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Generalized regression and feed forward back propagation neural networks in modelling flammability characteristics of polymethyl methacrylate (PMMA)

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ABSTRACT

The capability of artificial neural networks in predicting microscale combustion calorimeter (MCC) parameters of polymethyl methacrylate (PMMA) was carried out in this study. Using values of sample mass and corresponding heating rate, feed forward back propagation (FFBP) and generalized regression neural network (GRNN) models were developed to predict MCC parameters. On the whole, GRNN outperformed FFBP in predicting HRC data while FFBP model saw an improvement over GRNN when estimating pTime. It was also discovered that GRNN obtained better THR, pTemp and pHRR predictions during training but generated a relatively poor correlation when estimating the testing data. Sensitivity analysis on the ANN models revealed that heating rate had a more significant effect on the models' outcome. Also, the ANN models observed the least error deviation when compared with HRC results for PMMA from structure-property models. Hence, ANN presents a reliable method for predicting flammability characteristics of PMMA from MCC test.

1. Introduction

The continual use, processing and modification of polymers such as polymethyl methacrylate (PMMA), for the purpose of medicine, transportation, construction, aviation, etc. have heightened interests in flammability studies over the years. Flammability is a type of fire hazard that describes the ability of a material to ignite easily and burn rapidly with a flame [1]. Currently, there are various large-scale polymer tests that measure different aspects of flammability. UL 94 is an ignitability test that provides a qualitative ranking of polymeric materials. LOI determines the lowest concentration of oxygen that can support downward burning of a vertically oriented sample. Oxygen bomb calorimeter measures the potential heat or calorific value under high pressure and in a pure oxygen environment and cone calorimeter provides a broad range of ignition and combustion properties [2].

According to Lyon et al. [3], researchers failed to recognise flammability as an intrinsic material property up until the development of the microscale combustion calorimeter (MCC). The MCC test apparatus could relate polymer properties to flame and fire test by successfully producing separate condense phase (pyrolysis) and gas phase (combustion) [4]. By way of this, the MCC was able to provide quantitatively, the potential or capacity of a material to release heat in fire which is measured as heat release capacity, HRC [3]. It is therefore acknowledged that MCC technique can provide a more scientific and quantitative assessment of polymer flammability, as its principle of operation correspond to fire calorimetry rather than thermal analysis [5]. This has led to several studies [5–13] adopting the MCC to screen the flammability of pure polymers and plastics with flame retardants in recent years.

The premise that flammability parameters obtained from an MCC experiment are intrinsic material properties was further confirmed by Walters and Lyon [14] and Lyon et al. [15] when they calculated flammability parameters from additive molar group contribution. Additive molar group method is known to provide satisfactory agreement with measured MCC results [1] by employing the additive contribution of functional groups. However, additive molar group method exhibits a limitation as material property cannot be determined if its functional group or molecular moiety is not available in the database. By virtue of this, Parandekar et al. [16] proposed a computational quantitative structure-property relationship (QSPR) model based on genetic function algorithm to estimate flammability characteristics of polymers. Keshavarz et al. [17] also developed a simple model based on repeat unit

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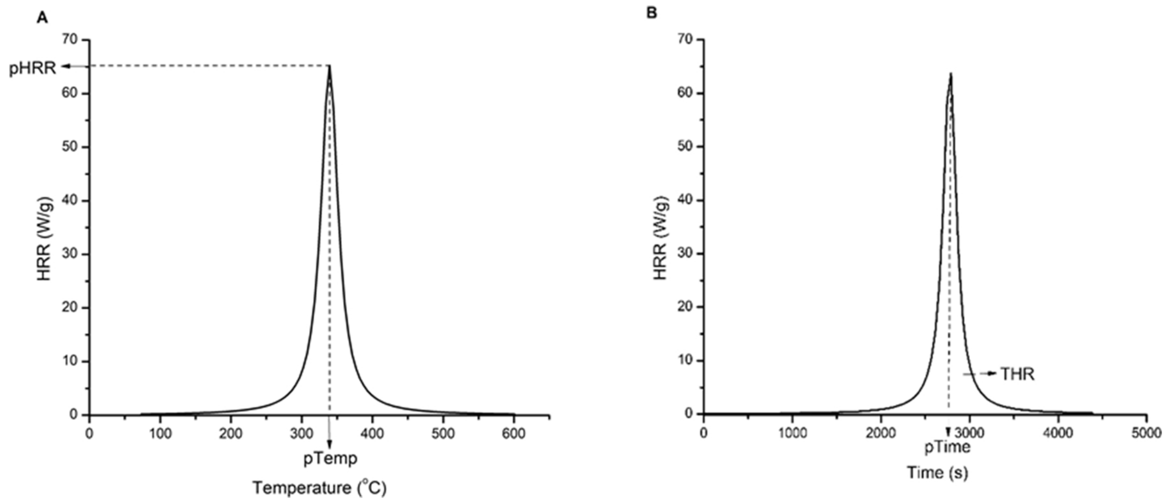

Fig. 1. Typical HRR curves as a function of (A) temperature and (B) time for PMMA.

