Singapore Section of the Combustion Institute

SSCI | Young Combustion Researchers Webinar

Model development for surrogate fuels: From reaction class method to automated generation and optimization

Dr. Jiaxin Liu

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Time: September 28, 2026, 17:00 Singapore

Host: Dr. Shangpeng Li (National University of Singapore)

Zoom meeting: https://nus-sg.zoom.us/s/87932445619

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ABSTRACT

Practical transportation fuels contain hundreds or even thousands of chemical components, making it impractical to include every constituent in a detailed chemical kinetic model. The surrogate fuel approach represents these complex fuels using a limited number of representative components selected to reproduce their key combustion characteristics. Reliable kinetic models for these surrogate components are therefore essential. This work begins with kinetic model development for large alkanes and oxygenated fuels using the reaction class method, focusing on *n*-decane as a representative large alkane and ethyl tert-butyl ether (ETBE) as a high-octane oxygenated fuel component. However, applying the reaction class method to numerous, structurally diverse surrogate components requires repetitive effort and complicates consistent rate rule assignment across fuels. This limitation motivated the advancement of model development to automated mechanism generation and rate rule optimization. The MAMOX++ framework was extended and upgraded in this work to generate detailed models for large hydrocarbons with minimal manual intervention, as demonstrated for linear and branched alkenes, while Optima++ was employed to optimize their rate rules consistently within prior uncertainty limits. Optimized models reproduce experimental data across different conditions and capture the reactivity trends among different alkene structures and chain lengths. Overall, automated generation and optimization improve the efficiency and transferability of kinetic model development for complex surrogate fuels.

ABOUT THE SPEAKER



Dr. Jiaxin Liu is an incoming Research Fellow at the National University of Singapore, working with Prof. Huangwei Zhang. He completed his doctoral research at the Combustion Chemistry Centre, University of Galway in 2026 under the supervision of Prof. Henry J. Curran. His research focuses on combustion chemistry and detailed chemical kinetic modeling of surrogate fuel components, particularly large alkanes, alkenes and oxygenated fuels. His doctoral work combined experimental measurements and kinetic modeling to investigate ignition chemistry and kinetic interactions in fuel blends. A central theme was the progression from reaction class method to automated generation and rate rule optimization. He extended the MAMOX++ framework for automated generation of alkene mechanisms and integrated it with Optima++ to optimize rate rules against experimental data. He also contributed to the development of core combustion chemistry in C3MechV4.0.1 and GalwayMech2.0. His work aims to improve the predictive capability and transferability of kinetic models across different fuel structures and combustion conditions. He received the 2026 BOC Postgraduate Award at the University of Galway in recognition of excellence in his doctoral research.