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Development and validation of a detailed NH_3 combustion mechanism CEU-NH3

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The usage of fossil fuels like coal, oil, and natural gas has caused serious challenges to human societies with pollution emissions as well as greenhouse gases like CO_2. According to the data of IEA, the global CO_2 emission in 2023 has reached 37.4 billion tonnes (Gt), with a 1.1% increase ratio[1]. More than 198 countries have signed the 2015 Paris Agreement. To control the global average temperature rise limited to 1.5 ºC, it's urgently needed by all countries switching fossil fuel-based energy systems to a renewable and sustainable one. As one of the most important zero-carbon fuels, ammonia is playing a more and more important role in the combustion area and is considered to replace typical fossil fuels[2]. The green ammonia can be synthesized through the Haber-Bosch process with green H_2 and N_2. Without carbon in the molecule, and easy for liquification it's one of the best H_2 carriers. Ammonia can be directly or co-fired with natural gas, oil, and coal in the existing gas turbines, engines as well as industrial boilers and furnaces.

The combustion of ammonia is a challenge due to low reactivity and risk of extremely high NO_x emission. Developing and validating of NH_3 combustion mechanism is essential for understanding the reaction process and developing a new type of combustion technology for NH_3 fuels. In this paper, the fundamental experiments based on heat flux methods and a detailed NH_3 combustion mechanism of CEU-NH_3 will be introduced[3,4]. Based on the kinetic simulation platform of CHEMKIN, the mechanism will be validated by a variety of experiment data like laminar burning velocity, ignition delay time, and species concentration obtained from experimental data for pure NH_3, NH_3/H_2, NH_3/CH_4, NH_3/Syngas, and NH_3/Methanol/Ethanol. A temperature dependence parameter α and pressure dependence parameter β model will be introduced and discussed. The over-rich phenomenon of different fuels will be discussed as well. The NO_x formation route and control strategy will be discussed based on kinetic simulation results. The sensitivity analysis and rate of production (ROP) for key species will be analyzed.

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