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Estimating the Saturation Thermodynamic Properties of Propene Using a Feed Forward Neural Network

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Abstract: A feed forward neural network model is applied to forecast the saturation thermodynamic properties of propene. The method has been used to estimate thermodynamic properties including the heat capacity, Joule-Thomson coefficient, viscosity, thermal conductivity and surface tension. Conducted experimental investigations show applicability of the proposed approach. Comparing with other theoretical models, this method is both simple and reliable. This will cause to open some potential research areas in order to avoid doing costly and some unnecessary experimental works.

Key words: Propene · Artificial neural networks · Heat capacity · Joule-Thomson coefficient · Viscosity · Thermal conductivity · Surface tension

INTRODUCTION

Propane is derived from petroleum products during oil or natural gas processing, it has widespread applications in industries, for instance, as a fuel gas is commonly applied by scrap yards for cutting carbon steel, where the cut quality is not critical, propane (R-290) can used as a replacement in mechanical refrigeration systems designed to use R-12, R-22 or R-134a chloro- or fluorocarbon based refrigerants. Propane is heavier than air and is compressible to the liquid that is transportable in containers,it is considered as a major commodity in the petrochemicals industry.

Propene has many important reactions in inustries such as, reactions with halogenes, hydrogen halides, sulphuric acid and the processes like polymerization (isotactic, atactic and syndiotactic), as a major industrial chemical intermediate that serves as one of the building blocks for an array of chemical and plastic products such as polypropylene, acrylonitrile, oxo chemicals, propylene oxide, cumene, isopropyl alcohol and acrylic. By considering the importance of propene, prediction the thermodynamic properties of it, is the purpose of this paper. Among many thermodynamic properties, heat capacity (Cp), Joule-Thomson coefficient, viscosity, thermal conductivity and surface tension, which are valuable are considered.

It is known that heat capacity data are important in the engineering design of chemical processes, for instance in generalization heat exchanger and energy balance design calculation or in gas-phase chemical reactions these data are essential for determine the energy necessary to bring the chemical reactants up to reaction temperature. Joule-Thomson coefficients are applied in the Linde technique as a standard process in the petrochemical industry for example, where the cooling effect is used to liquefy gases and also in many cryogenic applications. Viscosity data and also thermal conductivity data are required in many engineering applications in the chemical processing and petroleum refining industries. Surface tension data have special importance such as heat, mass and momentum transfer operations that involve process equipment, for instance heat exchanger, distillation columns, absorption and fluid-flow piping.

In recent years some scientists have tried to develop experimental methods of measuring these thermodynamic properties and on the other hand some investigators have been interested in developing theoretical models to predict these phenomenological behaviors of different substances. For some asymmetric systems, Queimada *et al*. [1] measured surface tension and also made corresponding state model of surface tension [1], Brooks and Mills measured the surface tension of melts by levitated drop method [2] and Sheikh

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and Boushehri applied corresponding state correlation for surface tension of melts [3]. In 2000 McGlashan and Wormald [4], had measured Joule-Thomson coefficient of water vapour by a calorimeter with an adjustable throttle, Diedrichs *et al*. [5] predicted liquid heat capacities by the group contribution equation of state VTPR [5] and Divi *et al*. [6] could measure heat capacities of organic materials by modulated differential scanning calorimetry [6]. Wang *et al*. [7] did a new approach to modeling the thermal conductivity of some materials in 2006 [7] and on the other hand Bhattacharya *et al*. [8] did characterization of the temperature oscillation technique to measure thermal conductivity of fluids [8]. Kadam *et al*. [9] worked on measuring viscosity [9] and Xu *et al*. [10] worked on prediction of viscosity [10]. It should be mentioned that most of the theoretical methods are so complex and require a lot of parameters, for instance, Eslami and Boushehri [11] proposed these formulas for calculating heat capacity and Joule-Thomson coefficient. Hattori and Kito in 2006 applied ANN by considering oxidation of propene [12]. However it was not related to thermodynamic properties of propene. Main contribution of current research is to apply an artificial neural network model as a solid theoretical model in practical experimental cases. To the best of our knowledge, no closely research found to help us present a comparative analysis among pervious methods and current proposed approach.

ARTIFICIAL NEURAL NETWORKS MODEL

Artificial neural networks: According to Filho *et al*. [13], artificial neural networks (ANN) presented by Mc Culloch and Pitts [14] in which ANN are born from approach of developing intelligent systems by simulating the biological structure and the work of human brain. Afterwards, the number of studies on ANN increased considerably. As indicated in Grossmand and Thursby [15] the theory of ANN is based on neurobiology, mathematics and physics. An ANN is composed of hierarchy organized neural bundles, bound parallel to each other. Unlike the classical systems, the use of ANN is based on their pervious experiences. Since information is processed in a parallel fashion by the neurons in ANN, the system is much faster than the classical models. As it is common in the ANN literature, application of those had been carried out in several researches in both classification and forecasting areas. For instance, Zorriassatine *et al*. [16] applied neural network to classify statistical quality control problem. Also Abounoori and Bagherpour [17] developed a generalized regression neural network to estimate industrial cost of production. However, in this paper ANN is applied to forecast several important chemical characteristics in which obtaining those in a library environment using experimental study seems to be much expensive and often impossible to do. Thus, applying an artificial forecasting system which is able to predict results with acceptable percentage of error is investigated.

