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Polycyclic Aromatic Hydrocarbon (PAH) formation in thermal degradation of Styrene Butadiene Copolymer (SBR)

Eilhann Kwon and Marco J. Castaldi*
Department of Earth and Environmental Engineering
Henry Krumb School of Mines, Columbia University
New York, NY 10027

ABSTRACT

This study has been initiated to quantify the release of the Polycyclic Aromatic Hydrocarbon (PAH) species from Styrene Butadiene Copolymer (SBR) during gasification. The identification and quantification has been determined experimentally using Gas Chromatography/Mass Spectroscopy (GC/MS) coupled to a Thermo-Gravimetric Analysis (TGA) unit. SBR samples were pyrolysed in a TGA unit in a N_2 atmosphere. The identities and absolute concentrations of over 32 major and minor species have been established, including a large number of aromatics, substituted aromatics, and PAHs. The light hydrocarbon species also have been determined simultaneously and identified as H_2, C_2H_2, CH_4, C_2H_6, and C_4H_{10} with lower concentrations of other hydrocarbon gases. Significant amounts of ethyl benzene, toluene, and styrene were observed between 330°C and 500°C. The largest PAH detected was the family of $C_{24}H_{14}$ (molecular weight 302), benzo[ghi]perylene with peak concentrations reaching 0.19 ppmv. The effluent species detected suggest that formation of PAH's occurs either through hydrocarbon addition reactions or benzene ring re-combination reactions. In addition, the chemical structure of SBR lends itself gas phase release of benzene molecules or radicals, thus facilitating the PAH production route. Preliminary calculations done using MOPAC provided some insight into the energy required to break the benzene ligand bond from the butadiene structure. The measurements supply information on the identities and levels of hazardous air pollutants, and provide useful new data for the development and validation of detailed reaction mechanisms describing their origin and fate.

INTRODUCTION

The disposal of used automobile tires has caused many environmental and economic problems. In the US, 750 million to 2 billion used tires have been stockpiled, which are increasing at a rate of 280 million per year[1]. Around 2,600,000 metric tons of used tire were produced in the European Union in 2001. A low percentage is re-capped or reused for reduced-quality rubber but around 80% of these tires are accumulated in dumps, posing hazards such as disease and accidental fires and adversely impacting the environment[2].

Tire disposal requires special solid waste management because of their particular properties. The durability and strength of tires make their