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Resumo: *This study aimed to develop Python computer codes addressing problems relevant to the discipline of Chemical Thermodynamics. The choice of language is due to its free nature, open source, and versatility, facilitating access to educational resources. The implementation of libraries and a graphical interface to the codes provides ease in execution and visualization of results. Four libraries were highlighted, including thermo and CoolProp, open-source software facilitating the determination of thermodynamic properties for pure substances and mixtures, allowing the use of various models for critical analysis and selection of the most appropriate. The iapws and XSteam libraries stood out in determining properties of water, steam, and aqueous solutions. All libraries are available on GitHub, a collaborative environment conducive to project contribution and sharing among researchers, constituting a valuable resource for student reference. This work enabled the implementation of more realistic GRAPHICAL ABSTRACT problems, demanding higher cognitive levels compared to traditional resolution with calculators. The computational approach presented offers an effective tool to enhance the teaching of Chemical Thermodynamics, expanding possibilities for analysis and understanding by student*

Palavras-chave: *chemical engineering, education, python, thermodynamics.*

IMPLEMENTING OPEN SOURCE PYTHON LIBRARIES IN TEACHING THERMODYNAMICS

1. INTRODUCTION

Increasingly complex skills have been required for engineers. The National Curricular Guidelines for Engineering (Brazil, 2019) demand from graduates holistic and humanistic analysis and decision-making, as well as aptitude for new technologies. Classes that utilize technological tools can foster not only aptitude for new technologies but also the acquisition of higher cognitive levels, such as analysis, evaluation, and creation (CONKLIN, 2005).

The use of software in Engineering is not new; software such as Engineering Equation Solver (EES), MATLAB, or Aspen HYSYS has been used for thermodynamic simulations. However, its use as a methodological teaching tool is not yet well-established, mainly due to the level of difficulty and high cost. Since its first appearance in 1991, Python has become one of the most popular dynamic languages, along with Perl, Ruby, and others (McKinney, 2017). Coupled with its freeness and ease of use, Python has contributed to the creation of fundamental libraries for expandability in software development. Thus, Python plays an important role as Information and Communication Technology (ICT), being employed in the creation of educational utilities that provide a practical approach to learning. According to Sweigart, A. I. (2015), its use has been effectively employed in offering practical activities in academic environments, with the potential to be adaptable to various teaching and learning styles and enabling the exploration of more realistic and, therefore, more complex problem-solving in the classroom.

As a demonstration of the possibilities of this implementation, this work uses a thermodynamic cycles problem, more specifically, the Rankine cycle, a common theme in Thermodynamics courses in various engineering disciplines. The sizing of this model is based on the determination of variables in the saturation region, traditionally obtained through thermodynamic tables. However, by using Python in conjunction with specific libraries, whose functionalities are listed in Table 1, this process becomes a simplified and efficient "mission" through a graphical interface, providing the student not only with an understanding of the calculations involved but also the apprehension of theoretical situations in different contexts.

Table 1 - Library Functionalities

Library	Use	Open-source	Modeling	Maximum Pressure (Mpa)	Maximum temperature (K)
CoolProp	Superheated Steam	Yes	Helmotz Free Energy	220640	-
Thermo	Superheated Steam	Yes	State Equations	-	-
IAPWSS	Saturation state	Yes	Regressive Equations	1000	1273
XSteam	Saturation state	Yes	IAPWS Extension	1000	1273

Source: Authors

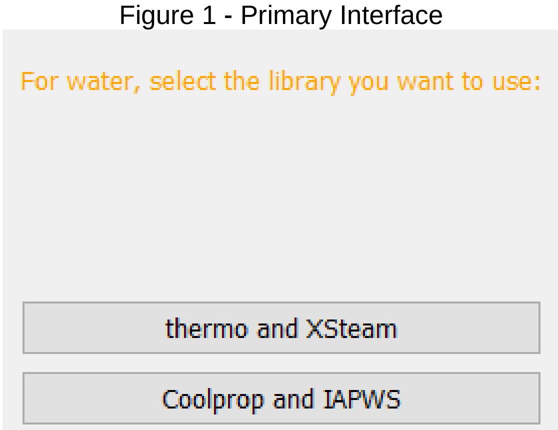
Therefore, this article aims to develop an educational methodology suitable for contemporary demands by incorporating Python as a working tool, analyzing different libraries in the thermodynamic context of a thermal machine.

