3. Genetic Algorithms

A Genetic Algorithm is a robust and efficient optimization technique imitating the principles of biological adaptation and evolution based upon the mechanics of the Genetic Survival of the Fittest Theory. The procedure involves a population of parameter sets undergoing a process of selection such that only those giving the best results (the fittest) of every generation survive. Children of best mating are reproduced from the parameter set pool of the parents, plus random mutations. The code used is GANNET by Tuckwell et al. [1] for Matlab.

The fitness function (kind of inverse of the error) used in this work is to measure the adaptation of each parameter set as defined by the fitness of the weight solution and the time derivative of the exponential data, for both the weight solution and the time derivative data.

4. Results & Discussion

Following the two mechanisms indicated above, the kinetic parameters that best fit the TGA experiments have been derived. The experiment in inert atmosphere (100% N₂) is used to extract the pyrolysis parameters, and an atmosphere to extract the oxidation parameters.

The 3-reaction mechanism in the inert atmosphere approximates well the solid weight profile but is not able to capture the two weight loss-rate peaks. In air atmosphere, the curve of weight-loss rate captures only two of the three peaks. These results point out that an initial reaction in stages in the mechanism. The 3-reaction mechanism is able to capture all the peaks in the weight loss-rate curves and approximates properly the solid weight profile, indicating the success of adding another pyrolysis step.

3-reaction Mechanism by Ohlemiller [2]

Narrowing the range from 5 to 20°C/min show two global pyrolysis reaction-paths and three global oxidative reaction-paths. The temperature range where each reaction takes place depends on the heating rate. The kinetics of polyurethane can be approximated by a few heterogeneous reaction: pyrolysis and oxidations. A three-step chemical reaction scheme for polyurethane foam was proposed by Ohlemiller [2] foam pyrolysis, foam oxidation and char oxidation, accounting for three solid species; foam, char and residue. However, TGA results suggest that a five-steps mechanism is more appropriate; two foam pyrolysis, foam oxidation and char oxidation. The two pyrolysis paths are associated with the main constituents of polyurethane foam; diisocyanate (di) and polyol (p).

5-reaction Mechanism

References