Accurate Prediction of Thermal Conductivity in Methane Binary Mixtures for Energy Applications Using a Convolutional Neural Network

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Abstract

Accurate prediction of thermal conductivity in methane (CH_4)-based binary gas mixtures is essential for enhancing the efficiency and safety of energy systems, gas separation processes, and the design of industrial equipment. Conventional empirical and theoretical models often lack sufficient accuracy when dealing with complex, nonlinear molecular interactions and require extensive experimental data. In this study, a novel framework based on one-dimensional convolutional neural networks (1D-CNNs) was developed to predict the thermal conductivity of CH_4 mixtures with seven gases (CO_2, CO, CF_4, H_2, N_2, Ne, and Ar) using fundamental input parameters such as temperature, pressure, and mole fractions. The model architecture was optimized through hyperparameter tuning, root mean square propagation (RMSprop) optimization, and dropout regularization to minimize overfitting while maintaining strong generalization capability. Quantitative evaluation demonstrated that the proposed model significantly outperformed traditional approaches, including random forest regression, feed-forward neural network (FFNN), support vector regression (SVR), and linear regression (LR), achieving $R^2 = 0.995$, mean absolute percentage error (MAPE) = 2.02%, mean absolute error (MAE) = 0.94 mW/m·K, and root mean square error (RMSE) = 1.59 mW/m·K. Residual analyses confirmed the model's excellent agreement with experimental data and minimal prediction bias. The results establish the proposed model as a powerful, scalable, and extensible tool for a wide range of industrial applications, including combustion modeling, thermal management in membrane technologies, cryogenic process design for liquefied natural gas (LNG) systems, and safety analysis of natural gas transmission pipelines.

Author keywords

convolutional neural networks (1D-CNNs); machine learning models; methane binary gas mixtures; thermal conductivity prediction; thermophysical properties

Indexed keywords

Engineering controlled terms

Binary mixtures; Convolution; Convolutional neural networks; Cryogenics; Errors; Feedforward neural networks; Forecasting; Gas mixtures; Gas permeable membranes; Industrial research; Learning systems; Mean square error; Membrane technology; Methane; Product design; Support vector regression; Thermal conductivity of gases; Thermal modeling

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