are positioned at distances of 50 mm, 100 mm, and 200 mm from the bottom of the combustion chamber. Additionally, as seen in Figure 1, high-speed camera measurements and photomultiplier measurements are performed through the available optical access windows.

Results

Due to the 2-page limit, not all figures and tables could be included. However, in addition to the 30 kW and 50 kW pure methane tests, six different hydrogen/methane blends with hydrogen molar fractions ranging from 20% to 100% were tested at 30 kW thermal power. As a result of these tests, the heat release rate measured by the photomultiplier tube was compared with the pressure measurements. In addition, spectral proper orthogonal decomposition (SPOD) analysis

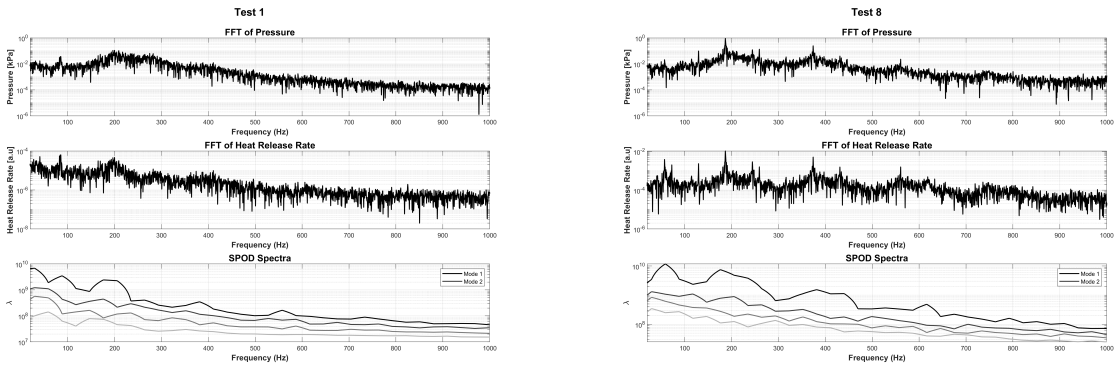


(a) Dynaf Combustor **(b)** Experimental Setup

Figure 1. Dynaf Combustor and Setup

was performed on the images obtained from the 7500 fps high-speed camera recordings[1],[2]. In these analyses, which have a 14 Hz resolution, the FFT of the SPOD energy matrix was taken and compared with the pressure and heat release rate data.

The similarity in dominant frequencies led to the conclusion that a single camera may be sufficient for thermoacoustic instability analysis, even if the data is not intensively provided. Moreover, it was observed that the addition of hydrogen increases thermoacoustic activities. The FFT comparison of one of the tests is presented in Figure 2 However, due to page limitations, the SPOD modes could not be included and will be shown during the presentation via video.



(a) Pure Methane Test **(b)** Pure Hydrogen Test

Figure 2. Experimental Results

References

[1] O. T. Schmidt, "Spectral proper orthogonal decomposition using multitaper estimates," *Theoretical and Computational Fluid Dynamics*, vol. 36, no. 5, pp. 741–754, 2022.

[2] O. T. Schmidt and T. Colonius, "Guide to spectral proper orthogonal decomposition," *AIAA Journal*, vol. 58, no. 3, pp. 1023–1033, 2020.

H2FLEX: THE DEVELOPMENT OF A HYDROGEN TURBINE BURNER PROTOTYPE

Thijs Bouten*, Teja Donepudi, Rene Pecnik**, Jurriaan Peeters**, Sikke Klein** and Lars-Uno Axelsson***
thijs.bouten@destinus.energy
*Destinus Energy, Hengelo, The Netherlands
**Delft University of Technology, Delft, The Netherlands

Abstract

With the phasing out of natural gas, hydrogen appears to be a cost-effective solution for continuing to use the gas grid, and at the same time to realize clean electricity and heat in the industry. Destinus Energy and TU Delft worked together in the H2Flex project on the development of the next-generation hydrogen combustion technology. This technology meets the future requirements of a cost-effective, ultra-low emission combustion system for the OP16 gas turbine that can operate on 100% natural gas and 100% hydrogen, and any mix thereof.

Approach

Destinus' radial swirl stabilized DLE combustor has been optimized. Various design variations have been created and tested in Destinus' atmospheric combustor test rig. It is operated in (partially) premixed mode to reduce emissions. This combustor has originally been designed for natural gas application [1]. The challenge of increasing the hydrogen operability is to do this without compromising efficiency (e.g. flashback combustion control and injection strategy), startup times, and emissions of NO_x.

The use of CFD is an integral component of the combustors' design and optimization process. The commonly used approaches are URANS and Scale-Resolving Simulations such as LES and hybrid RANS/LES methods. URANS models are widely used by industry due to their low computational costs. Hybrid models such as the algebraic WMLES reduce the need for mesh resolution close to the walls, leading to lower computational times than classical LES. In this approach, RANS formulation is used close to the walls, while a modified LES formulation

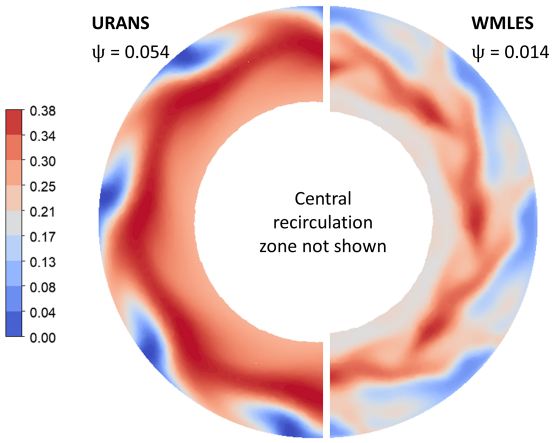


Figure 1. URANS (left) and WMLES (right) predictions of instantaneous equivalence ratio (ϕ) contour in pre-combustion plane

is used in the outer part of the boundary layer. More details of this modelling approach have been discussed in [2].

Results

The instantaneous fuel equivalence ratio contour at a typical flame location is shown in Figure 1 where the time-averaged mixing level is under-predicted by 74% in URANS compared to WMLES. The highly diffusive nature of hydrogen and high-density gradients in the system could lead to additional underlying physics, which are not accounted for by URANS-based methods, introducing uncertainty and limitations in the accuracy of predictions. This indicates the need for high accuracy mixing simulations to optimized combustor designs for low NO_x and flashback resistance.

Various combustor configurations have been tested in Destinus' atmospheric combustor test rig. It has been found that for the baseline (natural gas) combustor configuration, the amount of hydrogen is limited. An increased hydrogen contents, increases the NO_x emissions significantly, until flashback occurs at a specific hydrogen contents. By optimizing the fuel injector design, with a focus on the fuel mixing, 100% hydrogen operation has been achieved (Figure 2) while low NO_x emissions were maintained ($<$15 ppmv at 15% O_2)

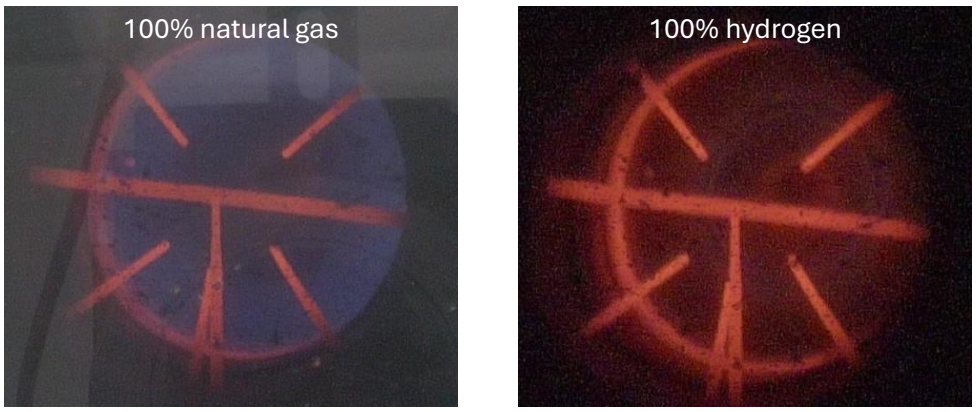


Figure 2. Comparison of natural gas and hydrogen flame during atmospheric testing of optimized combustor

Acknowledgement

The project has received financial support from TKI Energie under grant number: TKI-2021-H2-23.

