A Quantitative Property-Property Relationship for the Internal Diffusion Coefficients of Organic Compounds in Solid Materials

Indoor releases of organic chemicals encapsulated in solid materials are major contributors to human exposures and are directly related to the internal diffusion coefficient in solid materials. Existing correlations to estimate the diffusion coefficient are only valid for a limited number of chemical-material combinations. This paper develops and evaluates a quantitative property-property relationship (QPPR) to predict diffusion coefficients for a wide range of organic chemicals and materials. We first compiled a training dataset of 1103 measured diffusion coefficients for 158 chemicals in 32 consolidated material types. Following a detailed analysis of the temperature influence, we developed a multiple linear regression model to predict diffusion coefficients as a function of chemical molecular weight (MW), temperature, and material type (adjusted R2 of 0.93). The internal validations showed the model to be robust, stable and not a result of chance correlation. The external validation against two separate prediction datasets demonstrated the model has good predicting ability within its applicability domain (R2ext > 0.8), namely MW between 30 and 1178 g/mol and temperature between 4 and 180 °C. By covering a much wider range of organic chemicals and materials, this QPPR facilitates high-throughput estimates of human exposures for chemicals encapsulated in solid materials.

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Authors: Huang, L. (Ekstern), Fantke, P. (Intern), Jolliet, O. (Ekstern)
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