Network design: According to complex nature of chemical processes, a fully connected feed forward neural network model was selected. Due to experimental data, five inputs and five outputs have been selected. In this section, temperature, pressure, volume, density and internal energy are taken into account as inputs. Also, heat capacity (Cp), Joule-Thomson coefficient, Viscosity, thermal conductivity and surface tension are assumed to be outputs of proposed system in Fig. 1, as it is well indicated there are five, six, four and five neurons on input layer, hidden layers and output layer respectively. Two selected hidden layers and corresponding nodes have been investigated through trial and error mechanism.

Also it is clear that number of input and output nodes derived form nature of problem as mentioned before. To avoid the effect of inputs variation in several domains, all inputs were normalized. Both hidden layers were designed the same as below: Powel optimization algorithm was conducted as learning rule to learn how to fit data based on pervious sets. Within all layer, Input function have been estimated through dot product approach. Moreover, linear transfer function has been used as activation function in all steps. The algorithm had run for more than 10000 times, each performed as it is mentioned. Moreover, Mean square of error had been applied to conduct the algorithm more accurate.

Comparative analysis: To evaluate validation of proposed approach the obtained results by neural network were compared with experimental data gathered in lab environment within 150 data series in which approximately 90 and 10 percent of whole data were selected as training and validation set respectively. However, validation set are derived from data in which never have given to the ANN model previously. The experimental data which are named actual in figures, are the saturation both liquid and vapor properties of Propene from T=197.67 Kelvin and P=0.023323 MPa to T=358.16 Kelvin and P=4.0815 MPa [18]. In order to investigate efficiency of proposed neural

