ХОЛОДИЛЬНА ТЕХНІКА ТА ЕНЕРГОТЕХНОЛОГІЇ

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Machine learning for refrigerants properties

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The interdisciplinary nature of new objectives aimed at the design of the working matters for environmentally friendly technologies requires a more dynamic use of information technology (IT) to ensure proper trade-off decisions under a competitive environment. Machine learning (ML) is the part of artificial intelligence (AI) methodologies that uses algorithms that are not a direct solution to a problem but learning through solutions to innumerable similar problems. Machine learning has explored a new path in the study of the thermodynamic behavior of emerging substances. Various computational tools have been provided with an effective approach to solving the actual problem of predicting the phase behavior of soft substances under strong exogenous influences. The aim of this study is to develop a new perspective on predicting the thermodynamic properties of soft substances using a methodology that provides artificial neural networks (ANN) and a global phase diagram to ensure correlation between structure and properties. In this study, we present applications of machine learning in engineering thermodynamics to predict azeotropic behaviour of binary refrigerants and determine the coefficient of performance (COP) for Organic Rankine Cycle (ORC) working media based on the data on boiling and critical points was studied. A new approach to predicting the formation of an azeotropic state in a mixture, which is developed and presented. This approach uses the synergy of neural networks and the global phase diagram methodology to correlate azeotropic data for binary mixtures based only on the critical properties and the centric coefficient of the individual components in refrigerant mixtures. It does not require intensive calculations. The construction of ANN correlations between the information attributes of working fluids and the criteria for the efficiency of the Rankin cycle narrows the scope of trade-offs in the space of competitive economic, environmental and technological criteria.

Keywords: *Machine learning; Refrigerants; Azeotrope prediction; Artificial neural networks; Global Phase diagram; Organic Rankine cycle; Coefficient of performance; Thermodynamic properties*

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1. Introduction

The innovative nature of the modern economy produces a breakthrough in the field of thermodynamics. The interdisciplinary nature of new objectives aimed at the design of the working matters for environmentally friendly technologies requires a more dynamic use of information technology (IT) to ensure proper trade-off decisions under a competitive environment. In this case, the competence and experience of the experts are replaced by the "wisdom of many". There is a shift in motivation for research: from traditional "just in case" to research "just in time."

Machine learning (ML) is the part of artificial intelligence (AI) methodologies that uses algorithms that are not a direct solution to a problem but learning through solutions to innumerable similar problems. The use of machine learning for the determination of fluid property correlations recently was applied in the study [1], equation of state for fluid properties was generated by the machine learning approach in [2]. The presented examples of machine learning applica-

tions in soft matter, including design of self-assembling materials, nonlinear learning of protein folding landscapes, high throughput antimicrobial peptide design, and data-driven materials design engines, are given in [3]. Prediction of activity coefficients with ML was performed in [4], a general-purpose machine learning framework for predicting properties of inorganic materials was presented in [5], computer-aided synthesis planning is discussed in [6]. The neural network is one example of machine learning algorithms applying to quantum physics [7], physical chemistry [8] and [9]. Recent trends of machine learning in the heat transfer sector are reflected in applying renewable energy [10].

In this study, we present applications of machine learning in engineering thermodynamics as an illustrative example of integration of data science paradigms and thermodynamic approach to predict azeotropic behaviour of binary refrigerants and determine the coefficient of performance (COP) for Organic Rankine Cycle (ORC) working media. The conventional artificial neural networks approach was applied to evaluate the data, capable of recognising complex input-output relationships.

Data science is the modern direction in poorly structured large data sets, in which hidden patterns between variables are revealed. Data science algorithms combine a wide range of scientific disciplines: machine learning, statistics, artificial intelligence, databases and others. The main methods and algorithms of Data science include the following: artificial neural networks, decision trees, symbolic rules, nearest neighbour methods, and k-nearest neighbour, support vector machine, Bayesian networks, including the Apriori algorithm; evolutionary programming and genetic algorithms, various methods of data visualisation and many other methods.