The developed algorithm demonstrates the implementation of a graphical user interface (GUI) in Python aimed at facilitating the analysis of properties and thermodynamic concepts involved in a vapor cycle, providing intuitive interaction for different states of the cycle.

2. METHODOLOGY

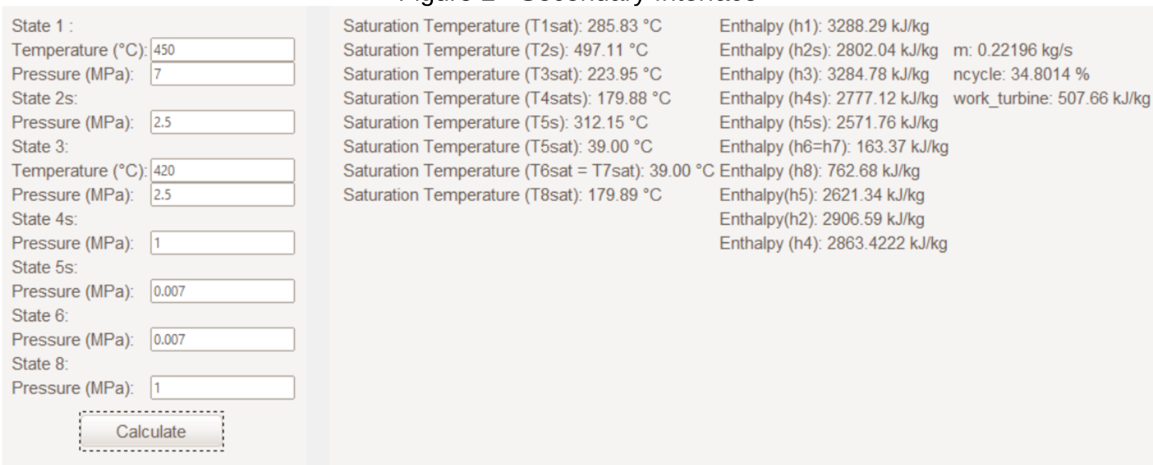
This tool consists of two main interfaces defined as frontends, both developed entirely in Python with the Tkinter library. In the initial interface, the user has buttons to select the thermodynamic libraries to be used. On the other hand, in the secondary interface, the user has indicative labels about the data that can be entered in each input field and the display of results in text form.

Figure 1 - Primary Interface



Source: Authors

Figure 2 - Secondary Interface



Source: Authors

The backend of the application refers to the part that deals with processing and calculation logic, composed of three classes. The main one, called "SteamCalculatorApp," plays a central role in the application, controlling the graphical interface and managing user interaction. By creating instances (represented by the use of the "self" function), this class allows the user to manipulate values in the input fields, which are then used to perform calculations and display results in the secondary window. Additionally, the "SteamCalculatorApp" class includes the algorithm responsible for determining each property of the vapor cycle based on the available libraries, whose function is implemented in the "calculate_enthalpies" method.

The second class, responsible for user interaction, is named "input_widgets." This class is responsible for creating labels and input fields in the graphical interface, facilitating the insertion of desired temperature and pressure values. Once the data is inputted by the user, the program utilizes these values to execute the calculations defined in the "SteamCalculatorApp" class when the "calculate" button is pressed.

Finally, the "output_widget" class aims to display the calculation results in text format, positioning them to the right of where the data is inputted for better user visualization.

It is important to highlight that the entire algorithm was developed based on the documentation provided by each library used.

3. RESULTS AND DISUSSION

To validate the program, we refer to the work of Joshi et al. (2023), in which a system composed of three distinct turbines was proposed: high pressure (h.p.), intermediate pressure (i.p.), and low pressure (l.p.). At the beginning of the cycle, steam is supplied to the turbine at a pressure of 7 MPa and a temperature of 450°C. After the first expansion in the high-pressure turbine, the steam is heated to 420°C. Then, expansion occurs in the intermediate-pressure turbine until reaching a minimum pressure, at which point some steam is extracted to heat the feedwater to 180°C. The remaining steam expands until reaching a pressure of 0.007 MPa in the condenser. The isentropic efficiencies of the turbines are provided: 78.5% for the high-pressure turbine and 83% for the intermediate and low-pressure turbines. In order to achieve these results, it is necessary to determine the enthalpies (Table 2) at each stage of the cycle (Table 3).

