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A neural network for predicting normal boiling point of pure refrigerants using molecular groups and a topological index

Shuai Deng, Wen Su, Li Zhao *

Key Laboratory of Efficient Utilization of Low and Medium Grade Energy (Tianjin University), MOE, Tianjin 300072, China

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ABSTRACT

An artificial neuron network based on genetic algorithm is presented to predict the normal boiling point (T_b) of refrigerants from 16 molecular groups and a topological index. The 16 molecular groups used in this paper can cover most refrigerants or working fluids in refrigeration, heat pump and organic Rankine cycle; the chosen topological index is able to distinguish all the refrigerant isomers. A total of 334 data points from previous experiments are used to create this network. The calculated results, which are based on a developed numerical method, show a good agreement with experimental data; the average absolute deviations for training, validation and test sets are 1.83%, 1.77%, 2.13%, respectively. A performance comparison between the developed numerical model and the other two existing models, namely QSPR approach and UNIFAC group contribution method, shows that the proposed model can predict T_b of refrigerants in a better accord with experimental data.

Un réseau neuronal pour prédire le point d'ébullition normal de purs frigorigènes en utilisant les groupes moléculaires et un indice topologique

Mots clés : Point d'ébullition normal ; Frigorigène ; Prévision de propriété ; Réseau neuronal artificiel ; Groupes moléculaires ; Indice topologique

* *Corresponding author.* Key Laboratory of Efficient Utilization of Low and Medium Grade Energy (Tianjin University), MOE, Tianjin 300072, China. Tel.: +86 022 27404188; Fax: +86 022 27404188.
E-mail address: jons@tju.edu.cn (L. Zhao).
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Nomenclature

Standard

A	adjacency matrix of compound
a	element of adjacency matrix
AAD	absolute average deviation, %
ANN	artificial neural network
ANN-GCM	artificial neural network-group contribution method
ARD	absolute relative deviation, %
Bias	average percent deviation, %
CAMD	computer-aided molecular design
CFCs	chlorofluorocarbons
EA	extended matrix of compound
ea	element of extended matrix
EATII	topological index
f	fitness function
GA	genetic algorithm
GWP	global warming potential
HCFCs	hydrochlorofluorocarbons
HFEs	hydrofluoroethers
m	number of hidden nodes
MSE	mean squared error
N	total number of data points
n	number of groups found in the molecule
NC	network's complexity function
ODP	ozone depletion potential
ORC	organic Rankine cycle
QSPR	quantitative structure property relationship
T	temperature, K
Radii	covalence radii of groups, $\mathring{A}$
RMS	root mean square error

Greek symbols

ω	weight of an edge connecting two groups
δ	connected degree of molecular group

Subscripts

i	index of a matrix or data for i_{th} sample
j	index of a matrix
b	normal boiling point
cal	network's calculation of normal boiling point
exp	experimental value of normal boiling point

Superscripts

*	sum of power series of extended matrix

1. Introduction

Investigation of refrigerants is the basis of refrigeration, heat pump and organic Rankine cycle (ORC) system research. The accuracy of thermal physical properties is an important consideration in engineering design and fundamental research. Although a large number of physical properties for refrigerants have been measured and published in the literature (Calm and Hourahan, 2011), it is urgent to design alternative refrigerants with desired properties (Samudra and Sahinidis, 2013a) due to the growing concerns regarding the depletion of the ozone layer and the greenhouse effect. Approximate property models to predict a set of desired properties are necessary in the process of computer-aided molecular design (CAMD) of refrigerants (Khetib et al., 2009; Samudra and Sahinidis, 2009). Therefore, prediction models in high accuracy are required for scientists and engineers working in this field.

Normal boiling point (T_b) is one of the most important thermal properties of refrigerants. Most other thermal properties are predictable from T_b (Poling et al., 2001). T_b is defined as the temperature at which a liquid's vapor pressure equals to an atmospheric pressure. There are a number of methods proposed for prediction of T_b (Poling et al., 2001). Joback and Reid (1987) proposed a group contribution method that presents an approximate value of T_b for aliphatic and aromatic hydrocarbons. T_b is estimated with the sum of contributions of all structural groups that occurred in the molecule. This method is not particularly accurate but can be acceptable for preliminary calculations. Later, Devotta and Pendyala (1992) modified the Joback method to calculate T_b of halogenated compounds much more accurately. Then Constantinou and Gani (1994) developed an advanced group contribution method based on the UNIFAC group. The accuracy was enhanced by providing contributions at a "second order" level for T_b. A different group contribution model was presented by Marrero-Morejón and Pardillo-Fontdevila (1999). They called the model a group interaction contribution technique. Wang et al. (2009) predicted the T_b of organic compounds based on the position group contribution method, which could distinguish most isomers. There are already some group-contribution models improved by the introduction of molecular descriptors (Abooali and Sobati, 2014); the main molecular descriptors are the symmetry number and the flexibility number (Wang et al., 2009). A quantitative structure property relationship (QSPR) approach for pure refrigerants was proposed by Abooali and Sobati (2014) based on solely five molecular descriptors. It should be noted that the proposed models above have some important disadvantages. For example, these models have limited applicability for distinction of isomers because the isomers have the same number and kind of groups. Besides, the existing property estimation models are for all the organics, and their accuracy in refrigerant is deficiency; they are very complicated in dividing molecular groups for a quick prediction of refrigerant properties.

Artificial neural network (ANN) is a suitable alternative to model the different properties of organic compounds. The primary advantage is that ANN can simulate the nonlinear relationship between structural information and properties of compounds during the training process and then generalize the knowledge among homologous series without the need for theoretical formulas (Liu et al., 1997). A few attempts have been made for predicting properties of refrigerants using ANN. Liu et al. (1997) set up five topological indexes, such as the connection index and the polarity number, as input parameters of a neural network to predict T_b and other properties