High-fidelity chemical kinetic models are critical in predictive modeling during design and optimization of next generation energy systems. Shock tube provides an ideal tool to investigate high-temperature chemical kinetics. Non-intrusive laser absorption diagnostics provide in-situ measurements of quantitative, time-resolved species concentration data in this complex chemically reacting system. In this work, shock tube and laser absorption spectroscopy were utilized to measure species concentration time-histories during pyrolysis and oxidation of organophosphorous compounds (OPCs). The experiments data obtained were used as benchmark to develop an improved kinetic model of OPCs combustion.

Interest in combustion chemistry of OPCs is associated to their use as fire suppressants and as chemical weapons. Pyrolysis and oxidation of OPCs were carried out behind reflected shock wave and laser absorption spectroscopy utilizing quantum cascade laser at mid-IR wavelength region was used to measure time resolved intermediate CO concentration produced during the process. Utilizing the experiments data, an improved chemical kinetic model for combustion of an OPC - Triethyl Phosphate (TEP) was developed. Various steps taken to develop the improved model include: calculation of thermochemical properties; updating hydrocarbon kinetics; calculation of reaction rates and addition of alternative TEP decomposition pathways. The prediction of TEP combustion, in terms intermediate CO concentration yield during its pyrolysis and oxidation, made by the improved model is in much better agreement with the experiments. Such an accurate kinetic model is critical in predicting the effectiveness of OPCs as flame retardants when used as dopants in hydrocarbon fuels; and in devising counter weapon of mass destruction strategies to destroy chemical weapons.

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The public is welcome to attend.