EDUCATIONAL TOOL FOR THE PREDICTION OF THERMODYNAMIC STATE PROPERTIES OF PURE SUBSTANCES IN A GASEOUS STATE

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Abstract. *It is proposed an educational tool in Thermodynamics development in portuguese language. It consists of a software called Softtermo V1.0, for the prediction of Thermodynamic State Properties, of pure substances in a gaseous state, using the Equations of State: Clapeyron, Van der Waals, Redlich-Kwong and derivatives, Peng-Robinson and modifications, Berthelot and its reduced form, and Clausius. From the theoretical basis of these Equations of State, it was developed a software, within Matlab platform, capable to predict the following Thermodynamic Properties: pressure, volume, temperature, heat capacity, internal energy, enthalpy and entropy. For the solution of Cubic Equations of State, the software makes use of numerical methods of Briot-Ruffini and bisection. Softtermo V1.0 presents also other functions, such as: support, theories, converting units and reports, when required by the User. The considerations taken to the property(ies) prediction(s) and to the comparison of selected equations can also be reported at the output of the program. The proposal presents three main advantages with regard to the most software available. The first one is that is not restricted only to the fundamental prediction of PVT properties, extending the prediction of heat capacity, internal energy, enthalpy and entropy proprieties that are obtained from their own by definitions not only of ideal gases but also real gases, the second one is that it works with up to three simultaneous equations of real gases, the third one is that it presents a larger number of substances available in your library, one hundred and fifty, including various gaseous and refrigerants commonly used in engineering.*

Keywords: *Thermodynamics, Software, Prediction of properties.*

1. INTRODUCTION

The determination of the thermodynamic behavior of real fluids had a great importance to the engineering project and industrials process. In the last three decades there was a theoretical advancement follower of the increasing of the technical of numeric calculus due the use of the computers. The use of the equations of states to predict of the thermodynamic properties of the real gaseous is due to restriction of the equation of ideal gaseous when submitted to high pressure or low temperature to produce volume to spread to zero, which is impossible in the real situation (Shapiro and Moran, 2002).

In 1873, to take aim eliminate the restrictive of the Clapeyron's equation, Johannes Diderik Van der Waals added an constant in the equation of ideal gaseous corresponding to correctness of the volume occupied by the molecules of the gaseous, this term was relating to the attraction power of the molecular themselves, (Müller, 2006).

After that, others equations of states arose with more precision than Van der Waals's equation, actually there are around of one hundred equations of state. Many of these equations consist in nonlinear equations which makes difficult to learn them and their applications, in general, there are necessity of the application of numeric methods to obtain the solution, especially the specific volume.

This work proposes an educational tool for the Thermodynamics, which helps the learning process while reduces the time for the execution of equations, as the equations of Van der Waals, Redlich-Kwong, Peng-Robinson, Berthelot and Clausius, between others, in order to predict the Thermodynamics Properties of Real Gaseous. Beyond that, to the prediction of the Thermodynamic Properties, the Software Menu provides Help, Theories (regarding Thermodynamics Properties and Equations of State), Units Converter and Calculus Reports.

Is important to emphasize that the educational software proposed, called Softtermo V1.0, don't ought to substitute in any moment the direct resolutions made by the student during the process of learning. However the Softtermo V1.0 will find applications if utilized for engineering's, chemistry's, and physical's students and correlated areas during solutions of exercises and also for engineer in your activities. For teachers in Thermodynamic field, the Software will increase the velocity of calculus and also provides the possibility the comparison between Equations of State when upon obtained final results, providing more flexibility and objectivity in the analyses of results.

The Softtermo V1.0, moreover, disposes of a comparative study between Equations of State, allowing the prediction of Thermodynamic Properties on until tree simultaneous equations and providing the results to the graphic interface.

2. A BRIEF LITERATURE REVIEW

The Work and Minzoni Santilio (2004) entitled Software for the Calculation of Thermodynamic Properties of Real Gases, is particularly useful for predicting the fundamental properties (pressure-volume-temperature).