References

[1] W. J. Ramaekers, F. A. Tap, T. Bouten, and L.-U. Axelsson, "Comparison of different cfd models for predicting emissions in an opra dle combustor," in *Proceedings of the ASME Turbo Expo 2019: Turbomachinery Technical Conference and Exposition*, (Phoenix, Arizona, USA), vol. Volume 4B: Combustion, Fuels, and Emissions, 2019.

[2] T. Donepudi, R. Pecnik, J. W. R. Peeters, S. Klein, T. Bouten, and L.-U. Axelsson, "Shear-Driven Hydrogen-Air Mixing in OP16 DLE Combustor: A Comparative Study Between URANS and LES," in *Proceedings of the ASME Turbo Expo 2024: Turbomachinery Technical Conference and Exposition*, vol. Volume 2: Ceramics and Ceramic Composites; Coal, Biomass, Hydrogen, and Alternative Fuels, 2024.

DEEP LEARNING DYNAMICAL LATENCIES FOR THE REPRESENTATION OF COMPLEX CHEMICAL KINETICS

L. Castellanos*, R. S. M. Freitas, A. Parente***, F. Contino*.**
luisa.castellanos@uclouvain.be
*Université Catholique de Louvain, École Polytechnique de Louvain, Institute of Mechanics, Materials and Civil Engineering, Ottignies-Louvain-la-Neuve, Belgium
**School of Engineering and Materials Science, Queen Mary University London, London, United Kingdom
***Université Libre de Bruxelles, École polytechnique de Bruxelles, Aero-Thermo-Mechanics Laboratory, Brussels, Belgium

Abstract

The efficient modeling of reactive flows is an ongoing research topic, due to their importance in industrial processes and the computational overhead from the chemical kinetics modeling, which increases exponentially with the number of chemical species under consideration. Therefore, dimensionality reduction can significantly improve such calculations.

With the increasing importance of Machine Learning (ML) applications, many techniques have been used to improve combustion science. Among these applications, dimensionality reduction takes place with techniques such as Principal Component Analysis (PCA) [1], Autoencoders (AEs) [2], etc. Among these, the application of Time-lag Autoencoders (TAE)[3] has been proven to efficiently reduce the dimensionality of mechanisms while providing a physical interpretation of the reduced manifold. However, TAE methodology has been applied to hydrogen combustion, therefore, this work aims to develop a further understanding of TAE application for complex mechanisms. TAE is strongly based on the AE structure, in which a state vector is fed to the network, which applies an encoding operation (E) to reduce dimensionality, producing a reduced manifold on a bottleneck layer. This reduced manifold goes through a decoding operation (D), and produces a reconstructed state as the output vector. The output of the AE network is the same input vector, while in TAE, the output is a time-shifted version of the input state vector (value in the following time-step).

For analyzing chemical mechanisms with many species, it is proposed to study specific subspaces representing different chemical pathways, or mixtures with different equivalence ratios. The analysis is performed for methane combustion with the GRI-mech 2.11 mechanism (31 active species). The composition sampling includes different equivalence ratios from $\phi \in [0.45, 1.25]$ varying by 0.2 at pressure $P_0 = 4.33$ atm and inlet temperature $T_0 = 1418$ K. All ignition cases will be reduced to a manifold size 3.

A TAE is trained for each ignition case according to the guidelines described in [3]. The obtained manifolds are analyzed to obtain the associated chemical species (chemical carriers [3]), and a permutation importance test will help to analyze their quality as parameters for the remaining chemical species while assessing a linear hypothesis. An importance index will be associated between each chemical species that is observed as an output of the model, and the chemical carrier working as an input. The index value is proportional to the chemical carrier quality as a parameter for the specific output. 9 chemical carriers are identified and available in Table 1. The ignition case with $\phi = 1.25$ is analyzed in detail. The permutation importance indexes are visualized in Figure 1. Each axis represents the permutation importance index for the associated chemical carrier, while each scatter point represents one of the parameterized chemical species. It is observed that most chemical species can be described by the chemical carriers or a combination of them.

Table 1. Chemical Carriers GRI-mech 2.11

ϕ	Chemical Carriers
0.45	O2, O2, O2
0.65	HO2, CO, OH
0.85	H, CH2OH, CH4
1.05	H, CH2OH, H
1.25	OH, CH3OH, CH3

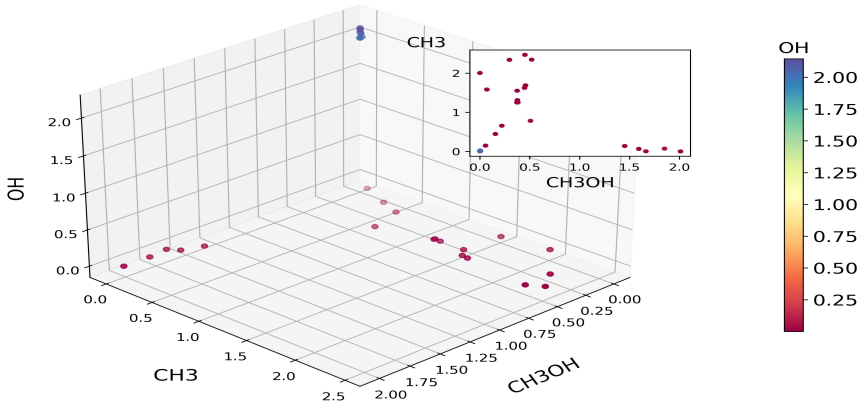


Figure 1. Permutation importance indexes for GRI-mech 2.11 mechanism ($\phi = 1.25$), the 3D scatter plot shows the three branches of sensitivities, according to the obtained chemical carriers; in small, the top view of the plot is available.

The identified species play a role in many important chemical reactions. As an example, CH3 is an important product of CH4 dehydrogenation and plays a role in CH4 formation through reactions N162 (CH3+CH3OH <=> CH2OH+CH4) and N163 (CH3+CH3OH <=> CH3O+CH4); this explains the appearance of CH2OH and CH3OH as chemical carriers. Radicals such as H, OH, and HO2 react with CH4, promoting oxidation. Therefore, chemical carriers are selected according to their role in the chemical reactions. A similar experiment is performed for the Aramco 2.0 mechanism; the experiment produces similar findings and allows a selection of 13 chemical carriers. Therefore, TAE has good capabilities for aiding efficient parametrization in chemical mechanisms while sampling the subspace in various kinetic regimes can provide chemical species that act as good parameters of the reactions' phenomena. Such chemical species can be used with adequate clustering to develop Reduced Order Models (ROMs); since they are strongly related to the chemical pathways present in the mechanism, they could be extrapolated to describe other subspaces with similar chemistry kinetics.

[1] J. C. Sutherland and A. Parente, "Combustion modeling using principal component analysis," *Proceedings of the Combustion Institute*, vol. 32, no. 1, pp. 1563–1570, 2009.

