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

By

Are you this author?

Motahar, S (Motahar, Sadegh) [1] ; Shams, M (Shams, Mohammadreza) [2] ; Jannati, M (Jannati, Mohsen) [3] ; Jami, MS (Jami, Mohammed Saedi) [4]

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Abstract

Accurate prediction of thermal conductivity in methane (CH4)-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 CH4 mixtures with seven gases (CO2, CO, CF4, H2, N2, 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

liquefied natural gas (LNG) systems, and safety analysis of natural gas transmission pipelines.

Keywords

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Author Information

Corresponding Address: Motahar, Sadegh (corresponding author)
Univ Isfahan, Dept Mech Engn, Shahreza Campus, Shahreza, Iran
E-mail Addresses :
s.motahar@shr.ui.ac.ir