FEATURED LECTURE - AI in Combustion
PLENARY LECTURE BY PROF. MATTHIAS IHME

Tuesday's Plenary Lecture on the status and challenges of machine learning (ML) applications in combustion was delivered by the brilliant Prof. **Matthias Ihme** (Stanford University and SLAC National Accelerator Laboratory, United States). It covered relevant topics such as introducing physical constraints on out-of-the-box ML tools. The virtues of foundation models were examined, accompanied by compelling case studies. AI (artificial intelligence) was described as a co-pilot to aid brainstorming and formulating research hypotheses. Finally, the Plenary assuaged any fear that AI will take our jobs (at least in the near-term), with Gemini 1.5 2024 not performing well enough to pass a PhD qualifying exam.

During the coffee break, we talked to Prof. Ihme about some of our curiosities…

How long have you used AI?
This started a while ago- during my PhD (which he got in 2008), where I developed an interest in neural networks and implemented a NN algorithm in Fortran 90 to replace conventional chemical tabulation. The novel idea at that time was to optimize the NN architecture, what is now know as hyperparameter optimization.

Besides his interest in AI applied to combustion research, Prof. Ihme suggests to rely on physics as much as possible, especially in data-sparse environments: physics-enhanced approaches might be a better solution to avoid "hallucinating" answers from AI. Also, as a scientist, he would "feel sad" to eliminate the physics entirely…

What do we need to make the most of ML and should we be concerned about its extensive application?
We need big data to train models. Some companies specialize in ML advancements to provide ML "challenges" and benchmark cases to test and train models for. As part of this, they often provide free storage space that we should exploit for data sharing. In this respect, we should bear in mind that model training is very energy intensive. Therefore, the sharing of ML-model architectures and weights more broadly wouldn't require regenerating them, which would also make AI applications greener. On the other hand, I trust that energy-efficient computing will make substantial progress over the next few years and dedicated hardware architectures will also help with reducing energy consumption from AI applications.

A packed house for Prof. Matthias Ihme's Plenary Lecture!

Prof. Matthias Ihme (Middle) with session chairs
Profs. Alessandro Parente (Left) and Terese Løvås (Right).
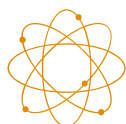
SCIENTIFIC HIGHLIGHTS

AI APPLIED TO FUEL DESIGN, AS EXPLAINED BY PROF. MANI SARATHY

Tuesday was AI day! After the Plenary Lecture, the morning's Topical Review, delivered by Prof. **Mani Sarathy** (KAUST, Saudi Arabia), focused on AI applications to fuel design. His talk provided an overview of early correlations developed for fuel properties and then moved to ML applications and challenges including the selection of molecular descriptors, GNN from large quantum mechanics datasets, fuel candidate selection for multicomponent mixtures, and uncertainty quantification.

After the talk, we were able to ask Prof. Sarathy some questions...

Are there already examples of novel fuels that have been designed using AI?
When it comes to individual components, it's a matter of screening different molecules to see which of them are potential fuel candidates. Designing new fuel mixtures, however, is novel and possible only with artificial intelligence.

What are the primary challenges faced when applying AI in fuel design?
Lack of data is a major issue. In the fuels and combustion field, the data available for machine learning models is much smaller compared to other domains. This scarcity makes it challenging to quantify the uncertainty of model performance on new chemical functionalities.

You mentioned lack of data, is this a call for experimental groups around the globe to provide such experimental data for fuel properties so we can better train our AI models?
Absolutely. In AI, you need open data sharing. You need larger databases, and in the combustion community there's few examples of this, but we need much more common databases. This is true for experiments but also for physics-based simulations.

