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Automated Approach to Pyrolysis and Oxidation Modelling for Sustainable Aeronautic Fuels (SAF)

Anthony BERGAUD[1,2*], Thomas LESAFFRE[1], Omar DOUNIA[1], Eleonore RIBER[1]
[1] *CERFACS, 42, av. Gaspard Coriolis, 31100 Toulouse, France*
[2] *SAFRAN AIRCRAFT ENGINES, Rond-point René Ravaud, 77550 Moissy-Cramayel, France*
**lead presenter: bergaud@cerfacs.fr*

In the context of decarbonizing the energy sector, and more specifically the aeronautical field, engine manufacturers have committed to the path of alternative fuels (Sustainable Aviation Fuels, or SAFs). In addition to experimental campaigns, numerical simulation proves to be an essential tool, capable of reproducing even slight "fuel effects" on engine performances.
One of the key challenges in Large-Eddy Simulations (LES) of complex fuel combustion lies in accurate and affordable chemical kinetics modelling. While Analytically Reduced Chemistry (ARC) [1-4] has significantly advanced our understanding of these processes, its use in LES remains computationally intensive and difficult to implement in industrial settings. To address this issue, it is proposed to model large fuel molecule combustion using a global mechanism encompassing both fuel pyrolysis and oxidation, following H. Wang et al. work [5,6]. It is intended to reproduce the key parameters governing both the internal and global features of the combustion of these large fuel molecules.
For the fuel fragmentation part, an automated methodology developed by L. Heberle et al. [8] is used to identify the most important species, the dominant reaction pathways and their associated kinetic parameters. The oxidation of pyrolysis products, resulting from the first step, is subsequently described using a global oxidation reaction scheme. The accuracy and generalization capabilities of the resulting chemical scheme are assessed through several canonical configurations.

References

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