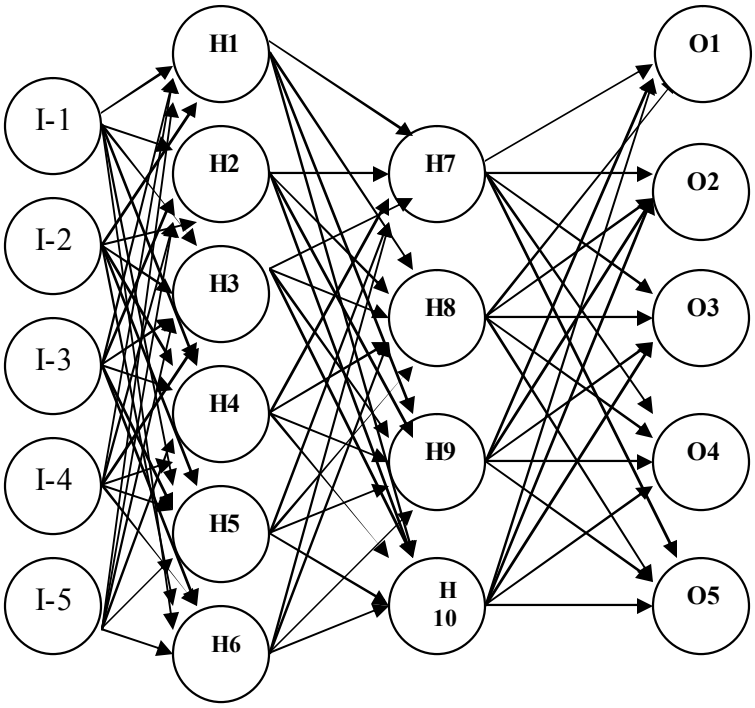

Fig. 1: The structure of proposed feed forward neural network

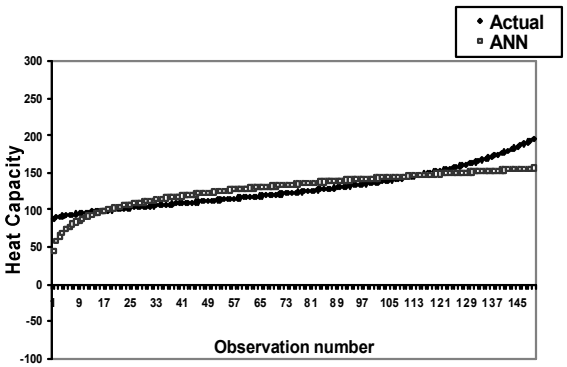

Fig. 2: Comparative analysis for Cp

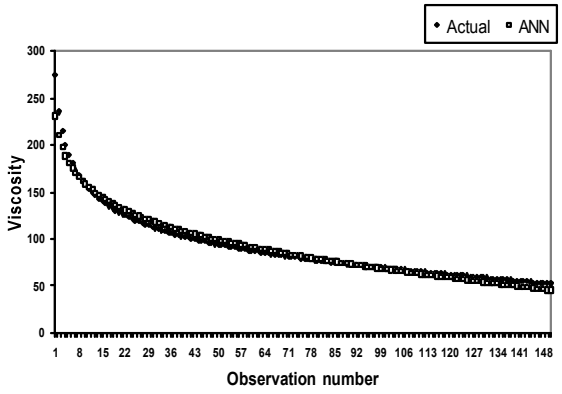

Fig. 4: Comparative analysis for viscosity

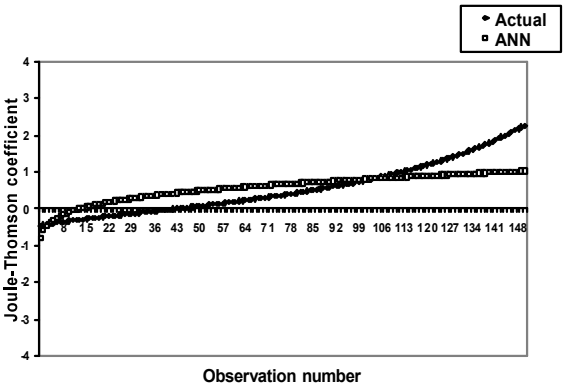

Fig. 3: Comparative analysis for Joule Thomson coefficient

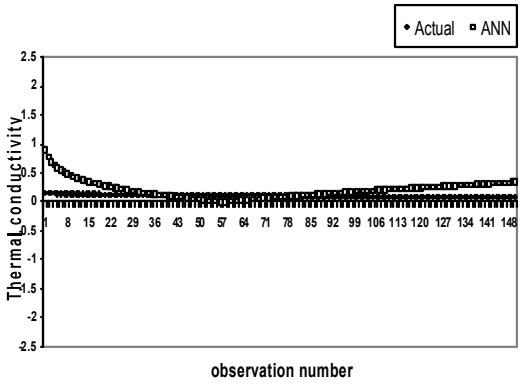

Fig. 5: Comparative analysis for thermal conductivity

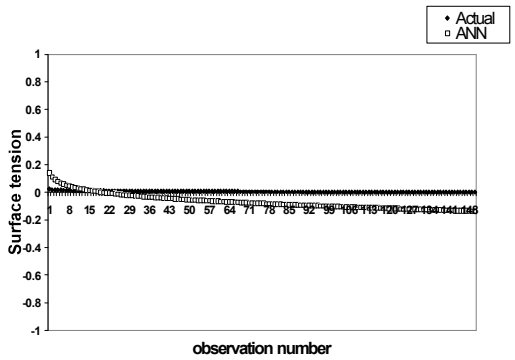

Fig. 6: Comparative analysis for surface tension

network significantly after running comparative analysis through Fig. 2-5, a statistical analysis is conducted through whole data as it is given in Table 1.

RESULTS DISCUSSION

Since correlation coefficient can be vary from -1 to 1, estimated results for heat capacity (Cp), Joule-Thomson coefficient and especially Viscosity show acceptable degree of correlation with actual data. However, further, Viscosity can be estimated using ANN due to its performance within history matching. It will cause cost decreasing. In other way, Thermal conductivity and surface tension have not been well fitted according to correlation coefficient results. That is why, low data variation seen in both of them. As a result, thermal conductivity decreased form 0.15 to 0.08 and surface tension decreased from 0.02 to 0.00 within 150 data series (whole data series). That is mean no fluctuation have seen and data trend for both seems to be straight as you may be seen through Fig. 4 and 5 respectively. Thus, due to this fact that ANN should be applied to forecast behavior of complex variables, both forth and fifth outputs can be taken into consideration as under control variable within libratory condition. Further, in such cases a sensitivity analysis can be conducted for more insurance. It is worth noting that this method is simple and applicable in compare with other theoretical methods such as [11].

CONCLUSION

In this research, five important properties of Propone have investigated through applying a feed forward neural network. The most advantage of proposed system is to estimate whole of required outputs in a unique neural network system simultaneously. This helps us to apply NN instead using costly experimental data. To the best of our knowledge, no closely research found in the literature in which able us to run comparative analysis among proposed and available commonly used approaches. Therefore, the obtained results were compared to experimental cases as well. The results show that three obtained outputs have strong correlations with actual cases. Hereby, other two outputs (forth and fifth outputs) hadn't strong correlation with actual data. However, regarding to low fluctuation and variation in forth and fifth output trends, the models can be efficiently used for the first, second and third outputs as well. Furthermore, the model can be applied for whole outputs with out loss of generality. Further research can be done on developing a customized neural networks application to chemical processes with well organized tuned parameters.

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