[2] P. Zhang and R. Sankaran, "Autoencoder neural network for chemically reacting systems," *Journal of Machine Learning for Modeling and Computing*, vol. 3, no. 4, pp. 1–28, 2022.

[3] L. Castellanos, R. S. M. Freitas, A. Parente, and F. Contino, "Deep learning dynamical latencies for the analysis and reduction of combustion chemistry kinetics," *Physics of Fluids*, vol. 35, no. 10, p. 107 143, 2023.

TURBULENCE EFFECTS ON THE NOX SUPPRESSION BY STRAINING LEAN PREMIXED HYDROGEN FLAMES

M. Fathi, S. Hickel, A.K. Doan, and I. Langella
e-mail of principal author: m.fathi@tudelft.nl
Delft University of Technology

Abstract

Ultra-lean combustion of hydrogen presents a feasible approach for reducing NOx emissions due to its potential to significantly lower the adiabatic flame temperature. However, numerous practical challenges, including flame blow-off, flashback, and thermoacoustic instabilities, limit its effectiveness as a single solution. These challenges require alternative methods to achieve efficient reduction in NOx under real-world conditions.

One promising strategy is to leverage the unique ability of hydrogen to withstand extremely high strain rates, unlike hydrocarbons. This property can be effectively utilized to limit NOx generation. Studies, such as those by Porcarelli et al. [1], have shown that increasing the tangential strain rate of the flame can effectively suppress NOx formation in hydrogen/air combustion. This suppression is primarily achieved by redistributing and shortening the lifespan of intermediate radicals, which are critical in the NOx formation process.

Previous investigations in this area have predominantly focused on laminar flows, leaving the impact of turbulence on NOx suppression largely unexplored. Therefore, the objective of this study is to examine the effectiveness of NOx suppression by straining under highly turbulent conditions. To comprehensively capture the effects of turbulence on NOx formation, we performed direct numerical simulation (DNS), employing a detailed NOx reaction mechanism.

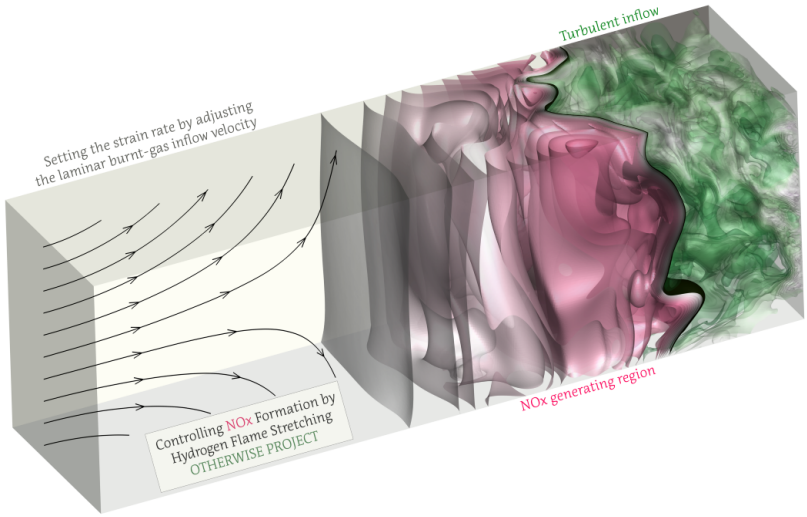


Figure 1. DNS of turbulent counterflow premixed hydrogen flame under intensive strain

To achieve this objective, a series of DNS simulations were conducted on turbulent reaction-to-product counterflow flames. The configuration involved two opposed rectangular nozzles, 3 x 4 mm in size, separated by a 12 mm gap. The flow setup consisted of a turbulent stream of premixed reactants, with an average inflow velocity of 10 m/s and a temperature of 300 K, supplied through the right nozzle. Turbulence was generated using an advanced digital filter

method, based on an integral length scale of 1 mm and a turbulent intensity of 40%. On the opposite side, a laminar stream of hot combustion products was introduced, with varying inflow velocities but at a fixed temperature of 2030 K. The bulk strain rate was adjusted by modifying the velocity of this laminar stream, while turbulent flow conditions remained unchanged. The reactant composition was set using an equivalence ratio of 0.7, and the composition of the combustion products was derived from equilibrium free-flame calculations assuming complete combustion for the reactant composition.

For the numerical analysis, the computational domain was discretized using a grid with $576 \times 192 \times 144$ points, and a minimum grid spacing of 20 μm was used to ensure sufficient resolution of key flow characteristics. The reacting compressible Navier-Stokes equations were solved, incorporating variable thermo-transport properties and a finite-rate chemistry model to accurately capture the combustion dynamics. Chemical reactions were modeled using the Sanchez-Williams hydrogen-air mechanism [2], coupled with the Capurso NOx formation mechanism [3], which involves 15 species and 37 elementary reaction steps, providing a detailed representation of both combustion and pollutant formation processes. Boundary conditions were carefully handled using an advanced reacting Navier-Stokes Characteristic Boundary Condition (NSCBC) treatment to ensure the stability and accuracy of the simulation.

For this DNS-based investigation, we utilized our in-house flow solver INCA (www.inca.cfd). The results clearly demonstrate that increasing the tangential flame strain effectively reduces NOx emissions under turbulent conditions. Through detailed analysis of DNS data and reaction pathways, we identified the primary mechanisms contributing to NOx suppression at high strain rates, even amidst turbulence. These insights provide a promising direction for the development of cleaner combustion strategies that exploit the unique properties of hydrogen under turbulent conditions.

References

[1] A. Porcarelli, B. Kruljević, and I. Langella, "Suppression of nox emissions by intensive strain in lean premixed hydrogen flamelets," *Int. J. Hydrog. Energy*, vol. 49, pp. 413–431, 2024.

[2] A. L. Sánchez and F. A. Williams, "Recent advances in understanding of flammability characteristics of hydrogen," *Prog. Energy Combust. Sci.*, vol. 41, pp. 1–55, 2014.

[3] T. Capurso, D. Laera, E. Riber, and B. Cuenot, "Nox pathways in lean partially premixed swirling h2-air turbulent flame," *Combust. Flame.*, vol. 248, p. 112 581, 2023.

DATA-DRIVEN PREDICTION AND WATER INJECTION-BASED PREVENTION OF FLASHBACK IN A LEAN HYDROGEN REHEAT COMBUSTOR

M. Floris*, I. Langella*, K. Aditya and N. A. K. Doan***
M.Floris@tudelft.nl
*Faculty of Aerospace Engineering, Delft University of Technology, Delft, Netherlands
**Department of Computational and Data Sciences, Indian Institute of Science, Bengaluru, India

Introduction

Hydrogen will play a key-role in the decarbonization of combustion-based energy conversion and propulsion systems. However, hydrogen increases the risk of flashback and it therefore becomes crucial to develop techniques which can predict the onset of flashback with sufficient warning time to allow for mitigating action. In previous work [1], a promising data-driven technique which combines Co-Kurtosis PCA and modularity-based clustering was shown to be efficient in identifying precursors of flashback. Co-K PCA was used to obtain a a latent reduced representation of the reacting system, while modularity-based clustering could identify precursors in this reduced representation. However, that work did not investigate whether the precursor could provide sufficient warning time to prevent the full effects of flashback. This aspect is investigated in the present study through the use of water injection, timed with the identified precursors, to prevent the flashback.