Recently, estimates based on the theory of fuzzy sets have become widespread. SVM (Support vector machines) algorithm provides users with the most robust and accurate method to solve machine-learning problems. Linear or nonlinear regressions are often used in modelling and predicting thermodynamic properties. However, real-world problems do not fit well-developed statistical methods for this case. The main algorithms and solution methods are reduced to the following: Statistical methods – Neural network algorithms – Genetic algorithms – Evolutionary algorithms – Decision trees – Bounded search algorithms – Fuzzy logic algorithms – Systems for visualisation of multidimensional data along with classical schemes of correlation, regression, and factor analysis. Artificial neural networks (ANNs) allow the learning process to establish relationships between input data and output characteristics of any degree of complexity. These models consist of interconnected groups of artificial neurons, which are, in fact, process and transform input data according to the neuronal architecture.

In most cases, ANNs are adaptive systems that change their structure under the influence of information flows entering the network during the learning process. The goal of training is to find the coefficients of connections between neurons, which determine the ability of a neural network to identify hidden relationships between input and output values. After training, the network can predict new data based on a limited sample of known relationships between input and output values.

2. Azeotrope prediction by artificial neural networks

The rate of global warming has set the task of accelerating the phase-out of ozone-depleting substances in all areas of activity. The demands of the world community have posed a serious scientific and technical challenge for refrigerant manufacturers. Attempts to find new working fluids that would combine the best energy and environmental performance led to the fact that binary mixtures became the most promising substances. Among this class of substances, azeotropic mixtures show significant advantages over zeotropic mixtures since the difference in the composition of the vapour and liquid phases leads to a negative impact on the efficiency of the cycles.

The article discusses a general approach to predicting the appearance of azeotropy in binary mixtures, which does not require cumbersome calculations of vapour-liquid equilibrium and provides valuable information on azeotropic liquids. An azeotrope is a mixture of two or more pure compounds (chemicals) in such a ratio that its composition cannot be changed by simple distillation. When an azeotrope is boiled, the resulting vapour has the same ratio of constituents as the original mixture of liquids. The word azeotrope comes from the Greek words "α ζειν τρόπος", meaning "no change on boiling".

The desire of refrigerant manufacturers to create an "ideal" fluid, which would simultaneously combine conflicting indicators, such as

• environmental (natural origin, low global warming potential (GWP), zero ozone depletion potential (ODP), non-flammable and non-toxic as well as non-corrosive);

• economic (low price);

• energy efficiency (high critical temperature, good solubility with refrigerant oil, low triple point, acceptable thermophysical properties, etc.).

It is clear that the fact among pure substances such a fluid does not exist.

3. Global phase behaviour of binary refrigerants

A theoretical analysis of the topology of phase diagrams is a handy tool for understanding the phenomena of phase equilibrium observed in multicomponent refrigerant blends. The pioneering work of van Konynenburg and Scott [11] demonstrated that the van der Waals one fluid model has vast possibilities of qualitative reproducing the main types of phase diagrams of binary fluids. The proposed classification was successful and is now used to describe the different types of phase behaviour in binary mixtures. Conventional phase diagrams visualize the state of a substance as a function of temperature *T*, pressure *p*, and component concentration *x*. Therefore, they are used as a tool for visual analysis of the physical picture of the solubility phenomena. These variables are inherently different. Pressure and temperature are the "field" variables that are the same for all phases coexisting in equilibrium. The molar fraction is the "density" that is in principle different for different phases. Global phase diagrams of binary mixtures represent boundaries between different types of phase behaviour in a dimensionless space of equation of state parameters. For the first time, the idea of mapping the surface of phase equilibria onto the space of field variables, i.e., parameters of an equation of state, was proposed by van der Waals. The boundaries of the global phase diagrams (tricritical points (TCPs), double critical endpoints (DCEPs), azeotropic line, etc.) divide the space of model parameters into the regions that correspond to the different types of phase behaviour. The mapping of the global surface of a thermodynamic equilibrium onto the space of parameters of an equation of state is the most extensive and sequential system of criteria for predicting the phase behaviour of a binary mixture. The types of phase behaviour within the Van Konynenburg and Scott classification scheme of interest are characterised (Fig. 1). Contrary to apparent ideas, it turns out that the lines connecting the critical points of pure components are not continuous, and the picture of the phase behaviour of solutions is not limited to the relatively simple diagrams shown in Fig. 1.

