Prediction of Thermodynamic Properties of Steam

Group 13

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**Overview**

The Gibb’s phase rule asserts that, for a pure compound, its set of thermodynamic properties (TP) are fully determined by specifying any two of the thermodynamic state variables. However, no model to date can calculate the TP of water, the most widely used industrial chemical, with satisfactory accuracy for engineering purposes. This project aims to capture the complex equation of state that governs the TP of water using artificial neural networks.

**Background**

Industrial steam is primarily used in steam cracking of naphtha to produce light weight hydrocarbons, in steam turbine to generate electricity, and in heat transfer to control temperature. The efficiency of all three processes above depends heavily on the TP of steam, which are complex functions of operating conditions, typically specified as temperature and pressure. Therefore, accurate prediction of TP is fundamental to efficient operation.

The traditional approach to TP prediction is empirical; the TP of steam is measured at a wide range of operating conditions and compiled into tables, and the TP at desired operating conditions is obtained by linearly interpolating within the table.

Chemists and physicists have developed numerous first-principle models for TP prediction, most of which are in the form of Equation of State (EOS). The most popular EOS includes Peng-Robinson EOS and Redlich-Kwong EOS. Despite the great advancement in EOS in the 20th century, its inaccuracy forbids the use of EOS in practical TP prediction.

**Statement of Work**

**Datasets**

The TP of steam is available on NIST in the form of csv files. The dataset includes temperature, pressure, specific volume, specific energy, specific enthalpy, and specific entropy. This dataset is referenced by many authors and used regularly as part of chemical engineering undergraduate curriculum.

**Method**

We will build a multilayer perceptron (MLP) neural network, train the network using the dataset indicated above, and compare its performance to both the linear interpolation method and the EOS method. The use of MLP in predicting thermodynamic properties of different substances has been demonstrated by a few researchers with promising degree of success [1] [2], which motivates the choice of this type of neural network

**Outcome and Performance evaluation**

The outcome of this project will be a neural network that can predict the thermodynamic properties of steam given the operating conditions in temperature and pressure. The quality of prediction will be assessed by comparing the results with experimentally measured values, linearly interpolated values, and with Peng-Robinson EOS predicted values. The neural network will only be useful if it out-performs the EOS method, and it will be practically relevant if it out-performs the linear interpolation method.

**Project Plan**

The GitHub repository for this project can be accessed [here](https://github.com/Bill-Yan-666/CS539). The project timeline is presented in the Gantt chart (Table 1) below.

Table . Project timeline Gantt chart

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  | Week 1 | Week 2 | Week 3 | Week 4 | Week 5 | Week 6 | Week 7 |
| Preprocess data |  |  |  |  |  |  |  |
| Build the MLP neural network |  |  |  |  |  |  |  |
| Build linear interpolator for comparing results |  |  |  |  |  |  |  |
| Build PR-EOS for comparing results |  |  |  |  |  |  |  |
| Write progess report |  |  |  |  |  |  |  |
| Train the network and determine optimal hyper-parameters |  |  |  |  |  |  |  |
| Write final report |  |  |  |  |  |  |  |
| Prepare presentation |  |  |  |  |  |  |  |

**References**

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| --- | --- |
| [1] | R. S. Andrade, R. Magalhaes and M. Iglesias, "Artificial neural network model to predict thermodynamic properties of low molar mass protic ionic liquid," *World Wide Journal of Multidisciplinary Research and Development,* vol. 2, no. 2, pp. 1-6, 2016. |
| [2] | F. Yousefi, H. Karimi and Z. Gandomkar, "Equation of state and artificial neural network to redict the thermodynamic properties of pure and mixture of liquid alkali metals," *Fluid Phase Equilibria,* vol. 370, pp. 43-49, 2014. |