ABSTRACT

Acrylic rubber is a special class of saturated polar rubbers with excellent resistance towards swelling in hydraulic oils, engine oils and transmission fluids. The current challenge is to improve the heat resistance and mechanical strength of the elastomer further in view of the stringent application requirements. This can be achieved by first studying the degradation behavior of the pristine elastomer followed by suitable modification of the elastomer. A series of Reactive Force Field (ReaxFF) molecular dynamics simulation was performed on polyacrylicester (ACM) terpolymer to understand its thermal decomposition characteristics. Evolution mechanisms of dominant products (alkyls and alkenes) were explored in detail based on the simulation approach. The fracture of ester linkage is the typical initiation step for the formation of alkyl radicals. The pathway for yielding alkenes mainly consists of the β-hydrogen elimination from the side chain ester groups. The findings were further verified with the experimental results from thermogravimetry coupled with Fourier transform infrared spectroscopy (TGA-FTIR) and simultaneous thermal analysis coupled with gas chromatography and mass spectroscopy (STA-GC-MS). Having been motivated by the quest to develop an elastomer with enhanced thermal as well as mechanical properties for the application at extreme environmental conditions, ACM based nanocomposites with nanosilica, modified nanoclay and graphene oxide were prepared by solution casting method and its thermal, as well as mechanical properties, were investigated. Incorporation of nanofillers enhanced thermal, dynamic mechanical and mechanical properties of ACM. The service life was also improved with the presence of nanofillers. Apart from the experimental analysis a series of reactive force field molecular dynamics simulation was performed on the polyacrylicester model chains ACM10 in presence of model silica and model graphene oxide. The initial decomposition temperature and the final degradation temperature were increased while the rate of degradation of ACM10 decreased with the introduction of model silica and graphene oxide molecules. The activation energy of degradation for ACM calculated from the reactive simulation was also consistent with the results obtained from the non-isothermal thermogravimetric analysis. Furthermore, optimization of the compounding formulation for the vulcanized compounds was carried out with the help of Taguchi method. Different dianiline curatives were used in the optimized formulation for the improvement of heat resistance and mechanical properties of the vulcanizates. Finally, different levels of nanosilica were used in the optimized formulation to enhance the thermal stability and mechanical properties further. Time-temperature superposition (T-TS) principal was utilized to evaluate the activation energy for degradation of the cross-linked samples. This current study would help in understanding and improving the thermal stability as well as mechanical strength of various elastomers in industrial applications.

Keywords: Degradation, Polyacrylicester elastomer, Thermal stability, Reactive molecular dynamics simulation, Dianiline curative