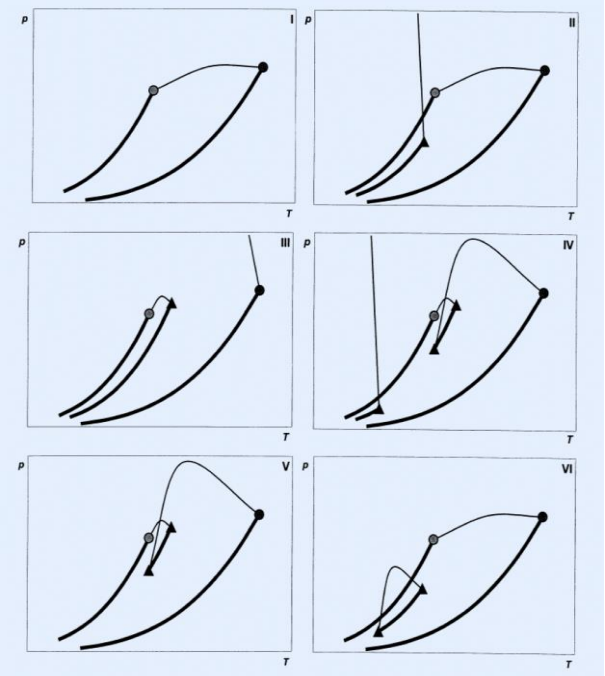

Figure 1 *– The main types of the phase behaviour of binary mixtures in the coordinates pressure-temperature*

It was found that there are 6 main types of the phase behaviour of binary solutions, which have been experimentally confirmed.

• Type I: a single permanent critical line between C_1 and C_2;

• Type II: one critical line connecting C_1 and C_2, another line going from C_m to a critical endpoint;

• Type III: one critical line going from C_1 to an upper critical endpoint, another line going from C_2 to C_m;

Type III-H: a subclass of III having heteroazeotropic three-phase curve.

Type III-A: a subclass of III with a genuine positive azeotropic line.

• Type IV: one critical line going from C_1 to an upper critical endpoint, a second critical line is going from C_2 to a lower critical endpoint, a third line is going from C_m to an upper critical endpoint.

• Type V: similar to IV, but without the low-temperature critical curve going to C_m.

• Type V-A: a subclass of V with a simple negative azeotropic line.

• Type VI: involving closed-loop liquid-liquid immiscibility at low temperatures and practically im-

possible for supercritical conditions.

Here C_1 and C_2 are critical points of refrigerant liquid; Cm is a hypothetic critical point beyond the solidification line.

At present, the topological analysis of equilibrium surfaces of binary fluid systems contains 26 singularities and 56 scenarios of evolution of the *p-T* diagrams [12].

4. Azeotrope classifiers

To describe the thermodynamic and phase behaviour of the binary fluids in this study, we use the one fluid model of the Redlich and Kwong (RK) [13]

$$p = \frac{RT}{v-b} - \frac{a(T)}{v(v+b)}, \tag{1}$$

where R is the universal gas constant and v is the molar volume; the model parameters a and b depend on the molar composition of x_i and x_j for the components i and j. The respective model parameters a and b are determined by quadratic dependences on composition and classical combining rules for the different pairs of interacting molecules a_{ij} and b_{ij}:

$$a = \sum_{i=1}^{N}\sum_{i=1}^{N} x_i x_j \sqrt{a_{ii}a_{jj}}\left(1-k_{ij}\right), \tag{2}$$

$$b = \sum_{i=1}^{N}\sum_{i=1}^{N} x_i x_j \frac{\left(b_{ii}+b_{jj}\right)}{2}\left(1-l_{ij}\right), \tag{3}$$

$$a_{ii} = 0,4274\frac{R^2T_{c_{ii}}^2}{p_{c_{ii}}}, \quad b_{ii} = 0,866\frac{RT_{c_{ii}}}{p_{c_{ii}}} \tag{4}$$

