הטכניון - מכון טכנולוגי לישראל

TECHNION - ISRAEL INSTITUTE OF TECHNOLOGY

הפקולטה להנדסה כימית
ע״ש וולפסון
The Wolfson Department of Chemical Engineering

Wolfson Department of Chemical Engineering Seminar

Monday, February 10th, 2025, at 14:00

Room 6

Automated Chemical Kinetic Model Generation of an Oxygenated Biofuel: Furfuryl

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MSc Seminar

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The global transition to sustainable energy has highlighted biofuels as promising alternatives to fossil fuels, offering the potential to mitigate greenhouse gas emissions. Among these, oxygenated furan compounds, such as furfuryl, stand out due to their renewable origin and favourable combustion properties (high energy density and potential applicability in spark-ignition (SI) engines). However, the limited availability of comprehensive kinetic models for furfuryl significantly hinders the understanding of its combustion behaviour and the optimization of its use in energy systems.

The present study addresses this critical gap by focusing on the development of a detailed and predictive chemical kinetic model for furfuryl combustion. Leveraging cutting-edge automated tools such as RMG (Reaction Mechanism Generator) and ARC (Accurate Rate Calculator), we accurately computed reaction rate coefficients and captured key reaction pathways under operational conditions. Our approach integrates high-level ab initio calculations and automated parameter refinement to deliver an accurate and reliable predictive model, validated against experimental data.

In this talk, I will present the predictive kinetic model developed for furfuryl combustion, showcasing its alignment with experimental findings and its ability to uncover the reaction mechanisms of other oxygenated furan biofuels. By advancing the understanding of these fuels, this research contributes to the broader effort to the design of tailored furan-based fuels for advanced engine technologies.

Refreshments will be served at 13:15.