How do you see the role of AI evolving in the field of fuel design over the next decade?
The uncertainty quantification aspects of being able to improve predictions with known uncertainty bounds for fuel design will be useful. And I think the hybrid approach combining AI methods with traditional physics-based modeling to give us interpretable AI will be more common.
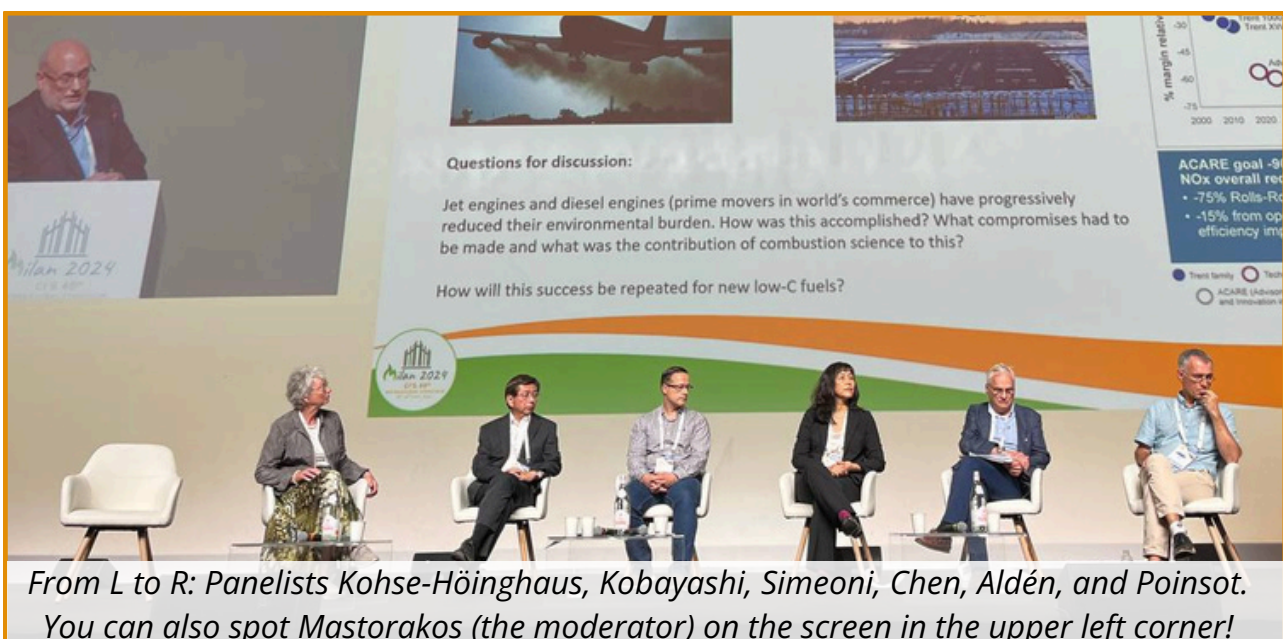
SPECIAL PANEL DISCUSSION SESSION

COMBUSTION RESEARCH AND IMPACT - PAST, PRESENT AND FUTURE

The first special panel session organized to celebrate the **70th Anniversary of The Combustion Institute** was held Tuesday afternoon in the Silver Room, and dealt with the past, present, and future of combustion research. To discuss the past, senior panelists were chosen -while future prospects will be dealt with more in detail in the panel on the future of combustion research on Thursday. Chaired by Prof. **Epaminondas Mastorakos**, introduced by videos with insights from Profs. **Derek Bradley** and **Forman Williams**, the session was guided by five selected speakers with long expertise in a variety of topics: **Marcus Aldén** (diagnostics), **Jacqueline Chen** (DNS/numerical combustion), **Hideaki Kobayashi** (gas turbines), **Katharina Kohse-Höinghaus** (chemistry), **Thierry Poinsot** (LES), and **Albert Simeoni** (fires).

Each of the panelists briefly introduced the past statuses and challenges of specific topics in a few minutes, then some researchers in the audience expressed their opinions and asked questions. Discussion topics were quite broad and included low emissions, CFD advancements, fires and safety, new fuels such as hydrogen, ammonia, biofuels, metals. Throughout the day, polls were conducted on the future of fuels in different applications and results were presented during the session. Opinions varied broadly; However, researchers agree that 1) hydrogen probably won't be "the" choice for marine applications in the future, 2) JET fuels and biofuels will probably be the most used in aviation in the future, and 3) power generation and heating will rely more and more on hydrogen as time goes on. Researchers also predict that future research focus will be more applied. i.e., TRLs between 3 and 6 - to Prof. Mastorakos' surprise. However, panelists did encourage scientists who like fundamentals to go for a "pen and paper" theoretical approach too!

From L to R: Panelists Kohse-Höinghaus, Kobayashi, Simeoni, Chen, Aldén, and Poinsot. You can also spot Mastorakos (the moderator) on the screen in the upper left corner!

COFFEE TALKS

SCIENTIFIC HIGHLIGHTS, AS CHOSEN BY ATTENDEES

Scientific discussion proceeded very fruitfully at the Poster Sessions and coffee break! Let's read about the impressions of young Symposium researchers:

Aysu Ozden and **Laura Donato** (Ph.D students, Université Libre de Bruxelles, Belgium):

"As young researchers in the multi-fidelity simulations and machine learning applied to the combustion applications, we came to the Symposium with high expectations of finding interesting discussion points and inspiration for our research, especially as these are relatively new topics. We found very inspiring this morning's Plenary! We are enthusiastic about the discussion held with other scientists after the oral presentation on possible application of our research and the opportunity of future collaboration"

Vincenzo Rosati and **Vicente Castro** (Ph.D students, Federico II and National Research Council, Napoli, Italy):

"The Early Career Mixer was amazing! We enjoyed the time together, the scientific discussion, but also singing the karaoke todos juntos! It was a wonderful opportunity to connect culturally with people from different parts of the world. As a Chilean, we consider that the instance of sharing beyond science is always important."

