

## **An Online Tool for Facilitating Thermodynamic Property Lookups**

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## **Abstract**

Property lookups are a critical element of undergraduate engineering thermodynamics courses. A student focus on the process of property lookups, however, can serve to obfuscate higher level learning objectives and analysis. We discuss application of PYroMat, an open-source, Python-based thermodynamic lookup package, to simplify property lookups and enable students to focus on deeper investigation of core concepts. While PYroMat has previously been reported as a classroom tool, the present study reports on development of a set of online calculators based on the PYroMat package to eliminate the need for students to learn programming skills alongside the thermodynamics content. Results from a survey indicate potential for the tool, but interpretations are somewhat limited by a small sample size. We believe that dissemination of these tools have the potential to facilitate student learning and encourage exploration of thermodynamics concepts.

## **1. Introduction**

Thermodynamics is a core topic in a number of traditional undergraduate engineering disciplines, so in the transition to Open Educational Resources (OER), it is essential that we develop not only sufficiently robust texts on the topic, but also the computational tools on which these courses rely. Finding open-source replacements for the software that is currently sold with thermodynamics texts is more than an imperative for OER, it is an opportunity to reimagine how students engage with the material.

For over a century, the thermodynamic properties of steam, refrigerants, air, and countless other substances of engineering relevance were contained in pages of tables thick enough to comprise multi-volume books of their own. A variety of styles of computational tools have arisen in recent decades to automate the tedium of extracting numerical values from tables, but they may suffer from a shortcoming. They may be platform-locked or available for purchase (e.g. [1]) or they might be circulated with texts on the topic (e.g. Engineering Equation Solver [2]). What open-source options exist are usually contained in specialized advanced packages designed for researchers, professionals, or at least students at the graduate level [3].

The PYroMat package for thermodynamic properties is an open-source Python-based package that has historically only been available for Python command lines. Prior works implementing it in thermodynamics classes have required students to learn at least a minimum amount of Python coding before they could benefit from the tool. In this work, we describe individual educational modules built on a web-based graphical interface for the PYroMat package.

The effort has two distinct but compatible goals:

1. To establish an open-source alternative to traditionally proprietary or specialized software packages providing thermodynamic properties,
2. To enable the use of more active problem-based approaches that are not typically practical with cumbersome table-based calculations.

The goal is not to eliminate the analytical skills obtained by practicing table look-ups, but to better establish the foundational concepts by empowering students to perform more exhaustive analyses than would typically be feasible.

## **2. Background**

Typically, students have performed the task of property lookups using property tables. Looking for methods to move beyond tables, faculty may encounter a number of modern, computer-based tools exist that have been created to provide thermodynamic data for a variety of commercial and academic purposes. A more detailed discussion of the state of available tools may be found in [3], however some key points are summarized here. In general, tools that are commonly employed for classroom purposes do not experience wide adoption in industry and vice versa. Codes that are useful in the classroom may be limited in accuracy or documentation, when scaling up to be used on real-world analyses. Conversely, those codes that are employed widely in industry frequently target specialized communities such as chemical equilibrium and combustion (STANJAN [4], Chemkin [5], Cantera [6]), or may have high barriers for entry in terms of costs. Tools targeting any audience may suffer from being limited to operation on a specific platform.

In general a universal thermodynamic data tool needs to meet the needs of three constituent groups with different needs: students, faculty and industry. Ultimately, in order for a tool to be useful in industry, it should be extensible, accurate (based on established data sources) and reliable. Students and faculty, on the other hand, are primarily concerned with ease of access (especially cost), ease of use and availability of documentation. Classroom time is limited, and reducing overhead for deploying a tool in the classroom is extremely valuable.

