International Conference on Numerical Combustion
Rome, Italy, October 14-17, 2025
www.icnc2025.com

Coupling virtual chemistry with filtered tabulated chemistry, a new approach to predict NOx in turbulent hydrogen combustion chambers

Etienne ESPADA[1]*, Samuel Dillon [2], Benoît Fiorina [1]
*Lead presenter: etienne.espada@centralesupelec.fr
[1] EM2C Laboratory, CNRS, CentraleSupélec, Université Paris-Saclay, 8-10 rue Joliot-Curie, 91190 Gif sur Yvette, France
[2] Safran Tech, Digital Sciences & Technologies Department, Rue des Jeunes Bois, Châteaufort, Magny-Les-Hameaux 78114, France

Hydrogen combustion in aircraft engines presents new challenges regarding engine operability and pollutant emissions. Novel injection systems are required, often leading to flame structures exhibiting multiple combustion regimes. To simulate and design such injectors, engineers require computational tools capable of capturing flame dynamics and predicting NO emissions with reasonable computational cost. The filtered tabulated approach has proven to be a reliable turbulent combustion model for predicting flame structure and has been recently extended to multi-regime combustion[1].

However, due to the different timescales governing nitrogen oxide production, tabulated chemistry approaches fail to accurately capture the chemical trajectories of NO formation without additional coordinates. To address this limitation, a hybrid strategy coupling the F-TACLES (Filtered Tabulated Chemistry for LES) model with virtual chemistry is proposed. Virtual chemistry [2] is a reduced mechanism in which real combustion products are replaced by virtual species, whose thermochemical properties and kinetic rates are optimized using machine learning algorithms.

The proposed methodology leverages F-TACLES to model the flame structure, while a virtual satellite mechanism predicts nitrogen oxide levels throughout the domain. This hybrid approach has been validated using one-dimensional canonical flamelets. In addition, it has been assessed on the HYLON burner [3], a three-dimensional coaxial turbulent combustion chamber operated jointly by IMFT and KAUST. The availability of recent in-flame NO measurements in this configuration provides a robust benchmark for evaluating the predictive capabilities of the hybrid model.

References

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