Test case and Methodology

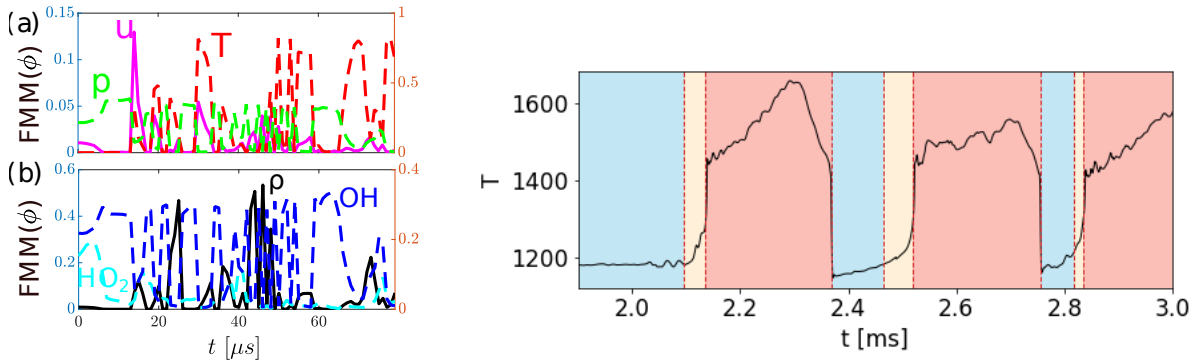
The configuration considered here is a simplified version of Anslado Energia's GT36 reheat combustor, operating at a pressure of 20 atm, with an inflow velocity of 200 m/s and a temperature of 1180 K. The incoming reactants consist of premixed hydrogen and air with an equivalence ratio of 0.35, which are stabilized through autoignition. Under these conditions, an intermittent flashback behaviour is observed, caused by pressure waves induced compressive heating in the mixing duct. The simplified combustor is simulated using LES, with a numerical setup as described in [2].

The simulation ran for a time long enough to acquire 8 flashback events. Then, a region near the inception of the early autoignition event on the mid spanwise plane was sampled for the co-kurtosis PCA method. In this method, a feature moment metric (FMM) is computed for each of the variables, determining their contribution to the overall kurtosis, and thus their importance for the apparition of extreme events. After the reduced representation is obtained, the modularity based clustering method is applied to the time-series of the identified variables sampled at the step location of the combustor. Here, a phase space representation is constructed, followed by tessellation into hypercubes, with the purpose of reducing the number of possible states the system can be in. A probability transition matrix, $\boldsymbol{P}$, is then computed and interpreted as a weighted and directed graph. Here, modularity-based clustering is applied. This algorithm maximizes modularity, where the greater the deviation from a random network created with the same degree sequence as the original graph, the higher the resulting modularity score. Using the newly obtained clusters, the precursor clusters are finally identified and used as an early indicator of an incoming flashback.

Results

In the feature reduction step, the co-kurtosis PCA method was applied to the full thermochemical state (all nine species mass fraction, temperature, pressure and density) and the components

of velocity. Following the procedure, the most important features [T, u, p , ρ, HO_2, OH] emerge based on their high values for the FMM, as shown in Figure 1 a). These features show a high activity before the inception of the flashback and confirm the physical intuition of the cause of the event. The time-series of these features are then used in the modularity-based clustering algorithm, where the extreme trajectories are defined as those for which $T > 1300$ K. It is then possible to estimate the time between the moment the combustor enters the precursor cluster and when it enters the extreme clusters, resulting in a mean prediction time of $t_{pred} = 32.1$ μs.



(a) **(b)**

Figure 1. a) Evolution of the FMM of the scalars of interest during a typical flashback event. b) Time-series of temperature where the background color indicates the type of cluster (blue: normal, orange: precursor and red: extreme)

The prediction time found using the proposed methodology gives sufficient warning time to take preemptive measures to suppress the propagation of the flame further into the mixing duct. This is demonstrated here using water injection. For this purpose the prediction time associated with the 2nd flashback shown in Figure 1 b) is used to time the water injection into the mixing duct through six sprays placed at the inlet. As shown from Figure 2, the water travels to the autoignition location before its inception and manages to stop it from travelling any further upstream.

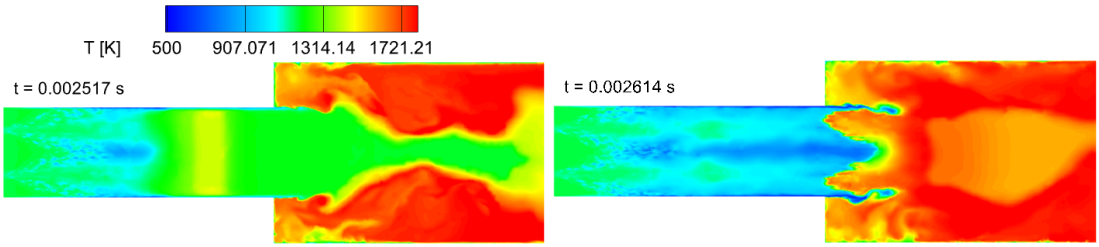


Figure 2. Contour of temperature showing the effect of the water spray on the flashback

[1] M. Floris, T. Shiva Sai, D. Nayak, I. Langella, K. Aditya, and N. A. K. Doan, "Data-driven identification of precursors of flashback in a lean hydrogen reheat combustor," *Proceedings of the Combustion Institute*, vol. 40, no. 1, p. 105 524, 2024.

[2] P. Rouco Pousada, N. A. K. Doan, K. Aditya, M. Düsing, A. Ciani, and I. Langella, "Flashback Prevention in a Hydrogen-Fueled Reheat Combustor by Water Injection Optimized With Global Sensitivity Analysis," Turbo Expo: Power for Land, Sea, and Air, vol. Volume 3B: Combustion, Fuels, and Emissions, V03BT04A003, 2024.

COMBUSTION DYNAMICS OF TWO HOT BLAST STOVE DESIGNS: FLAME TRANSFER FUNCTION ANALYSIS

J.W. Hofsteenge* and J.B.W. Kok
j.w.hofsteenge@utwente.nl
*Thermal Engineering, University of Twente, Enschede, The Netherlands

Abstract

The forced response of two different hot blast stove burner designs is determined. This is done by forcing the flow by perturbations in fuel mass flow rate and monitoring the response in terms of the heat release rate (HRR). The resulting flame transfer function (FTF) describes this response in terms of the gain and phase. A great deal of literature on the FTF is available for gas turbine systems, which exhibit combustion dynamics in the 100-500 Hz range. Due to the large size of hot blast stoves, the coupling between combustion and acoustics in these systems normally occurs below 100 Hz. The hot blast stoves are characterised by lengths of 30 m and diameters of 5 m and are fired by the low-calorific exhaust gas of the blast furnace. The fluid domain of the stoves is reduced by means of symmetry in periodicity, in order to keep the computational cost within a feasible range. The reacting flow is simulated using the SAS-SST URANS turbulence model and a non-adiabatic, diffusion flamelet-based FGM model for combustion. To reduce the computational cost further, the flow is forced using a superposition of four sine waves at distinct frequencies. Results show two very different flame shapes, due to the difference in burner dimensions. The larger C1 produces a much longer flame than C2 with a more distributed HRR. The FTFs similarly show differences: Burner case C1 is more responsive in terms of the gain over a larger frequency range than C2. The combustion time delay is also longer for C1 than C2: 50 ms to 30 ms, respectively.

Method

The two different burner designs are shown in Fig. 1, denoted C1 and C2. C1 has 20 fuel inlets and one large central air inlet. In C2, the air and fuel inlets are split into 9 fuel slits and 8 air slits, which then each split again left and right in an alternating fashion, resulting in a chequerboard pattern.