Table 2 - Enthalpies obtained from libraries by states along with their absolute errors

	Enthalpies (kJ/kg)			Absolute Error (%)	
State	**Reference**	**thermo x Xsteam**	**Coolprop X IAPWS**	**Reference - Thermo x Xsteam**	**Reference - CoolProp X IAPWS**
1	3287,949	3270,00	3288,00	0,546	0,002
2s	2801,964	2802,00	2802,00	0,001	0,001
2	2906,451	2902,00	2906,00	0,153	0,016
3	3284,477	3207,43	3284,78	2,346	0,009
4	2863,386	2850,00	2863,42	0,467	0,001
4s	2777,12	2777,12	2777,12	0,000	0,000
5	2621,29	2619	2621,34	0,087	0,002
5s	2571,747	2571,76	2571,77	0,001	0,001
6	163,342	163,37	163,37	0,017	0,017
7	163,342	163,37	163,37	0,017	0,017
8	762,525	762,00	762,68	0,069	0,020

Source: Authors

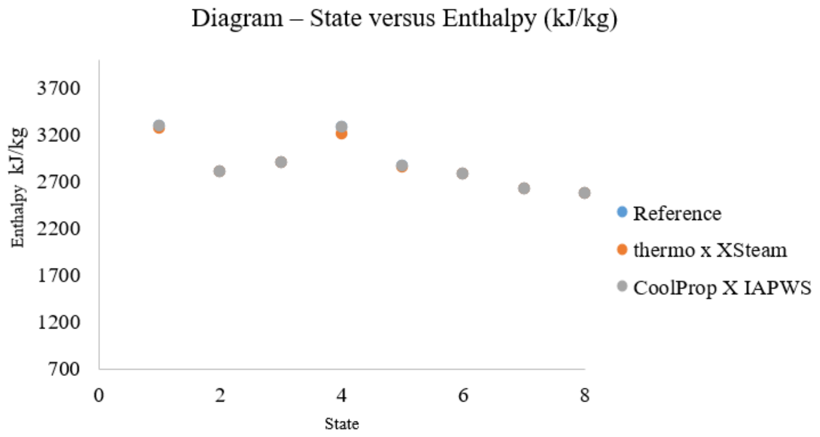
Table 3 - Entries and Outputs Present in Each State of the Cycle

State	Entry	Output	Isentropic Expansion
1	High pressure turbine	Reheater	-
2s	-	-	High pressure turbine
2	Reheater	High pressure turbine	-
3	Low pressure turbine	-	-
4	Intermediate pressure turbine	Intermediate pressure turbine	-
4	-	Feed Water Heated	-
4s	-	-	Intermediate pressure turbine
5	Condenser	Low pressure turbine	-
5s	-	-	Low pressure turbine
6	Pump 1	Condenser	-
7	Feed Water Heated	Pump 1	-
8	Pump 2	Feed Water Heated	-
9	Reheater	Pump 2	-

Source: Joshi et al. (2023)

The description of Graph 1 is a comparative analysis of the effectiveness of thermodynamic libraries used to determine water properties. The orange dot represents the thermo and Xsteam set, while the gray dot represents CoolProp and IAPWS. This approach highlights not only the speed of processing but also the accuracy, evidenced by the minimal discrepancy compared to reference values, noticeable by the uniformity of variables in each state. These results underscore the feasibility and usefulness of using open-source libraries as a complementary tool in educational environments.

Graphic 1 - Comparative Diagram Between Each State and the Obtained Enthalpies



Source: Authors

4. CONCLUSION

The use of this tool has enabled undergraduate students to pose questions and engage in a more critical analysis. Even after a theoretical lecture on the topic and conventional problem-solving, the questions raised during the use of the ICT demonstrated that a deeper understanding and even a critical sense of the process were occurring. Questions such as: What happens if the input of the fluid, which is superheated vapor, is replaced by saturated liquid or saturated vapor? Why is enthalpy used in efficiency calculations? What happens when I increase or decrease temperature and pressure values at each point in the system? And if I change the turbine's work, what happens to the cycle's efficiency? In classroom problems, the organic Rankine cycle is rarely discussed, despite its similarity to the classic Rankine cycle with water vapor. The focus for this utility was on implementing analysis for water vapor cycles; however, it is possible to extend the application to include other fluids, such as those used in organic Rankine cycles, without overly burdening classroom time. This way, comparative analyses can be proposed between cycles, their efficiencies, and the reasons for the differences found (Wanke, 2019).

5. REFERENCES

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