Global phase diagrams of binary fluids represent the boundaries between different types of phase behaviour in dimensionless parameter space. At present, the topological analysis of equilibrium surfaces of binary fluid systems contains 26 singularities and 56 scenarios of evolution of the *p-T* diagrams [12]. Global phase diagrams of binary fluids represent the boundaries between different types of phase behaviour in dimensionless parameter space. The dimensionless coordinates depend on the model of the equation of state; however, usually, they are represented by analogy with the coordinates introduced by van Konynenburg and Scott [11]:

$$\begin{aligned} Z_1 &= \left(a_{22}-a_{11}\right)/\left(a_{22}+a_{11}\right), \\ Z_2 &= \left(a_{22}-2a_{12}+a_{11}\right)/\left(a_{22}+a_{11}\right), \\ Z_3 &= \left(b_{22}-b_{11}\right)/\left(b_{22}+b_{11}\right), \\ Z_4 &= \left(b_{22}-2b_{12}+b_{11}\right)/\left(b_{22}+b_{11}\right). \end{aligned} \tag{5}$$

Global phase diagrams for all realistic models have a very similar structure, particularly for molecules of the same size. One may obtain the relationships for azeotropy boundaries from the global phase diagram [shaded A (Azeotropy) and H (Hetero-azeotropy)] regions in Fig. 2.

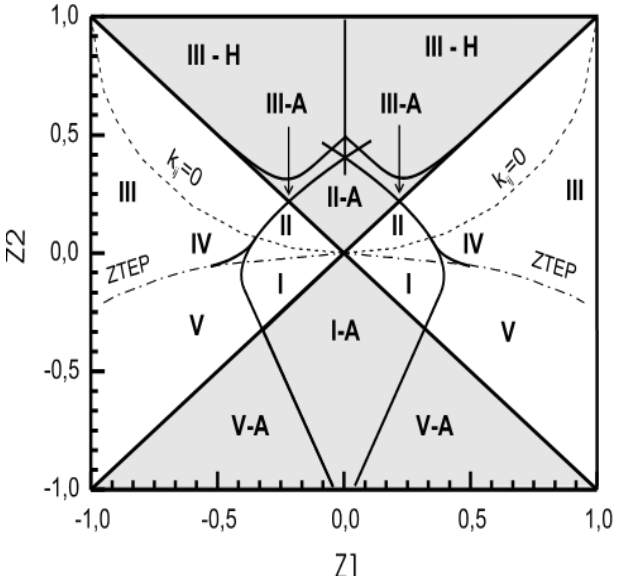

Figure 2 *– Global phase diagram of the RK model classifier ($Z_3 = Z_4 = 0$)*

The above azeotropic boundaries are straight lines in the (Z_1, Z_2)-plane that crosses at a single point near the centre for equal-sized molecules. It opens the opportunity for obtaining the series of inequalities to separate azeotropic and zeotropic regions of the global phase diagram. The selection criterion for azeotrope for the RK one fluid equation of state for binary mixture in global phase diagram variables [14]

$$Z_2 = \mp Z_1 - 0,67\left(1\pm Z_1\right)\left(\frac{1-Z_4}{1\pm Z_3}-1\right), \tag{6}$$

where the upper signs «+» or «-» correspond to the value of the composition of the critical azeotropic point at x_c = 0, the lower at x_c = 1. According to equation (6), in the Z_1 - Z_2 plane, at fixed values Z_3 and Z_4, the boundary that separates the zeotropic and azeotropic states is a straight line). If a characteristic

point is located in the northern or southern quadrants (Fig. 2), azeotropy phenomena should appear in the binary mixture.

For example, in the simplest case, for the van der Waals equation of state, the critical constants are related to the geometric (free volume – b) and energy parameters (a) well-known relations, which are found from the critical conditions. The boundaries separating the azeotropic and zeotropic states are determined by a system of thermodynamic equations [15], [16]. The relationship includes all the variety of azeotropic phenomena in binary mixtures, including azeotropic endpoint, critical azeotropic point, double azeotropic endpoint, azeotropic states in the so-called shield region and some others. A detailed list of the features of azeotropic states arising in two-component systems is given in [17]. In order to isolate the azeotropic regions, it is necessary to know the equation of state p (T, V, x) of the mixture and to map the above derivatives to a set of critical parameters of the components. Here we consider the cubic equations of state for a mixture in the one-fluid approximation, where R is the universal gas constant. Parameters a and b of the mixture, depending on the molar compositions x_i and x_j of components i and j include parameters and, as well as adjustable coefficients k_{ij} and l_{ij}, which characterise the imperfection of the solution as a result of intermolecular interactions between components i and j. Dimensionless variables, on which the thermodynamic surface of the mixture is mapped, is written either as a combination of parameters of the equation of state of pure components: or through the corresponding critical constants (T_{c1}, T_{c2}, P_{c1}, P_{c2}), as well as energy (k_{12}) and geometric (l_{12}) parameters of the interaction between the two components.