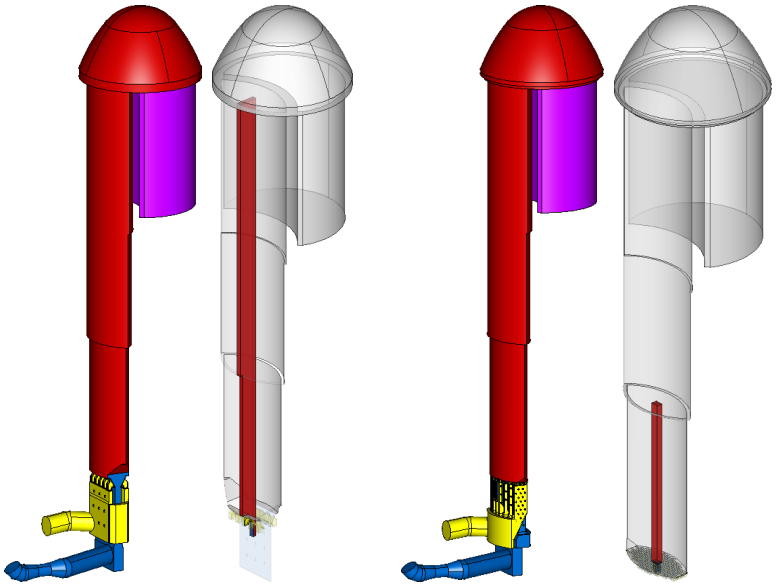
The axial velocity is forced at the domain inlet according to:

$$\tilde{u}_x(\vec{x},t) = \bar{u}_x(\vec{x})\left(1 + \frac{A}{N}\sum_i^N \sin(2\pi f_i t)\right). \tag{1}$$

In Tables 2a and 2b, the N forcing frequencies of each simulation are shown.

Results Highlights

From contours of the HRR it was found that the flame in C1 is much longer than that of C2. There, the flame is anchored at the wall, in the dead zone in between the fuel and air inlets. In Figure 4 the average HRR as a function of the convective time delay from the fuel inlet is plotted. This shows that the HRR is much more distributed and farther towards the tip of the flame in C1. This is in contrast with C2, where the maximum HRR is near the root of the flame, similar to a laminar non-premixed flame [1].



(a) Case C1 (b) Case C2

Figure 1. Overview of the total geometry (left) and reduced CFD fluid domains (right) of C1 and C2. The air inlet, fuel inlet and combustion chamber are coloured blue, yellow and red, respectively.

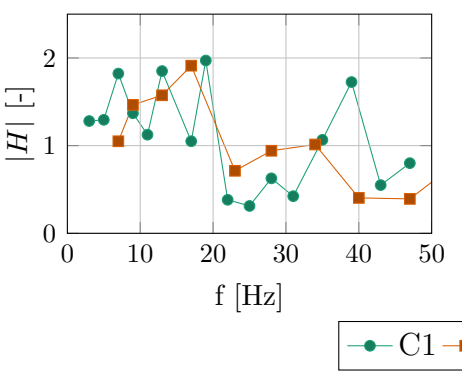
Table 2. Forcing frequencies applied in the simulations.

(a) Case C1

Sim	f_1	f_2	f_3	f_4
B1	3	5	11	19
B2	7	9	13	17
B3	22	25	35	39
B4	28	31	43	47

(b) Case C2

Sim	f_1	f_2	f_3	f_4
B1	7	9	13	17
B2	34	40	47	51
B3	23	28	83	91
B4	59	67	75	101



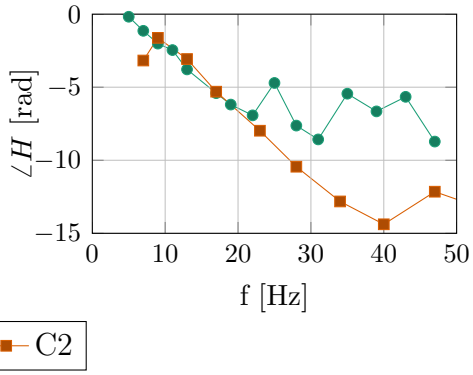


Figure 3. Gain (left) and phase lag (right) of the FTF for case C1 and case C2.

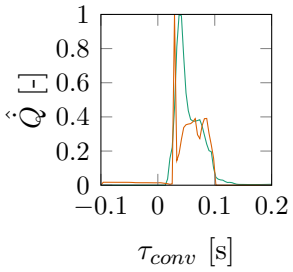


Figure 4. Normalised HRR distribution as function of the convective time delay from fuel inlet.

The resulting FTF is shown in Figure 3. Both cases show excess gain at frequencies below 20 Hz. Additionally C1 shows a peak at around 40 Hz. In terms of the phase, both cases have a constant initial slope of the phase (between 0 and 15 Hz for C1 and between 0 and 30 Hz for C2) that is very comparable between the two cases. The corresponding time delay, defined as $\tau = |\angle H|/(2\pi f)$, is approximately 0.05 s for C1 and 0.03 s for C2. Beyond 15 Hz, the phase of C1 starts to level off at around 2π. The same effect was seen in previous studies on other bluff-body non-premixed flames [2].

References

[1] N. Magina, V. Acharya, and T. Lieuwen, "Forced response of laminar non-premixed jet flames," Progress in Energy and Combustion Science, vol. 70, pp. 89–118, 2019.

[2] S. Klein, "On the acoustics of turbulent non-premixed flames," Ph.D. dissertation, University of Twente, Enschede, The Netherlands, 2000.

THERMOACOUSTIC ANALYSIS OF A LABORATORY-SCALE COMBUSTOR

Dario Passato*, Danilo Beli*, Ines Lopez Arteaga*
d.passato@tue.nl
*Department of Mechanical Engineering, Eindhoven University of Technology, 5612AE, Netherlands

Abstract

This abstract presents a comprehensive investigation of the thermoacoustic behavior of a 50 kW laboratory-scale cyclone burner using both experimental and numerical methods. The study addresses the fundamental problem of thermoacoustic instabilities, which can lead to destructive oscillations in combustors. These instabilities arise due to the interaction between the flame's heat release and the acoustic field within the combustion chamber. Understanding these phenomena is critical for the development of more efficient and stable combustion systems [1–3].

The system's geometry and boundary conditions are modeled using a finite element approach to solve the Helmholtz equation in the frequency domain. The model provides insight into the system's natural acoustic modes and identifies key frequencies where instabilities are most likely to occur. These results are compared with experimental data obtained from unforced oscillations observed during burner operation.

Numerical Methods and Experimental Validation

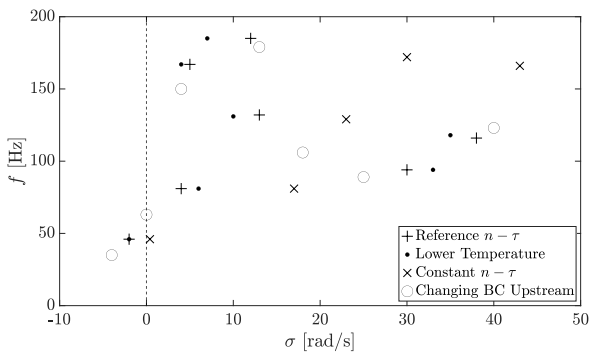
The finite element model (FEM) employs the Helmholtz equation to compute the acoustic pressure distribution within the combustor. Boundary conditions, such as impedance and flow conditions, are carefully defined to simulate real operational conditions. The introduction of a thermoacoustic source based on the $n - \tau$ flame transfer function allows us to capture the feedback mechanism between the flame and the acoustic field. The $n - \tau$ model parameters are extracted from computational fluid dynamics (CFD) simulations, which provide an accurate representation of the flame dynamics [4]. To evaluate the system's stability, we compute the complex eigenvalues of the modes. The real part of the eigenvalue corresponds to the growth or decay rate of oscillations, while the imaginary part gives the frequency. Unstable modes (with positive real parts) indicate regions where thermoacoustic instabilities may occur.