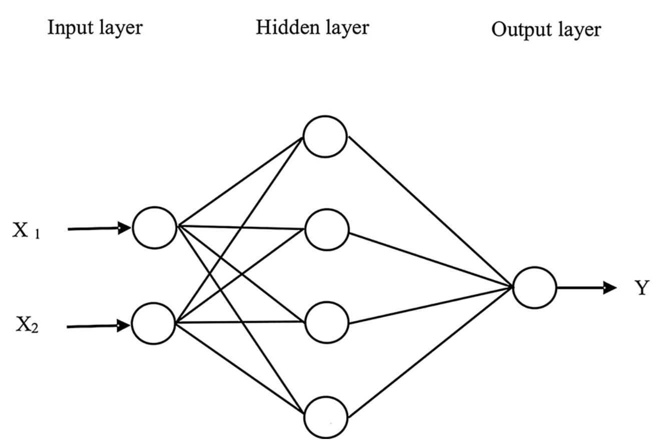

Fig. 2. Schematic diagram of FFBP architecture.

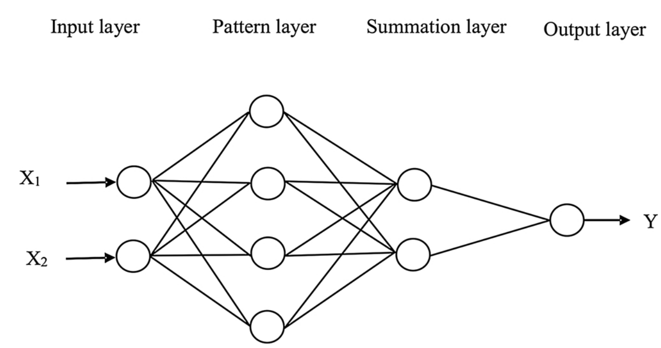

Fig. 3. Schematic diagram of GRNN architecture.

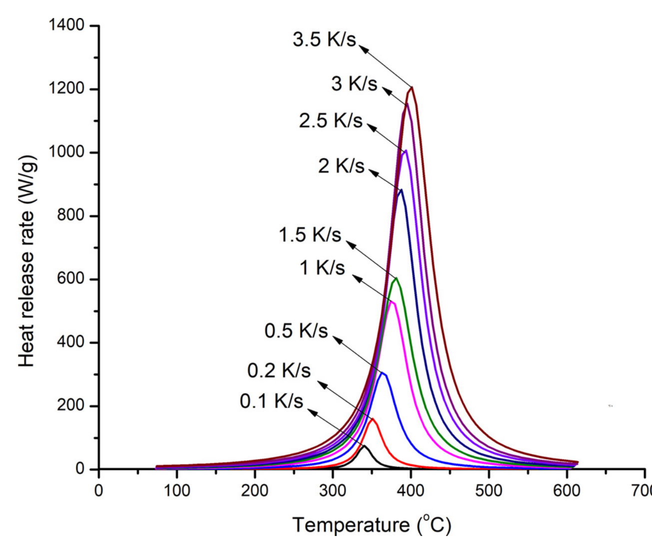

Fig. 4. Typical heat release rate (HRR) against temperature curves obtained from MCC.

of chemical groups/moieties like methyl, phenyl, carbonyl, ether, amide and ester to determine HRC.

It is important to note that flammability properties and MCC parameters can alternatively be predicted using artificial neural network (ANN) without the influence of molecular structure. With adequate MCC data, ANN model could evaluate flammability characteristics even beyond the conditions of the test performed. ANN is a computational model that tries to imitate the main workings of a biological brain [18]. Like the brain, ANN receives information as an input, processes it in the neurons and releases it out as an output. The transfer of information between neurons are done with the help of connection links. ANN has the propensity to model complex relationships between inputs and outputs or discover patterns in data [19]. Models created by ANN methods are mostly from non-linear and complex data systems with predictions falling within the range of the training data [20].

For this reason, ANN has proven to be superior compared to conventional mathematical-based modelling techniques due to its ability to provide high speed response when performing classifications and function approximations from large, noisy data. Among the many neural networks, feed forward back propagation (FFBP) neural network has been applied extensively in thermal analysis research including but not restricted to flammability limit in air of organic compounds [21], decomposition temperature of energetic cocrystals [22], kinetic analysis [23] and thermogravimetric measurements [24]. However, FFBP has some intrinsic drawbacks such as slow convergence speed during training, less generalizing performance due to overfitting and arriving at local minimum. Generalised regression neural network proposed by Specht [25] avoids the shortcomings of FFBP as it is known for fast and stable convergence without iteration when estimating continuous variables. GRNN trains by making use of radial basis function of non-linear regression method, contrary to the weight adjustment training technique employed by FFBP.

In view of the above, this study was performed to examine the potential of FFBP and GRNN in modelling flammability characteristics of PMMA. Performance comparison of FFBP and GRNN to accurately