Mapping the Flammability Space of Complex Refrigerant Mixtures Through Artificial Neural Networks Based on Molecular Descriptors

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With the European Union's regulations to phase out high-GWP refrigerants taking hold [1,2], the refrigeration sector is now confronting a novel, unexpected challenge: the introduction of more flammable yet environmentally acceptable alternatives. This paradigm shift underscores the urgency for a rapid, reliable screening methodology to evaluate the flammability of new 4th generation blends, providing a pragmatic alternative to the time-intensive traditional experimental assessments. In this contribution, an Artificial Neural Network (ANN) is meticulously constructed, evaluated, and validated to address this challenge, thus predicting the Normalized Flammability Index (NFI) for an extensive array of pure, binary, and ternary mixtures. The optimal configuration (61x14x24x1) presents an excellent fit to the data, with metrics like R^2 of 0.999, RMSE of 0.1735, AARD% of 0.8091, and SDev of ± 0.0434. Exhaustive assessments are conducted to ensure the most efficient architecture without compromising accuracy. Additionally, the analysis of Standardized Residuals (SDR) and Applicability Domain (AD) exhibits fine control and consistency over the data points. An external validation using quaternary mixtures further attests the model's adaptability and predictive capability. The exploration into the relative contribution of descriptors leads to the identification of 23 significant sigma descriptors derived from COSMO, responsible for 90.98% of the total contribution, revealing potential avenues for model simplification without substantial loss in predictive power. Moreover, the model successfully predicts the behavior of prospective industry-relevant mixtures [3], reinforcing its reliability and opening the door to experimentation with untested blends.

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