Experimental validation is conducted using pressure transducers placed in the combustion chamber to measure the acoustic pressure fluctuations. The system exhibits natural oscillations at specific frequencies, which are compared with the frequencies predicted by the FEM. The comparison shows good agreement, particularly for the lower-order modes, validating the accuracy of the numerical model.

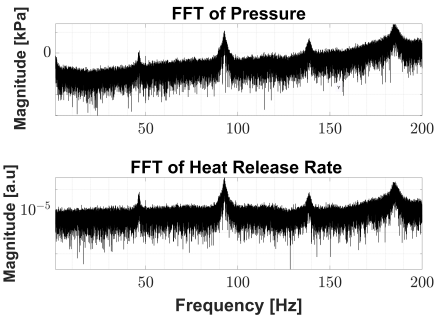
Results and Conclusions

The stability of the system is studied by searching for the complex eigenvalues. Referring to Fig. 1a, it is evident that reducing the combustor temperature (from 1500K to 1200K) does not affect the eigenvalue frequencies. This is expected, as the low-frequency modes observed correspond to oscillations in the long upstream duct and the temperature profile inside the combustor has minimal influence on these modes.

More significant effects are observed when modifying the parameters of the $n - \tau$ model and the upstream boundary conditions. With constant parameters of $n = 1$ and $\tau = 2.7 \times 10^{-3}$, substantial changes in the eigenvalue distribution occur, affecting both the real and imaginary



(a) Thermoacoustic System Eigenvalues



(b) Experimental Natural Oscillations Combustor

Figure 1. Comparison of Numerical Eigenvalues with Natural Oscillations Measurements

parts. Additionally, switching the upstream boundary condition from an open to a closed end further alters the eigenvalues. These results highlight the importance of accurate modeling of both the flame transfer function and the upstream boundary conditions for studying system stability, as oscillations predominantly occur in the upstream duct.

Considering these observations, comparisons with measurements from natural oscillations in the combustor, under the same conditions as the simulations, are possible. As shown in Fig. 1b (with pressure measurements taken via a downstream microphone), the odd modes identified in the simulation (*Reference* $n - \tau$ in Fig. 1a) are excited during natural oscillations. Peaks at 45 Hz, 90 Hz, and 136 Hz suggest that an unstable odd mode excites other odd harmonics. However, further research on the flame transfer function and upstream boundary condition frequencies, alongside an experimental campaign with multiple pressure acquisition points, is required for a complete system analysis.

The current model shows promising results: the harmonics from the natural oscillations align with the first identified mode. However, the model is sensitive to variations in upstream boundary conditions and the $n - \tau$ model parameters. Therefore, a combined numerical and experimental investigation is needed to evaluate the flame's response to upstream velocity fluctuations and validate the interaction index and time lag. Additionally, a deeper study of the upstream boundary conditions is necessary to improve accuracy.

References

[1] S. Candel, "Combustion dynamics and control: Progress and challenges," *Proceedings of the Combustion Institute*, vol. 29, pp. 1–28, 1 2002.

[2] F. Culick and P. Kuentzmann, "Unsteady motions in combustion chambers for propulsion systems," *NATO, Research and Technology Organization*, 2006.

[3] T. C. Lieuwen and V. Yang, "Combustion instabilities in gas turbine engines: Operational experience, fundamental mechanisms, and modeling," *American Institute of Aeronautics and Astronautics*, 2005.

[4] J. W. Hofsteenge and J. B. W. Kok, "Numerical analysis of swirl variation effect on cyclone burner flame transfer function," *29th International Congress on Sound and Vibration*, 2023.

INVESTIGATION OF KEROSENE-HYDROGEN MIXTURES: SPRAY MODELIZATION AND EMISSIONS ANALYSIS

P.Rouco Pousada*, K.A. Dave*, A. Gangoli Rao* and I. Langella*
p.roucopousada@tudelft.nl
*FPT department, Faculty of Aerospace Engineering, Delft University of Technology

Abstract

The growing emphasis on environmental sustainability has prompted a significant shift in the power generation sector, moving away from conventional fossil fuels towards more sustainable alternatives. Among these, hydrogen emerges as a promising solution for clean energy generation. However, hydrogen combustion presents major challenges, such as the formation of relatively high levels of nitrogen oxides (NOx), which have a high global warming potential [1]. Moreover, hydrogen is characterized by a wide flammability range, a very high flame propagation speed, and high diffusivity and reactivity [2]. Compared to natural gas, these properties impose more stringent requirements on combustor design [3]. In addition, hydrogen storage in aircraft is challenging due to the very high pressures required or the low temperatures needed to maintain it in liquid form. This means that fully hydrogen-powered aircraft face significant challenges, both in terms of combustion design and storage systems.

Before the development of fully hydrogen-powered aircraft, blending hydrogen with conventional aviation kerosene offers a practical approach to integrating hydrogen into aviation fuel [4]. Currently, TU Delft is engaged in research focused on developing a fuel-agnostic combustor capable of efficiently operating with hydrogen, kerosene, or a combination of both fuels. Since emissions from kerosene combustion are closely linked to the quality of fuel atomization, studying and controlling fuel spray properties are critical for designing and improving the performance of a multi-fuel combustor. Previous research at TU Delft has emphasized the utility of simple planar imaging techniques based on Mie scattering to measure droplet size and motion. This data is now being used to refine and validate CFD simulations of this multi-fuel combustor. The experimental droplet quantities are compared to numerical simulations with the aim of verifying key modelling choices, such as droplet distribution and associated parameters like the Sauter Mean Diameter (SMD) and the models employed. This information is then applied to simulate various engine-relevant operating conditions, including scenarios with pure kerosene, pure hydrogen, and a mixture of both fuels, in order to assess the effect on flame stability and emissions.

Methodology

The Mie scattering results are shown in **Figure 1 (left)**. The recorded intensity of scattered light depends on factors such as the intensity of the incident light sheet, collection angle, signal attenuation before collection, and the scattering cross-section. Therefore, analyzing the Mie-scattered images under these assumptions yields a relative size distribution of the droplets in the spray, which can then be used to derive the probability density function (PDF) and cumulative distribution function (CDF), as shown in **Figure 1 (center)**.

The spray model is evaluated and compared with experimental data using particle tracking velocimetry (PTV) for deeper insights. **Figure 1 (right)** presents the CFD simulation results, showing the positions of the injected droplets within the domain. The Sauter Mean Diameter (SMD) is estimated using empirical or semi-empirical models from the literature [5] and validated through this comparison. Once the spray model is established, simulations with kerosene

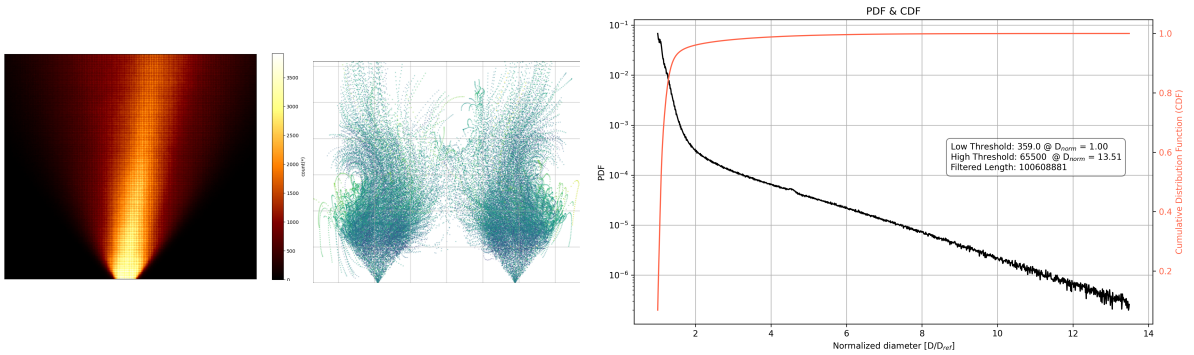


Figure 1. Left: Visualization of the particles detected on the Mie scattering analysis. Center: CFD simulation of the spray injected into the combustion chamber. Right: CDF and PDF of the distribution of particles detected by the Mie Scattering analysis.

and hydrogen are conducted. These simulations use Large Eddy Simulations (LES) with a Thickened Flame Model and Conjugate Heat Transfer. The results are compared with experimental data from TU Delft and sensitivity analyses of emissions and flame shape are performed. The power is kept the same on all the cases.