To construct artificial neural networks, models of linear networks and networks with backpropagation of an error were applied. The values of the critical temperature, critical pressure, and the acentricity factor (or normal boiling point) (T_{ci}, P_{ci}, Ω_i) for each of the components were used as the input vector (Fig. 3). The training was carried out using the standard algorithms of the Neural Network Toolbox package of the MATLAB program.

Reliability of the predictions of azeotropic behaviour in the binary mixtures of the refrigerants using neural networks relies on the choice of output value, which classifies mixtures as the azeotropic. We assume implicitly that the model contains submodels, including equation of state, mixing rules, thermodynamic relationships, neural networks models, phase equilibrium data, etc. Prediction of azeotrope can be obtained from the critical parameters and acentric factors of mixture's components. The algorithm is as follows: critical parameters and acentric factors for pure components are provided, and binary interaction parameter k_{12} (output value) is determined by neural network model and criterion of the azeotrope is calculated to classify an azeotrope membership [14].

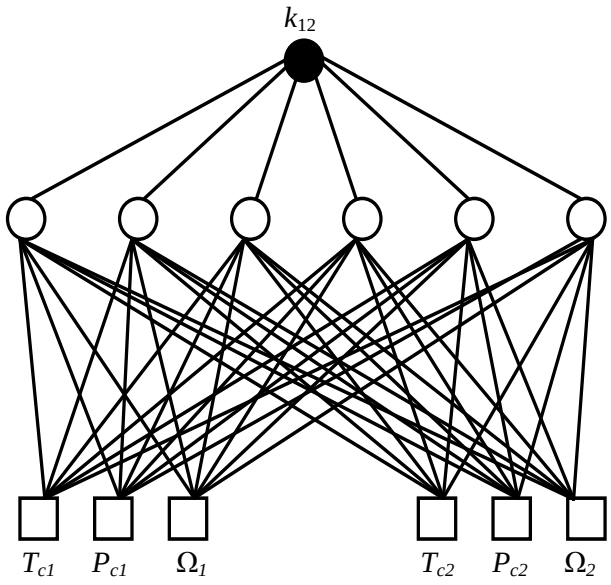

Figure 3 *– The inputs of simulated neural network*

The data on binary azeotropes were grouped into four subsets to obtain interaction coefficients using the available literature and experimental sources (binary synthetic refrigerants, hydrocarbon-synthetic refrigerants, and R744, hydrocarbons, R717, hydrocarbons). The correlation for k_{12} does not depend on the chemical structure of components. The subsets were selected to avoid the membership for allocated classes of substances to select training and validation sets. To demonstrate the universal approach, we included the systems formed with clearly different chemical nature of the components. Critical parameters and acentric factors applying to mixture components, as well as corresponding values k_{12} were included in the training set, which contained the data set for such systems as: R32, R143a, R32, R116, R32, R125, R32, R290, R23, R116, R744, and R125, R717 [18]. In addition, experimental data on phase equilibria for the temperature range 220-300K at different feeds were obtained to find interaction parameters of the RK equation of state for mixtures of natural and alternative refrigerants (CFCs, HCFCs, HCCs, HFCs, HFOs, hydrocarbons, ethers, and other). All potential cases of azeotropy appearance/absence are described for 1540

samples of natural and synthetic refrigerants.

5. Artificial neural network approach for determination of the organic rankine cycle COP

The sustainable development principle considers an integrated and balanced solution of the ecological, economic, social, and cultural challenges arising from the design processes. Power generation utilizing the low-temperature heat sources (320-570 K) as biomass, thermal solar, or waste heat has been becoming more and more significant during last few decades. ORC uses organic working fluids, obtaining higher thermal efficiency than with water used in traditional Rankine Cycles, because of the thermodynamic properties of these fluids. The problem of selection of the working media is intricately linked with a advanced technologies which incorporate concept of sustainable development. Challenge of the working fluid selection has been treated using recent achievements of molecular theory and experimental studies.