The softwares PROPVAP - V.3.03, entitled program to determination of thermodynamic properties of water" (PROPVAP), enables the determination of the thermodynamic properties of water only from the triple point up to 190 bar and 1300 ° C, and " PROPGAS - V03.02, entitled program for the determination of thermodynamic properties of mixtures of Ideal gases" (LLAGOSTERA, 2002), allows the determination of thermodynamic properties of ideal gases and mixtures up to temperatures of 1500 ° C.

The work of Silva and Monteiro Fidelis et al, (2007), VTP 1.0, entitled interactive software for estimating volumetric and thermodynamic properties using generalized correlations to pure gases, presents a database containing the properties of substances (critical temperature, critical pressure, critical volume, acentric factor) to estimating thermodynamic properties. The properties are calculated at the vapor phase through the analytical equations of state van der Waals, Redlich-Kwong and non-analytical BWR-Lee-Kesler.

In Engeering EES equation solver software allows the user to provide two independent properties for it to calculate all other thermodynamic properties of about one hundred substances, and provides numerous tables T_s, T_v, P_v, P_h and h_s. The methodology for calculating the dependent properties are only from The Peng-Robinson equation of state (Klein, 2010).

3. SOFTTERMO V1.0

3.1. Methodology

There are three methods in the Softtermo V1.0 to prediction of the thermodynamic properties, which is the "Single Method", "Semi-Linked Method" and "Linked Method". The Figures 1 to 3 show theses methods. The availability of these three methods aims to reach the necessity of the users, with more flexibility and facility.
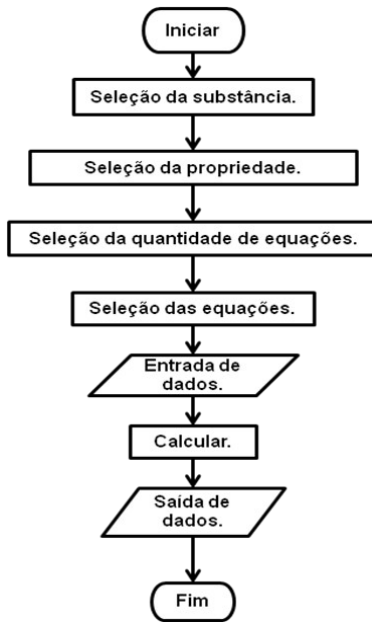
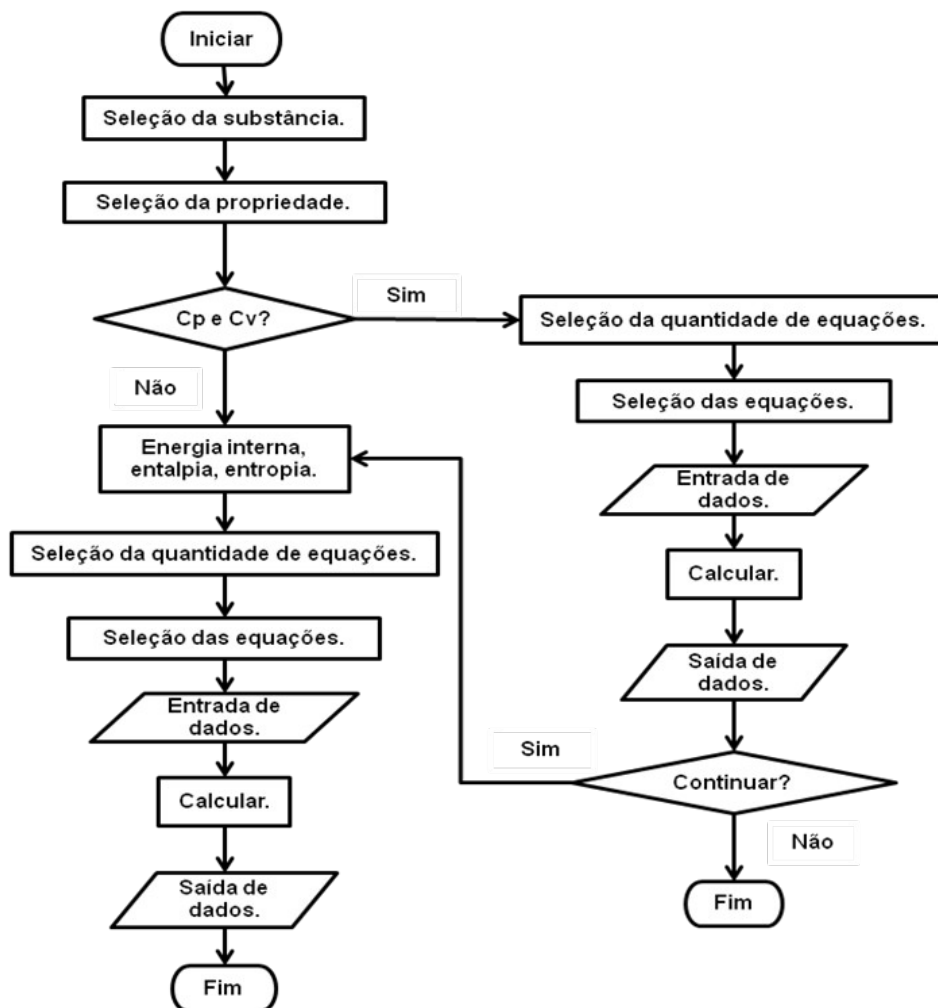Figure 1. Flowchart of the Single Method.
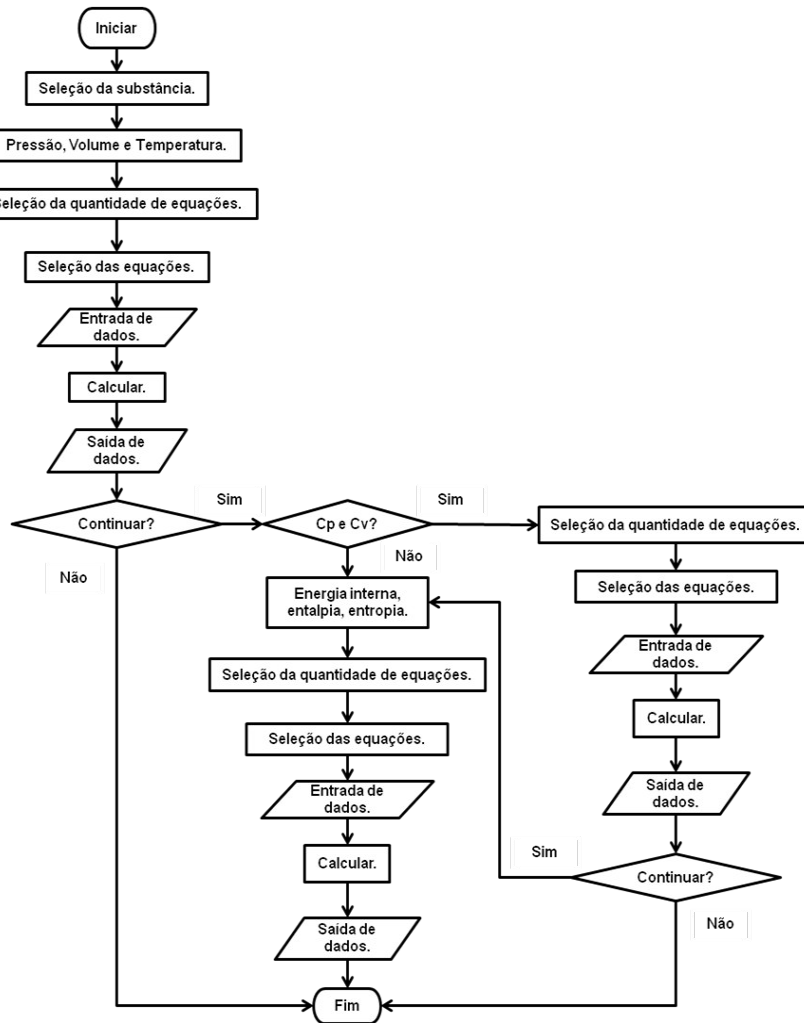
Figure 2. Flowchart of the "Semi-Linked" Method.

