

Transport, Pyrolysis and Combustion of two Flame Retardants in Polymers and Alkanes

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Flame retardants are added to polymers to avoid ignition or to reduce the flame propagation speed. There are physical and chemical mechanisms which lead to flame retardancy and flame extinction, and they can act in the condensed phase or in the gas phase. In our work we concentrate on the chemical action in the gas phase. In order to act as a flame retardant in the gas phase, several processes must occur successively and simultaneously. This starts with the diffusion and evaporation of the retardant from the condensed-phase polymer/retardant mixture. At least the polymer must pyrolyse in the condensed phase to form ignitable hydrocarbon vapors, while the retardant or its decomposition products have to evaporate at the same time. This is followed by gas phase reactions in different atmospheres, which may lead to an interaction between the chain carrier radicals (H, O, OH) and the retardant fragments, e.g. PO to reduce the radical concentrations.

To reduce complexity, our approach is to separate the processes and to simplify the systems, as far as possible, to get some insight into the partial steps. Two flame retardants are investigated here, ferrocene $\text{Fe}(\text{C}_5\text{H}_5)_2$ and aluminium diethylphosphinate $\text{C}_{12}\text{H}_{30}\text{AlO}_6\text{P}_3$.

In the presentation, four related experiments will be discussed: a) The investigation of the diffusion and evaporation of ferrocene out of a long-chained alkane (tetracosane) is described, showing the deviation from ideal-mixture behavior [1]. b) The pyrolysis of ferrocene in the gas phase is analyzed in a micro-reactor and mass spectrometry using synchrotron radiation and the i^2 PEPICO method [2]. c) The pyrolysis of AlPi in polyethylene mixtures is analyzed using mass spectrometry [3], and finally, d) the high-speed pyrolysis and combustion of such mixtures is analyzed using mass spectrometry and thermocouple measurements [4].

Although, the flame retardancy effect is often only deduced indirectly, the detection of reactive species in the gas phase is an important step to improve the mechanistic understanding of flame inhibiting effects. With such an approach, to simplify the processes, it should be possible in the long term to predict rate determining or limiting steps along the process chain and develop detailed models of flame ignition and retardancy starting with polymers.

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- [2] S. Grimm, P. Hemberger, T. Kasper, B. Atakan, Mechanism and Kinetics of the Thermal Decomposition of $\text{Fe}(\text{C}_5\text{H}_5)_2$ in Inert and Reductive Atmosphere: A Synchrotron-Assisted Investigation in A Microreactor, Advanced Materials Interfaces (2022), doi:10.1002/admi.202200192.
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