

SEMINAR

Challenges in Modeling Ammonia Combustion Using Methodologies Originally Designed for Hydrocarbons

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Context – The use of ammonia (NH_3) as a fuel for internal combustion engines has attracted increasing attention due to its carbon-free nature and established global production infrastructure. However, modeling NH_3 combustion using frameworks originally developed for and validated with hydrocarbon fuels presents significant challenges due to fundamental differences in chemical kinetics and combustion behavior, particularly when the goal is to accurately predict nitrogen oxide (NO_x) and nitrous oxide (N_2O) emissions. Ammonia (NH_3) is attracting interest as a carbon-free fuel for internal combustion engines, but modeling its combustion with frameworks developed for hydrocarbons poses significant challenges. Key differences in chemical kinetics — particularly the role of nitrogen-centered intermediates such as NH_2 , NH , and atomic nitrogen — lead to inaccurate predictions of ignition, flame propagation, and $\text{NO}_x/\text{N}_2\text{O}$ emissions.

Abstract – Dr. Cosmin Dumitrescu will discuss the research performed at West Virginia University towards the development of a 0D framework capable of predicting nitrogen-based emissions when NH_3 is used as fuel, neat or blended with another fuel. The model is built upon the SI Engine Zonal Simulator (SI EZS) in ANSYS Chemkin-Pro and extends its simplified flame-sheet representation by integrating additional reactors into a multi-stage reactor network. This configuration enables the modeling of detailed combustion and post-combustion kinetics, including reactions of unburned mixture released from crevices and during exhaust processes, while maintaining the low computational cost of the original SI EZS framework. The proposed approach allows the analysis of key reaction pathways influencing NH_3 consumption and nitrogen-based emissions and supports rapid evaluation of engine operating strategies such as equivalence ratio, spark timing, and engine speed.

Short Speaker Biography – Dr. Cosmin Dumitrescu is a Professor in the Mechanical, Materials, and Aerospace Engineering Department at West Virginia University, USA. He holds a PhD in Mechanical Engineering from The University of Alabama, Tuscaloosa. His field of specialty is thermal and fluid sciences, with a focus on experimental, computational and modeling research in fuels and highly efficient combustion systems for power generation and propulsion.

Info:

- **Where:** Aula Magna di Ingegneria
- **When:** Monday 22 June, 10:00 – 11:00
- The seminar will also include an overview of ongoing research at WVU on zero-carbon fuels and internal combustion engines, and available opportunities for thesis projects or student exchanges in these fields.