Figure 3. Flowchart of the "Linked Method".

3.2. Theoretical analysis

The measurable properties: pressure, temperature and specific volume, can be predicted by the States Equations referred above. Heat capacity, internal energy, enthalpy and entropy proprieties are obtained by their own definitions, together with the applications of Maxwell in relation to the calculus of partial derivates (Annamalai and Puri, 2020).

The mathematical formulation utilized to prediction the specific internal energy was the Eq. (1):

$$u = u_{ref} + \int_{T_{ref}}^{T} c_v \, dT + \int_{v_{ref}}^{v} \left[T \left(\frac{dP}{dT} \right)_v - P \right] dv \tag{1}$$

The Equation (2) corresponds to the mathematical formulation used to predict the specific enthalpy.

$$h = h_{ref} + \int_{T_{ref}}^{T} c_p \, dT + \int_{P_{ref}}^{P} \left[v + T \left(\frac{\partial P}{\partial T} \right) / \left(\frac{\partial P}{\partial v} \right) \right] dP \tag{2}$$

All thermodynamics properties can be expressed in function of two other independent properties (Annamalai, 2002), as so the entropy is calculated with the Eq. (3).

$$s = s_{ref} + \int_{v_{ref}}^{v} \left(\frac{\partial P}{\partial T} \right)_v dv + \int_{T_{ref}}^{T} \frac{c_v}{T} dT \tag{3}$$

The relations between Specific Heats are given by the Eq. (4):

$$c_p = c_v + \left[T \left(\frac{\partial P}{\partial T} \right)_v - P \right] \left(\frac{dv}{dT} \right)_p + P \left(\frac{dv}{dT} \right)_p = c_v + \left[T \left(\frac{\partial P}{\partial T} \right)_v \left(\frac{dv}{dT} \right)_p \right] \tag{4}$$

Another way to show these relations is by Eq. (5):

$$c_p = c_v - \left[T \left(\frac{\partial P}{\partial T} \right)^2 / \left(\frac{\partial P}{\partial v} \right) \right]$$

(5)

4. RESULTS AND DISCUSSIONS

The following are some results of the main menu and secondary, the Graphical Interfaces of In and Out, and the Validation Tests of Softtermo V1.0, used for the Prediction of State Properties of Thermodynamic
Figure 4 consists of the Inicial Interface for Softtermo V1.0.

Figure 4. Inicial Graphical Interface.

By selecting the bottom "Iniciar", the Softtermo V1.0 shows the Interface of Substances and Thermodynamic Properties Selection to be worked by the software, Fig. 5. The option to turn back to the previous interface is available on down-right corner of the Softtermo V1.0.
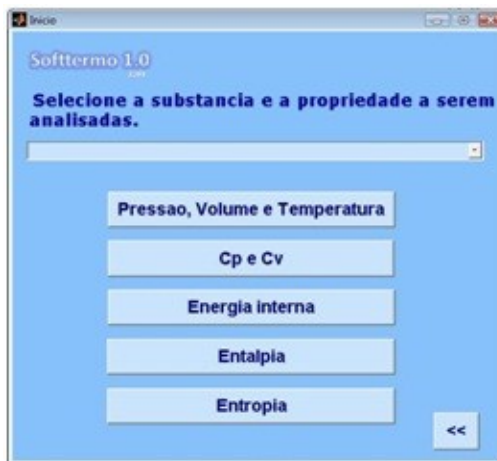

Figure 5. Substances and State Properties of Thermodynamic selection.