Results

Preliminary analysis of the spray data suggests that the droplet size distribution can be approximated by a Rosin-Rammler distribution, with an SMD ranging from 20 to 35 m. This range is consistent with predictions in the literature. While the parameters defining the Rosin-Rammler distribution are still being refined, early simulations show a close match to the experimental results in terms of particle distribution and velocity profiles within the combustor.

In the combustor simulations, the pure kerosene flame is characterized by two lobes and high CO emission levels. For the pure hydrogen flame, where the fuel enters the combustor fully premixed with air, a central flame is formed. This flame is expected to produce no CO emissions but higher NOx levels due to the elevated combustion temperatures. When hydrogen and kerosene are mixed, a central flame forms within the shear layers, resulting in an increased evaporation rate of kerosene droplets due to recirculation zones. Smaller droplets, with a lower Stokes number, follow the recirculation flow more effectively, enhancing mixing compared to larger kerosene droplets, which tend to be convected downstream. In this scenario, CO emissions decrease compared to pure kerosene combustion, but NOx emissions rise. Further comparisons between the standard kerosene burner and the hydrogen-kerosene mixture will be conducted.

[1] G. Lammel and H. Graßl, "Greenhouse effect of nox," *Environ. Sci. Pollut. R.*, vol. 2, 1995.

[2] A. C. Benim and K. J. Syed, *Flashback Mechanisms in Lean Premixed Gas Turbine Combustion*. Elsevier Academic Press, 2014.

[3] J. Strohle and T. Myhrvold, "An evaluation of detailed reaction mechanisms for hydrogen combustion under gas turbine conditions," *Int. J. Hydrogen Energy*, vol. 32, no. 1, 2007.

[4] X. Hui, C. Zhang, M. Xia, and C.-J. Sung, "Effects of hydrogen addition on combustion characteristics of n-decane/air mixtures," *Comb. and flame*, vol. 161, no. 9, 2014.

[5] A. H. Lefebvre and V. G. McDonell, *Atomization and Sprays*. CRC Press, 2017.

FGM MODELING OF HYDROGEN BOUNDARY LAYER FLASHBACK IN A TURBULENT CHANNEL

Stijn N.J. Schepers* and Jeroen A. van Oijen*
s.n.j.schepers@tue.nl
*Mechanical Engineering, Eindhoven University of Technology, Eindhoven, the Netherlands

Abstract

Introduction

Due to hydrogen's high reactivity most premixed combustion systems are sensitive to flame flashback. In the work of Endres et al. [1], flashback limits in a turbulent channel at two conditions, Re $= 9722$ and Re $= 19444$, are obtained numerically using an implicit LES approach with detailed chemistry. They compared their outcomes to the experimental results of Eichler et al. [2]. In this work, the flashback limit at Re $= 9722$ is reproduced using a Flamelet Generated Manifold (FGM) [3] approach to model the chemistry, enabling a significant reduction in simulation time.

Numerical Model

Before flashback limits can be determined, a cold flow solution with fully developed turbulence is needed as a base for the reactive simulation.

Cold Flow Simulation

The rectangular domain as a length $L = 6\delta$ and width $W = 3\delta$ with δ being the half channel height with a value of $\delta = 8.75$ mm, which is in line with the experiments of Eichler et al. [2]. The mesh size is chosen such that the y^+ at the boundary is less than unity, corresponding to a fully resolved boundary layer. The subgrid scale (SGS) turbulence is modeled using the WALE turbulence model, which has proven to be accurate for wall bounded flows. To fully develop the turbulent flow, cyclic boundary conditions are prescribed at the inlet and outlet, and a bulk velocity $\bar{U} = 10$ m/s is enforced via a pressure gradient over the channel length.

Reactive Simulation

The chemistry is modeled using the Flamelet Generated Manifold (FGM) method [3]. To account for heat losses to the channel walls and local changes in mixture composition due to the preferential diffusion, a 3D-manifold is spanned by running flamelets for a varying inlet enthalpy and equivalence ratio. The corresponding control variables are a progress variable, enthalpy and mixture fraction. The preferential diffusion terms in all control variables are modeled by reducing the full term to solely the contributions of a limited set of major species: H, H_2 and H_2O. A schematic of the reactive case is depicted in Figure 1. This set up is very similar to the work of Endres et al. [1]. Slices of the turbulent velocity field obtained from the cold flow solution are fed to the inlet and the outlet pressure is fixed at ambient. The top wall is entirely isothermal and the lower wall is half isothermal and half adiabatic. By doing this, the flame is able to stabilize on the border between the isothermal and adiabatic wall, as depicted by the orange lines. The equivalence of the mixture is increased until the flame is able to cross this border and propagate through the boundary layer towards the inlet. This equivalence ratio is defined as the flashback limit.

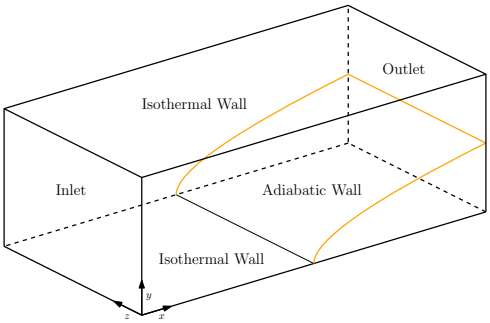
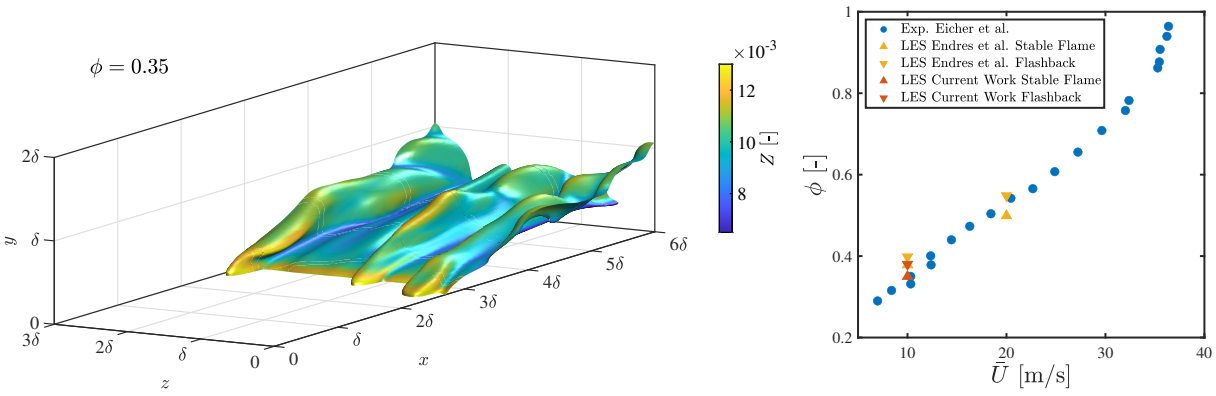


Figure 1. Schematic figure of the reactive simulation case.