The selection of the working fluids with predefined set of properties as inter alia greenhouse effect, flammability, toxicity, thermodynamic properties, performance specifications is one of the most important stages in simulation and the process design. Strategy for working fluid selection is an inverse problem of incorporating the technological performance parameters directly into the design of the ORC plants. However, algorithms for searching optimal working media that possess optimal combination of the properties can be formalized mathematically based on the multicriteria decision-making theory. The generalized efficiency criterion can be represented for the whole system by the vector *K*, including the local criteria K_i as the components for mapping the multiple requirements imposed on the ORC system. A final decision is defined as the intersection of all fuzzy criteria. The fuzzy criteria are represented by its membership function $\mu(X)$.

The membership function can be selected of a linear or nonlinear type upon the nature of the problem. One of the possible fuzzy convolution schemes is presented below. Maximum (minimum) values for each criterion K_i are established via scalar maximization (minimization). Results are denoted as "perfect" X^0 points.

The matrix [*T*], where the diagonal elements are "perfect" points, is defined as follows:

$$[T]=\begin{bmatrix} K_1\left(X_1^0\right) & K_2\left(X_1^0\right)... & K_n\left(X_1^0\right) \\ K_1\left(X_2^0\right) & K_2\left(X_2^0\right)... & K_n\left(X_2^0\right) \\ : & : & : \\ K_1\left(X_m^0\right) & K_2\left(X_m^0\right)... & K_n\left(X_m^0\right) \end{bmatrix}. \quad (7)$$

Minimum and maximum for criteria are defined:

$$\begin{aligned} K_i^{\min} &= \min_j K_j\left(X_j^0\right) = K_i\left(X_i^0\right), i=1...n; \\ K_i^{\max} &= \max_j K_j\left(X_j^0\right), i=1...n. \end{aligned} \quad (8)$$

The membership functions are assumed for all fuzzy goals as follows:

$$\mu_{K_i}\left(X\right)=\left\{\begin{array}{cc} 0, & if\ K_i\left(X\right)>K_i^{\max} \\ \dfrac{K_i^{\max}-K_i}{K_i^{\max}-K_i^{\min}} & if\ K_i^{\min}<K_i<K_i^{\max} \\ 1, & f\ K_i\left(X\right)\le K_i^{\min} \end{array}\right\}. \quad (9)$$

A decision is determined as the intersection of all fuzzy criteria under constraints represented by its membership functions. The solution of the multicriteria problem discloses the meaning of the optimality operator and depends on the decision maker experience and problem understanding. The criterion is written in the ***C***-metrics form

$$K_C=\sum_{i=1}^{N}\left|\mu_i\right|. \quad (10)$$

The level of energy efficiency (Fig. 4) using the HFE – $C_5H_2F_6O_2$ looks more attractive among HFEs: (CF_3OCF_2H – HFE-125), (CHF_2OCHF_2 – HFE-134), (CF_3OCH_3 – HFE-143a), ($CF_3OCFHCF_3$ – HFE-227me), ($CF_3CHFCF_2OCH_3$ – HFE-245mf), (n- $C_3F_7OCH_3$ – HFE-700-347mcc), ($C_4F_9OCH_3$ – HFE-7100 (HFE-449mccc)), and ($C_4F_9OC_2H_5$ – HFE-7200).

Working fluid selection problem has been tackled using achievements of molecular theory, engineering experience and experimental studies. The COP comparison among the ORC with HFE working fluids (Fig. 4) shows the maximum value 4.1% for $C_5H_2F_6O_2$ and minimum COP – 3.6% for C_2HF_5O.