By selecting the "Volume" at the interface of Fig. 5, the available interfaces after the selection of Quantity of Equations (Fig. 6) will be in agreement with Fig. 7, varying according to the quantity of selected equations.
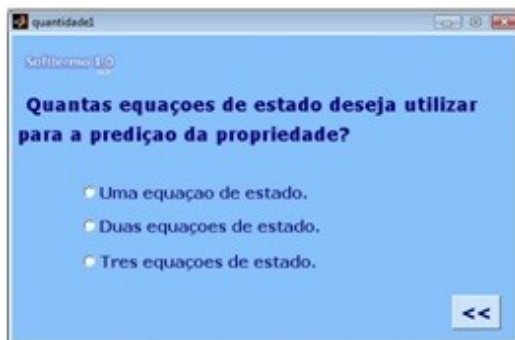
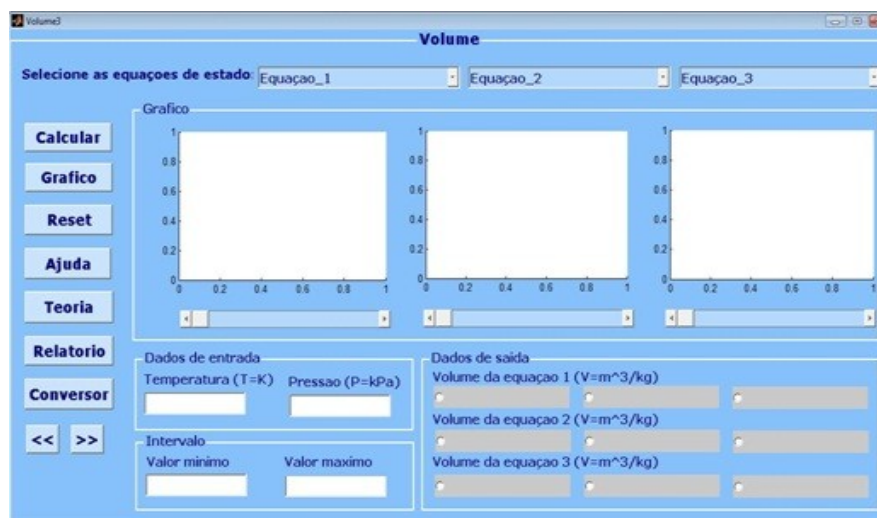Figure 6. Selection of Quantity of Equations

Figure 7. Interface to predict the Volume by using three Equations of State.

The option Reset, available on all graphic interfaces used to predict the States of Thermodynamic, resets all data entries on the interface.

Selecting the bottom "Ajuda", the Softtermo V1.0 shows a graphical interface that teaches the user how to make use of the software, Fig. 8.

Figure 8. Example of "Ajuda" function.

The function "Teoria" presents thirty graphic interfaces containing information about State Equations to Prediction of Thermodynamic Properties and other equations used by Softtermo 1.0, Fig. 9.
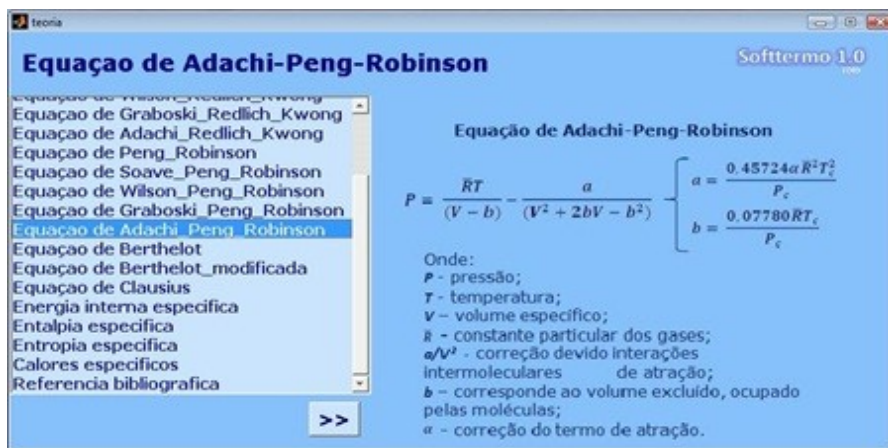
Figure 9. Example of "Teoria" function.

