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Recent developments in N-fuels, NO_x and NO_x/hydrocarbons interaction chemistry

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The investigation of nitrogen chemistry is gaining extreme attention in relation to sustainable energy technologies and clean combustion. Beside the long-lasting interest in nitrogen oxides (NO_x) chemistry for pollutants emission mitigation and abatement, additional challenges are outlined by the imminent needs of the energy transition.

(1) Ammonia (NH_3) is a promising carbon neutral fuel of interest also for diesel fuel mixtures. (2) Biomass conversion to bio-oils (FPBO) with (fast) pyrolysis is a sustainable way to produce bio-fuels for transportation engines, heat and power applications. Despite the intrinsic carbon neutral nature, FPBO combustion carries some concern in relation to the impact of fuel-N on NO_x emissions. (3) Demand for fuel-flexible combustion systems (e.g. NH_3/Diesel, $NH_3/H_2/CH_4$), (4) optimization or retrofitting of consolidated technologies (EGR), and (5) design of new processes (e.g. MILD combustion) require improved understanding of fuel/NO_x interactions. From a microscopic chemical kinetics perspective, all of the above share a common core set of relevant N-species and reactions, making the development of a physically meaningful, consistent and single model mandatory.

This work presents the recent developments in the N-fuels (NH_3, pyrrole, pyrrolidine), NO_x and NO_x/hydrocarbons subsets of the CRECK kinetic model. From the molecular scale calculation of rate constants and thermochemistry, criticisms and model development/optimization strategies for such interconnected subsets are discussed, together with applications in more complex reactor-scale simulations.