QSAR/QSPR in Polymers: Recent Developments in Property Modeling

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ABSTRACT

Predictive modeling of the properties of polymers and polymeric materials is getting more attention, while it is still very complicated due to complexity of these materials. In this review, we discuss main applications of quantitative structure-property/activity relationships (QSPR/QSAR) methods for polymers published recently. The most relevant publications are discussed covering this field highlighting the main advantages and drawbacks of the obtained predictive models. Examples dealing with refractive index, glass transition temperatures, intrinsic viscosity, thermal decomposition and flammability properties are shown, together with a fouling-release activity study. Finally, some considerations are discussed in order to give some clues that could lead to the improvement in the efficient computational design and/or optimization of new polymers with enhanced properties/activities.

KEYWORDS

Polymer Informatics, Polymers, QSAR, QSPR, Virtual Screening

INTRODUCTION

The discovery of new materials with enhanced properties is one of the main goals in contemporary science, but most of this discovery has been done by using trial and error methods. Among these materials, the polymers are one of the most widely distributed in commercial products. In this way, some researchers have developed some experimental designs to study the behavior of some properties with the variation of the type of substituents, percentage of monomers in the cross-linking polymers, the variation of the monomeric units in the monomers, and so on (Ma et al., 2017; Galhenage et al., 2017; Selim et al., 2017). The fact is that most of them have performed their analysis through a Factorial Design that allows the researchers to manipulate two or more independent variables (factors) simultaneously to observe their effects on the dependent variable (properties) (Creswell, 2013). However, this do not allow to get a deep understanding of the relationships between the structures and properties.

The main drawbacks for the study of polymeric materials in QSPR/QSAR-related studies is the way that the chemical structure is encoded, since in most of the cases the polymer has as a

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common characteristic long chain length and a polydispersity that make very difficult a complete characterization of the structure and the further translation in this case to accurate molecular graphs for the calculation of features to describe these chemicals. Some approximations and studies were carried out, using monomeric units and/or small chains consisting in repeating monomers with end-capped hydrogens (Yu et al., 2006; Afantitis et al., 2006; Ajloo et al., 2008; Gao et al., 2007).

Although more powerful computers and algorithms are introduced each day and at a fast pace, only few studies related to the quantitative structure-property relationships of polymers were published, covering to some extent how they can advance the mechanistic understanding of some process or the successful design of novel or optimized molecules (Yu et al., 2007; Yu et al., 2010). Based on this knowledge, most of the QSPR/QSAR studies follow a general scheme as depicted in Figure 1. In this review, some of the more recent advances in the computational polymer studies are discussed, mainly those related to in silico prediction of properties from the structure.

**QSPR/QSAR APPLICATIONS IN POLYMERS**

The impact of this field was analyzed by retrieving data in the Scopus database using the search criteria (“QSAR” AND “Polymers”) or (“QSPR” AND “Polymers”). Besides that, we also limit the study to the last five years to visualize the most recent trends in this field. The mentioned query was plotted, and the results are shown in Figure 2. As can be observed in the figure, there is a small amount of published manuscripts related to this subject, with a small increase over the time for both QSAR and QSPR studies with 45 and 60 documents, respectively. This is understandable, because the complexity of the structures in this field is increasing, and in most of the cases the data set comprises a matrix of different chemicals/components with different compositions and with not completely known structure.

From another side, we plot two graphics depicting the world distribution by countries by using the above-mentioned query (Figures 3 and 4). It is important to highlight that the main contributors to this field are as usual the developed countries, and in this case, it could be related with the chemical industry as a factor that is correlated with the level of research efforts in polymers.

In a recent publication Duchowicz et al. (2015) performed a QSPR study using MLR for the modeling of refractive index in five datasets of 78 polymers, each one with a size varying from 1-5 monomer units. In this case, the authors used a dimeric polymer consisting of two monomeric units, which gave the model with $R^2_{train} = 0.96$, $R^2_{validation} = 0.95$, and $R^2_{test} = 0.85$. According to statistical coefficients, the model shows a very good performance. Although the same monomeric units are used for the assembly of the co-polymers, some influence can be detected related to the property investigated. In this case, it would be very good to study the polymers based on higher than five monomeric units’ theoretical structures, since most of the polymers are having a long backbone chain.
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