Figures 10 and 11 show some of the values obtained by Softtermo V1.0, observing that the entries data are inserted on the blanks while the exit data are found on the gray spaces. The Figure 12 show the report generated.
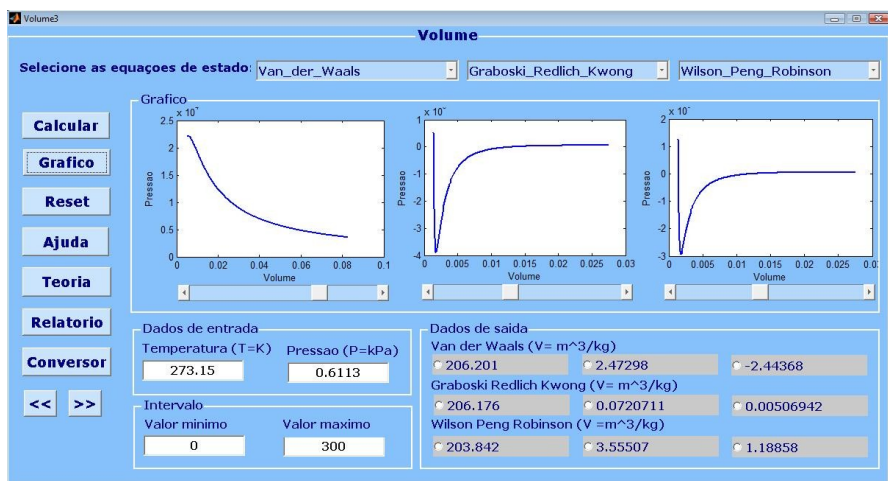

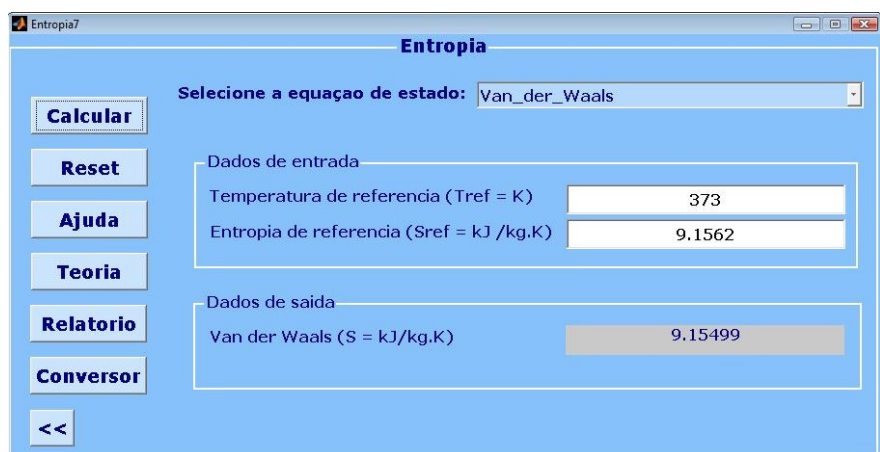Figure 10. Demonstration of "Volume" Calculus.

