

## Wolfson Department of Chemical Engineering Seminar

Monday, July 3<sup>rd</sup>, 2023 at 13:30

Room 6

### Automated Kinetic Model Generation of NH<sub>3</sub> and NH<sub>3</sub>/H<sub>2</sub> Combustion

**José María Velasco**

Grand Technion Energy Program

**MSc Seminar**

Advisor: Asst. Prof. Alon Grinberg Dana

Department of Chemical Engineering, Technion-Israel Institute for Technology

In the current renewable energy landscape, there has been a growing interest in studying the potential and versatility of ammonia as an energy carrier, serving as a viable alternative to conventional fossil fuels. Multiple research has been done to study ammonia and its chemistry by generating and testing kinetic models of ammonia combustion. Although several models have been proposed over the past five years, it's still evident that there are still discrepancies in species thermochemistry and kinetic parameters which causes a complex and difficult situation amongst scientists when it is necessary to decide on which one to use.

With the aim of overcoming this notable challenge, an innovative approach to kinetic model building is proposed. The present work focuses on generating, for the first time, a chemical kinetic model for the oxidation of ammonia and ammonia/hydrogen mixtures using a data centric approach. Using state of the art software tools and methods like the Reaction Mechanism Generator (RMG) developed at MIT, and the Automated Rate Calculator (ARC) developed in our group, we generated and refined a chemical kinetic model for ammonia combustion. This model includes top of the line data and computations that encompass all the available knowledge in the field currently available.

Furthermore, we will present a thorough sensitivity analysis and validation of the kinetic model, incorporating diverse experimental setups and varying conditions. Subsequently, a comprehensive discussion will be presented, highlighting the conclusions drawn from the analysis and addressing the potential, challenges, and future for this innovative approach.

Refreshments will be served at 13:15.