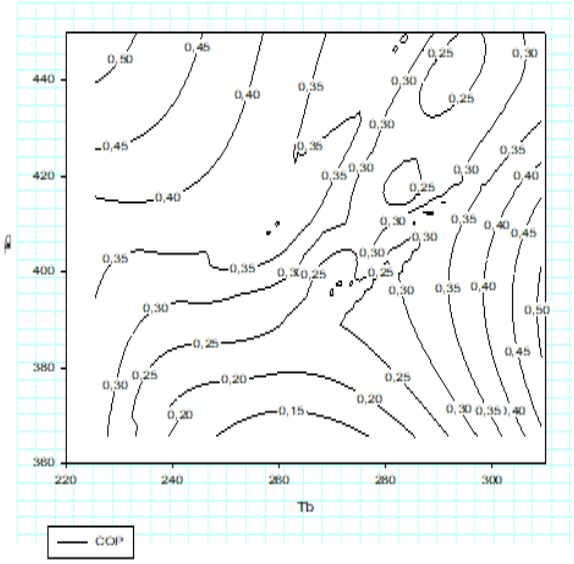

Figure 4 *– COP of the organic Rankine cycle with ANN as a function of boiling point (T_b) and critical point (T_c)*

6. Conclusions

A new approach to predicting the formation of the azeotropic state in a mixture is developed and presented. This approach employs synergy of neural networks and global phase diagram methodologies to correlate azeotropic data for binary mixtures based only on critical properties and acentric factor of the individual components in refrigerant mixtures and does not require intensive calculations.

The most reliable and straightforward way to transform heat into mechanical work is to apply the Rankine cycle. The typical working fluid for such high-temperature cycles is water vapour. Low-temperature heat sources (industrial heat discharges, geothermal sources, solar ponds, etc.) can also be converted into work if organic substances with a normal boiling point are lower than the boiling point for water vapour, are used as working fluids.

This study is one of the first attempts to apply the methodology of tailored, smart substances to select optimal working fluid for the ORC. Construction of ANN correlations between information attributes of the working fluids and efficiency criteria of the Rankine cycle narrows the area of compromise in the space of competitive economic, environmental, and technological criteria.

CRediT author statement

Sergiy Artemenko: Conceptualization, Methodology, Investigation, Data Curation, Formal analysis, Visualization, Software, Project administration, Writing – Original Draft. **Viktor Mazur**: Funding acquisition, Resources, Validation, Writing – Review & Editing, Supervision.

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Машинне навчання для властивостей холодоагентів

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Міждисциплінарний характер нових цілей, спрямованих на розробку робочих матеріалів для екологічно чистих технологій вимагає більш динамічного використання інформаційних технологій (IT) для забезпечення правильних компромісних рішень у конкурентному середовищі. Машинне навчання (ML) — це частина методології штучного інтелекту (AI), яка використовує алгоритми, які не є прямим рішенням проблеми, а навчаються за допомогою рішень незліченної кількості подібних проблем. Машинне навчання відкрило новий шлях у дослідженні термодинамічної поведінки нових речовин. Різні обчислювальні інструменти були застосовані для вирішення актуальної проблеми - прогнозування фазової поведінки soft речовин під значними екзогенними впливами. Метою цього дослідження є розробка нової точки зору щодо прогнозування термодинамічних властивостей м'яких речовин за допомогою методології, яка передбачає штучні нейронні мережі (ANN) та глобальну фазову діаграму для забезпечення кореляції між структурою та властивостями. В роботі представлено застосування машинного навчання в інженерній термодинаміці для прогнозування азеотропної поведінки бінарних холодоагентів і визначення коефіцієнта продуктивності (COP) для роботи органічного циклу Ренкіна (ORC). За даними про кипіння та критичні точки. Запропоновано новий підхід до прогнозування утворення азеотропного стану в суміші, який розроблено та представлено. Цей підхід використовує синергію нейронних мереж та методології глобальної фазової діаграми для кореляції азеотропних даних для бінарних сумішей на основі лише критичних властивостей та ацентричного коефіцієнта окремих компонентів у сумішах холодоагентів. Це не вимагає інтенсивних розрахунків. Побудова кореляцій ANN між інформаційними атрибутами робочих рідин та критеріями ефективності циклу Ренкіна звужує область компромісів у просторі конкурентних економічних, екологічних та технологічних критеріїв.

Ключові слова: *Машинне навчання; Холодоагенти; Прогнозування азеотропного стану; Штучні нейронні мережі; Глобальна фазова діаграма; Органічний цикл Ренкіна; Коефіцієнт перетворення; Термодинамічні властивості*

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