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 13:30

Room 6

Automated Chemical Kinetic Modeling of Surrogate ScramJet Fuels: Thermolysis and Combustion

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MSc Seminar

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One of the primary challenges in designing efficient scramjet engines is controlling the vehicle's temperature. Another closely related challenge is minimizing heat losses to maximize energy conversion into useful thrust. One potential solution is to use an "endothermic hydrocarbon fuel" to insulate the combustion chamber from the cold atmosphere. This approach involves subjecting the fuel to pyrolysis around the combustion chamber, allowing the fuel to absorb heat by breaking chemical bonds. The resulting pyrolysis products are then combusted, thereby retaining the released thermal energy within the system.

A major gap in designing such systems is the challenge to identify the exact composition of the pyrolysis products that constitute the mixture that undergoes combustion. To address this, a chemical kinetic model of the thermolysis process is required to predict the composition of the actual mixture entering the combustion. Understanding the thermal decomposition of jet fuel, which consists of many components, presents a complex challenge. Surrogate fuels are commonly used for modeling complex fuels due to their efficiency and controllability.

This study focuses on the automated generation of a chemical kinetic mechanism for the thermolysis of a surrogate fuel mixture composed of seven large fuel molecules: n-dodecane ($C_{12}H_{26}$), n-undecane ($C_{11}H_{24}$), 2,3-dimethyldecane ($C_{12}H_{26}$), 2,4-dimethylundecane ($C_{13}H_{26}$), decalin ($C_{10}H_{18}$), 1,2-dicyclohexylethane ($C_{14}H_{26}$), and octyl butanoate ($C_{12}O_2H_{24}$). Several advanced computational tools were employed in this study. The Reaction Mechanism Generator (RMG) was utilized to automatically generate chemical kinetic mechanisms based on known rate rules and reaction templates. Additionally, the Automated Rate Calculator (ARC) was used to automate electronic structure calculations relevant to chemical kinetic modeling, enabling accurate predictions of reaction pathways and rates.

Refreshments will be served at 13:15.