USE OF PCFC TO PREDICT THE FLAMMABILITY PARAMETERS OF POLYMERS FROM THEIR CHEMICAL STRUCTURE

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Predicting the flammability parameters of a polymer from its chemical composition would open up many opportunities like the selection of the best structure without using an expensive trial and error approach. In a recent study Lyon *et al.* have proposed to calculate the main flammability parameters of polymers using a Van Krevelen approach [1]. Such approach allows predicting roughly the heat release capacity (HRC) and the total heat release (THR) as measured in microscale combustion calorimeter (PCFC) [2]. A first empirical database was proposed with the contributions to HRC and THR for almost 40 chemical groups. Figure 1 shows the good agreement between measured and calculated HRC for various EVA or EMA copolymers.

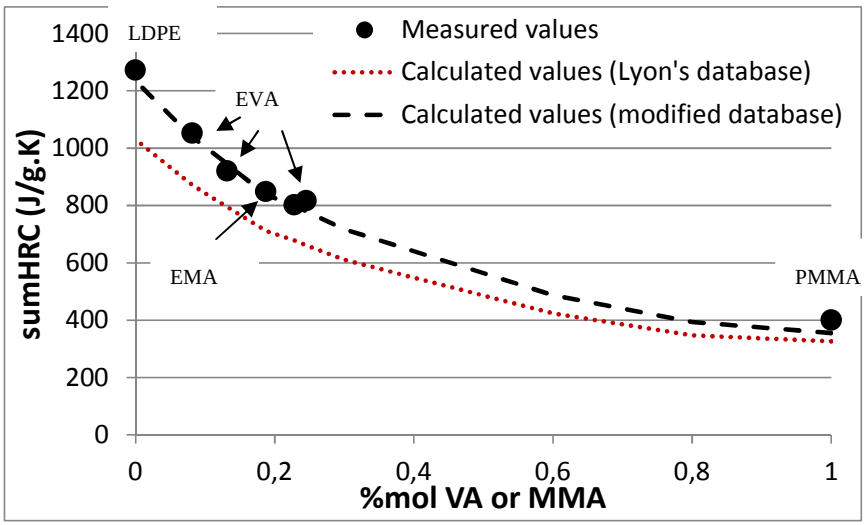

Figure 1 – Measured HRC and calculated HRC using Van Krevelen's approach for various EVA and EMA copolymers

The limits of this method are the interactions that may occur between chemical groups of a same structure during thermal decomposition. We have attempted to calculate the contributions of new chemical groups (not proposed in the Lyon's database) [3]. Figure 2 plots the calculated and experimental sumHRC of various molecules containing dioxaphosphorinane (series A) or phosphonate (series B) groups. A good agreement is observed when the contributions to sumHRC are fixed at 400 and 500 J/g.K (respectively for dioxaphosphorinane and phosphonate groups. Nevertheless the calculations fail to fit properly to the measured points for series C. This series gather molecules containing phosphonate and ester groups and possible interactions between these groups are believed to explain this absence of agreement.

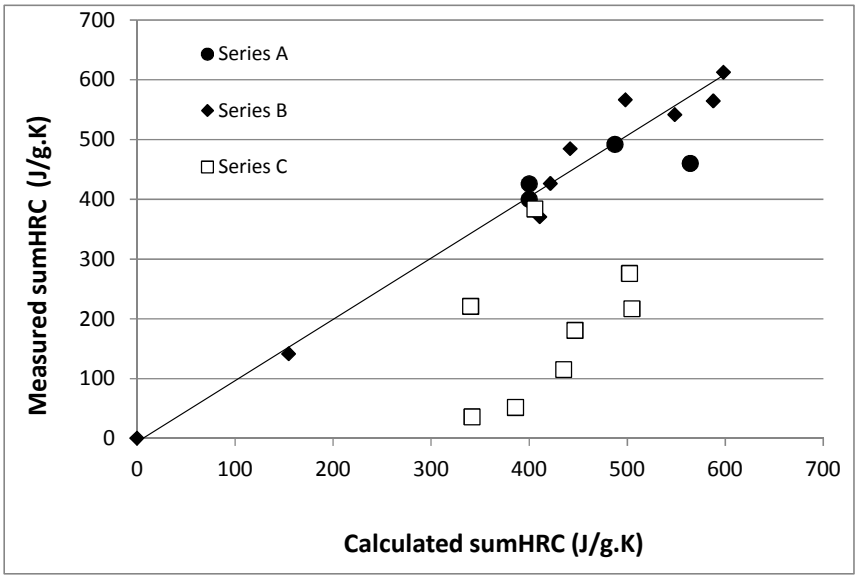

Figure 2 – Measured and calculated sumHRC for various phosphorus containing molecules [3]

Nevertheless in absence of agreement this method can be used as a tool to estimate interactions that occur during the thermal degradation [3]. The influence of fine details of the chemical structure on the flammability of a polymer can be evaluated by this method.

[1] R.E. Lyon, M. T. Takemori, N. Safronova, S.I. Stoliarov, R.N. Walters, **Polymer** 50 (2009), 2608-2617

[2] R.E. Lyon, R.N. Walters, **J. Anal. Appl. Pyrolysis** 71 (2004), 27-46

[3] R. Sonnier, C. Negrell-Guirao, H. Vahabi, B. Otazaghine, G. David, J-M. Lopez-Cuesta, **Polymer**, *In Press*, DOI: 10.1016/j.polymer.2012.01.055