(a) **(b)**

Figure 2. Snap shot of the flames surface at flashback colored with mixture fraction (a) and flashback limits of experiments [2], numerical results [1] and the results of the current work (b).

Results & Conclusion

In Figure 2a, the flame surface at flashback is depicted. It can be observed that the flame is able to cross the isothermal boundary through the boundary layer at this equivalence ratio ($\phi = 0.35$). This limit is shown in Figure 2b together with experimental results of Eichler et al. [2] and the implicit LES results with detailed chemistry of Endres et al. [1]. The numerical model in this work, using implicit LES and FGM chemistry, is able to reproduce the detailed chemistry simulations at much lower cost and predict the flashback limit in a rectangular channel at $\bar{U} = 10$ m/s with reasonable accuracy.

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References

[1] A. Endres and T. Sattelmayer, "Large Eddy simulation of confined turbulent boundary layer flashback of premixed hydrogen-air flames," *International Journal of Heat and Fluid Flow*, vol. 72, pp. 151–160, 2018.

[2] C. Eichler, G. Baumgartner, and T. Sattelmayer, "Experimental investigation of turbulent boundary layer flashback limits for premixed hydrogen-air flames confined in ducts," *Journal of Engineering for Gas Turbines and Power*, vol. 134, no. 1, 2012.

[3] J. A. van Oijen, A. Donini, R. J. Bastiaans, J. H. ten Thije Boonkkamp, and L. P. de Goey, "State-of-the-art in premixed combustion modeling using flamelet generated manifolds," *Progress in Energy and Combustion Science*, vol. 57, pp. 30–74, 2016.

Experimental study on the combustion characteristics of millimeter-sized iron particles

W. Tian[1], Y. Shoshin[1], V. Kornilov[1], L.P.H. de Goey[1], X.C. Mi[1,2]

w.tian2@tue.nl, x.c.mi@tue.nl

[1] Power & Flow Section, Department of Mechanical Engineering, Eindhoven University of Technology, Eindhoven, The Netherlands
[2] Eindhoven Institute of Renewable Energy Systems (EIRES), Eindhoven University of Technology, Eindhoven, The Netherlands

Abstract

Iron powder is considered a promising clean cycle fuel. For better utilization of iron particles for power generation as well as designing new combustors, the fundamentals of single iron particle combustion process should be understood. Current research is mainly focused on micrometer-sized iron particles, which is mainly because they are more suitable for use in power generation. However, due to the short combustion time scales and small particle sizes of micron-sized iron particles, it is difficult to visualize the combustion behavior in situ as well as to collect particles with different levels of oxidation to analyze their internal composition and structure. This limits the understanding of the combustion mechanism of iron particles to a certain extent. Therefore, we experiment with millimeter-sized iron particles to further understand the combustion mechanism of iron from longer burning time and more macroscopic visualization. In this work, we use a laser to ignite an isolated millimeter-sized iron particle and record the morphology and temperature change process through optical diagnosis. After combustion, we collect the iron oxide to do some material characterization to analyze their internal structure and composition. The combustion mechanism of iron particles is further discussed in terms of some combustion characteristics, formation of oxides, and the reaction process of oxygen with the particles. The results will enable us to further understand the iron particle combustion mechanism and provide more data to the theoretical modeling of iron combustion.

Figures

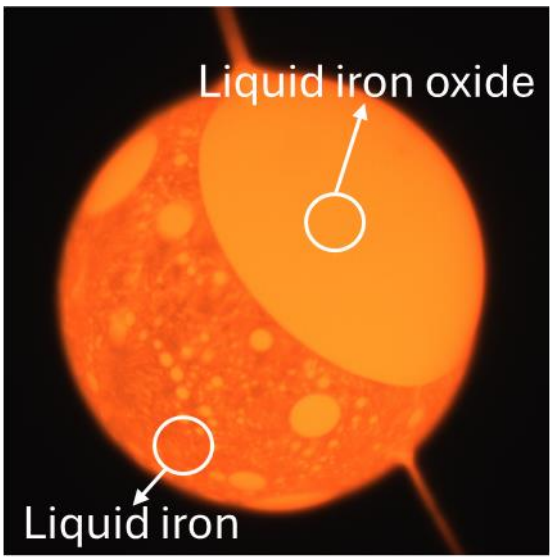

Figure 1. Immiscibility on the surface of iron droplets

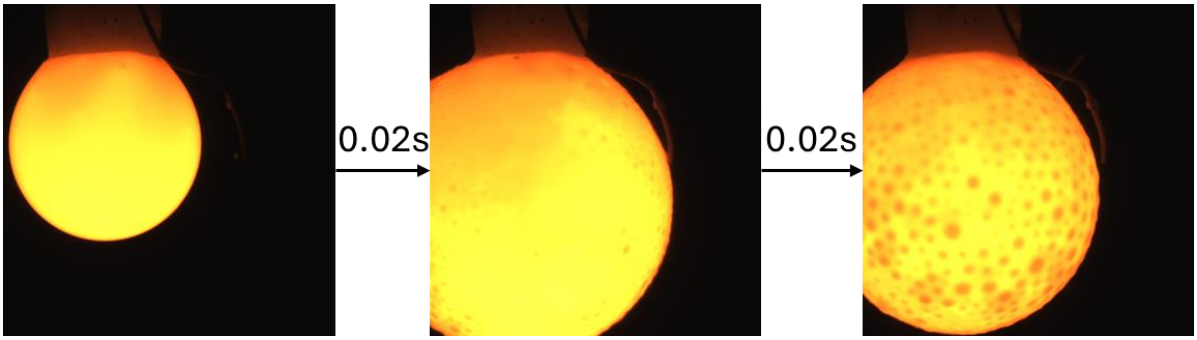

Figure 2. Rapid expansion of particle volume during combustion

NUMERICAL SIMULATION FOR THE EFFECT OF HYDROGEN DIFFERENTIAL DIFFUSION ON PREMIXED NH3/H2/N2 FLAME EXTINCTION

B. Xu* and R.J.M. Bastiaans*
b.xu1@tue.nl
*Power and Flow, Department of Mechanical Engineering, Eindhoven University of Technology, Eindhoven, The Netherlands

Abstract

Different blow-off behaviour was previously observed in premixed bluff-body stabilized flames with different ammonia/hydrogen/nitrogen blends, highlighting their different response to strain rate, and the role of rapid $\mathrm{H_2}$ consumption, which may be caused by the non-unity Lewis number effect of $\mathrm{H_2}$ and preferential diffusion. To study these effects on flame extinction, the Lewis numbers of species were artificially modified in 1D simulation for twin laminar premixed counterflow flame under different fuel blends, which is the fundamental counterpart that can easily be resolved. The results show that the non-unity Lewis number effect of $\mathrm{H_2}$, more accurately, the mass diffusivity of hydrogen is the main factor to determine the extinction strain rate. The high mass diffusivity of hydrogen makes the $\mathrm{NH_3/H_2/N_2}$ flames more resilient to extinction with increasing laminar flame velocity. In contrast, while preferential diffusion does not significantly change the laminar flame velocity, it makes extinction easier. However, preferential diffusion plays an important role in flame temperature only with a high $\mathrm{NH_3}$ ratio.