COFFEE TALKS

AN INDUSTRY PERSPECTIVE

Tuesday's Plenary Lecture reflected the most innovative advancements we are experiencing in all research fields and, of course, in combustion: the application of AI techniques to boost the energy transition and the main potentiality of machine learning methods to extrapolate knowledge from all the fields of interest.

Building on the reflections of the morning lecture, during the coffee break we had the interesting point of view from the industrial perspective of **Alessandro Della Rocca** (Tenova, Italy). He pointed out the several key aspects related to the effective exploitation of the AI techniques in different industrial sectors. From his perspective, AI could strongly help the automation of control processes and support the modeling stages of industrial equipment, especially during the screening phase before the development of prototypes. He wishes, as future perspectives, AI could also make feasible the application of LES in the development and analysis of industrial equipment, by reducing its computational cost.

SOCIAL EVENTS - ECR MIXER
MONDAY NIGHT FUN

The CI's Early Career Researchers (ECR) Mixer was held on Monday night at Politecnico di Milano (POLIMI), bringing together early career students and researchers in a vibrant and engaging outdoor venue. The event started with a warm welcome speech from the main organizer of the event, Prof. **Matteo Pelucchi**, followed by Prof. **Isabella Nova**, who shared the visionary aspirations of POLIMI. Then, Prof. **Wenting Sun** introduced the Early Career Advisory Committee and played a video message from Dr. Jenni Sidey-Gibbons, detailing her experience with becoming a successful combustion scientist and achieving her current position with the Canadian Space Agency.

After the speeches, the food and bar opened! Attendees enjoyed a lively atmosphere, mingling and exchanging ideas. Even the most shy PhD students broke the ice while playing table tennis, table football, and cornhole toss (thanks to the organizer for their home-made game!). The event culminated in entertaining activities including a trivia quiz, arranged and moderated by the lively Andrea Locaspi, leaving everyone with fond memories and new connections. But the best was yet to come... Isabella Branca kicked off the karaoke, and everyone grouped together, singing and dancing in front of the stage. Besides Tullio and Isabella, this author has no comment on the quality of the singing... Unfortunately, at 11 pm our lively guests were kicked out of POLIMI, though some attendees continued chatting at the closest brewery!

The mixer provided a unique platform for networking, learning, and having fun, reinforcing The Combustion Institute's commitment to fostering a supportive community for early career professionals. See you next time!

Attendees enjoy some karaoke at the Early Career Researcher Mixer!

SOME MORE PHOTOS FROM THE ECR MIXER!

SOCIAL EVENTS - WiC LUNCHEON
CONNECTING AS A COMMUNITY

A great Women in Combustion (**WiC**) Luncheon was held on Tuesday! Open and free to all registered participants of the Symposium, the event aimed to foster networking, collaboration, and mutual support among women in combustion from around the globe. Sponsored by King Abdullah University of Science and Technology (**KAUST**) and The Combustion Institute, the event was enthusiastically attended by academics, students, young researchers and industry professionals, who participated in insightful discussions contributing to the future of combustion research. **Maria Alzueta** started off the event, highlighting the combustion community's growing commitment to supporting women in this field. She invited **Katharina Kohse-Höinghaus** on stage, the former and **first female President of The Combustion Institute**. She shared relevant statistics about the community of women in the combustion field, and she reinforced the CI's ongoing mission to empower women to shape the future of combustion research.

Then the lunch started! The event was organized by dividing the participants into different tables, mixing young and senior attendees, from diverse countries and with different expertise. During the lunch, several key discussion topics were addressed, each highlighting different aspects of the professional experiences and challenges faced by women in combustion. These spanned **from future perspectives in combustion research to personal experiences and challenges**, as well as rising issues, such as work-life balance and implicit biases. Participants emphasized the need for clear and respectful communication within research teams to ensure that all voices are heard and valued. The value of mentorship in career development was a focal point of discussion. One of the most impactful outcomes of the event was the **proposal of a mentoring initiative**. Attendees were encouraged to volunteer as mentors or mentees, to build the support network within the WiC community. We closed the event with a great group photo, which you can see below!

SOME MORE PHOTOS FROM THE WiC LUNCHEON!

What is the Symposium Tribune? It's a daily bulletin that will keep you updated on all the key highlights and events happening at the Symposium, including interesting scientific talks and interviews to speakers, organizers, awardees. You will also find opinions from participants, and insights into social events in case you can't make it!

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Feedback is always welcome, and can be submitted via Telegram: https://t.me/CombustionSymposium2024/2