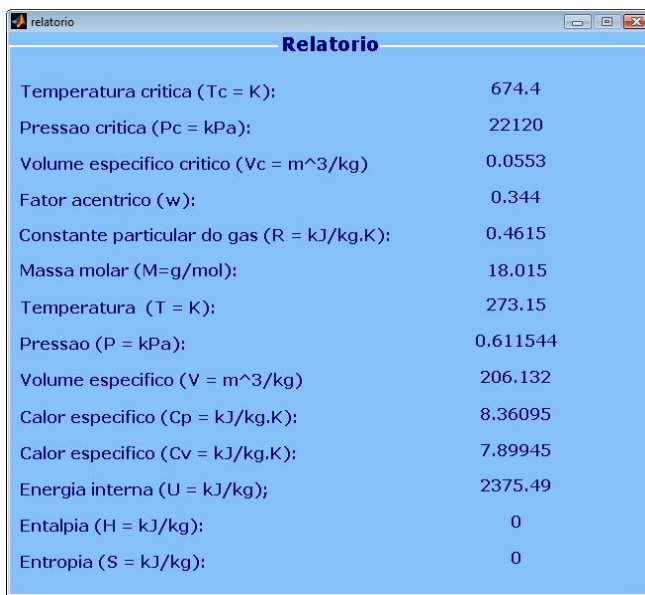Figure 11. Demonstration of Entropy Calculus by the Linked Method.

Figure 12. Demonstration of the function "Relatório".

Table 1. Specific heat of ammonia at constant volume obtained by the equation of Soave-Redlich-Kwong compared to the ideal gas.

Ammonia: vapor saturated						
Tabelated values				Calculated values		
Temperature (K)	Pressure (kPa)	Specific volume (m³/kg)	Cv do gás ideal	Cv do Softtermo (kJ/kg.K)	Absolute deviation (kJ/kg.K)	Relative deviation (%)
255.37200	209.73900	0.56909	7.82067	7.78181	0.03886	0.4968884
257.59400	230.76800	0.52021	7.83467	7.79197	0.0427	0.5450134
259.81700	253.52000	0.47626	7.84868	7.80178	0.0469	0.5975527
262.03900	277.92800	0.43675	7.86268	7.81121	0.05147	0.6546114
264.26100	304.19700	0.40110	7.87667	7.82021	0.05646	0.7168004
266.8300	332.39600	0.36895	7.89067	7.82875	0.06192	0.7847242

The results presented at Table 1 indicate average absolute deviation in module 0.04972 m³/kg and average relative deviation 0.6326%. Such deviations are a consequence of the equation used.

5. CONCLUSION

Given the above and the results presented, an educational tool in Thermodynamics was developed, called Softtermo V1.0 in Matlab, for the prediction of thermodynamic properties of pure substances in a gaseous state using various equations of state, which presents a user friendly platform.

The results showed that for each particular case are shown in the used equations, the characteristic data of each substance and the calculated thermodynamic property.

The validation test of Softtermo V1.0 had shown resulted satisfactory since the limit of application of each equation of state was rejected and that it was used random values of references during the validation procedure.

In relation to the pedagogical aspects the Softtermo V1.0 allows to reproduce quickly and accurately the contents treated in the classroom in terms of mathematical models (equations of state and thermodynamic relations), and the teaching function to start the student's cognitive actions in the external field as well as having the function gnoseological to induce the student to the fundamental representations. It also has a teaching function to enable the student to perform the action of identify the main parameters of the simulations.

In comparison to other software available, its great advantage is that it allows the classroom teacher in the prediction of thermodynamic properties for fifteen different equations of state, besides to allow a comparative study of up to three states simultaneously equations, which is not possible in commercial software available.

The Softtermo presents also a user-friendly interface, with well-designed screens, compact, pedagogically defined so that meets the needs of learning defined according to previously evaluated, i.e, from diagnosis made with the students of this institution, and a robust library and a system very efficient help

The relationship between teacher, student in this system, mainly due to their characteristic design teaching, shows extremely efficient and reflects on the student learning that through "step by step" using the same has been shown to be effective.

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7. RESPONSIBILITY NOTICE

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