Statistical methods and data-driven models to predict glass melt properties

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Abstract

In situations where theoretical models cannot be efficiently applied to calculate glass properties, empirical statistical models are often required. It is typically the case when glass contains a high number of components. Since the end of the 19th century, it is known that under certain conditions, silicate glass properties can be expressed as a simple linear combination of oxide contents. This "Principle of Additivity" was initially introduced to calculate heat capacity of glass, before being extended during the 20th century to a larger number of properties: optical, thermal, mechanical or rheological properties. In the 1990s, American scientists from PNNL developed a statistical methodology to establish robust property-composition models applicable to the formulation of nuclear waste conditioning glass. Since the 2000s, significant increase in the power of computer tools has allowed to use highly efficient algorithms in the predictive methods of data mining. For example, glass transition temperature can be accurately predicted by using neural networks. Glass viscosity prediction is much more challenging because of huge variability of this property on temperature and composition scales. An innovative methodology recently developed by glass formulation scientists at CEA, with the support of Orano and EDF, combines statistical techniques of experimental designs, multilinear regression and neural networks. It uses glass formulation data generated at CEA over the past 30 years as well as large amount of data collected from the literature and from commercial database. Results obtained for glass transition temperature and viscosity predictions are very accurate, compared to other statistical models already published in the literature.

Keywords: Machine Learning, viscosity, prediction, database

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