In an ideal world, students would be able to apply their classroom skills directly in the workplace upon graduation. When choosing a thermodynamic property tool for academic purposes, we suggest three key characteristics that an ideal tool would exhibit:

- Should be low cost (preferably free) and easily accessible across platforms
- Should be simple enough for novices to use
- Should be attractive to industry and thus useful for the students beyond their academic career

Our group has previously tried to address these three areas in the classroom through implementation of PyroMat, a computerized thermodynamic property lookup tool developed in Python [3]. PYroMat is licensed under the GNU Public License version 3, and is carefully documented as an open-source package. PYroMat uses standard property equations from the literature and can be used on any platform that can run Python.

In discussing the use of technology tools for education, Karimi [7] recommends that when utilizing such tools, care should be taken to ensure that they are not treated as “black-boxes,” such that students fail to take time to gain physical insights. We have demonstrated the use of PYroMat relative to this recommendation previously by using this tool to enable Problem Based Learning techniques in a thermodynamics course [8]. By utilizing PYroMat, we were able to encourage more student exploration of thermodynamic processes, which provides them opportunities to explore the physics more deeply.

At present, use of PYroMat relies on a code-level interface utilizing Python function calls to compute properties. In this paper, we report on further development of PYroMat as an educational tool through an Open Educational Resource format, in the form of an online tool that was developed to allow students to utilize PyroMat from any computer, and without the need for learning Python programming. This serves to improve platform independence and access to PYroMat and simplifies the use of the tool for novices and hopefully to better achieve the three goals that guide the platform development stated previously.

### **3. Description of the Online Tool**

Previous work has detailed has provided a summary of the design of PYroMat and has given snapshots of its key features. A summary of the current status of the library is as follows:

- Support for property lookups for a wide range of ideal gases
- Support for property lookups for three multi-phase substances (Water, R-134a, CO<sub>2</sub>), with a clear framework established to add more.
- An introductory framework for a cycle analysis toolkit (primarily focused at an undergraduate audience)
- A set of live webpages that provide a server-side implementation of several common calculations (described in further detail below)

The online tools being detailed herein consist of active content webpages that allow for computation of thermodynamic properties and perform related calculations. These are currently hosted on the PYroMat homepage. The simplest page provides for complete calculation of a

thermodynamic state, with two modes for user interaction: 1) entering property values as fields to obtain precise lookups and 2) clicking on property diagrams to provide a more visual representation of the lookup. A second, similar page, provides a similar interface for calculating saturation properties. A third page was created that facilitates computations for a simple Rankine cycle design. This tool is used to support the previously reported Problem Based Learning assignment previously reported on [8]. All of these pages serve as an interface layer between the user and the Python function calls that obtain property data from PyroMat, to eliminate the need for manual programming. These tools are provided as Open Educational Resources that can be adapted or built upon by users, and expanded for use in their own courses.

Functionally, these pages were developed using an interface that communicates with a server-side Python installation using CGI. The interactive plot element uses JavaScript to identify the position of the mouse cursor and map it into graph space coordinates. In the case of user entry or plot coordinates being found, the requested state is sent via CGI to the PYroMat backend, and used to generate a new HTML response with the updated text and graphics.

From a pedagogical perspective, the use of this tool provides a means by which exploration of problems can be fostered. Utilizing traditional table lookups makes iteration on cycle problems time prohibitive, making it very difficult to provide students with opportunities to explore cycle design space and observe the effects of changing variables. In this paper we discuss the functionality and capabilities of the tool and provide a few example use cases that can serve as a launching point for instructors who may consider adopting it in their courses.

**State Parameters**

Fluid: mp.H2O  
 Pressure: 101.325  
 Temperature: 300  
 Specific Enthalpy:   
 Specific Entropy:   
 Specific Volume:   
 Quality:   
 Update

**Units (Show/Hide)**  
 Pressure: kPa  
 Temperature: K  
 Energy: kJ  
 Matter: kg  
 Volume: m3

**State Properties**

T	p	v	h	s	x
K	kPa	m3/kg	kJ/kg	kJ/kgK	-
300.	101.325	0.001 003 45	112.655	0.393 062	liquid

Fig. 1 - Example of the single-point property calculator.

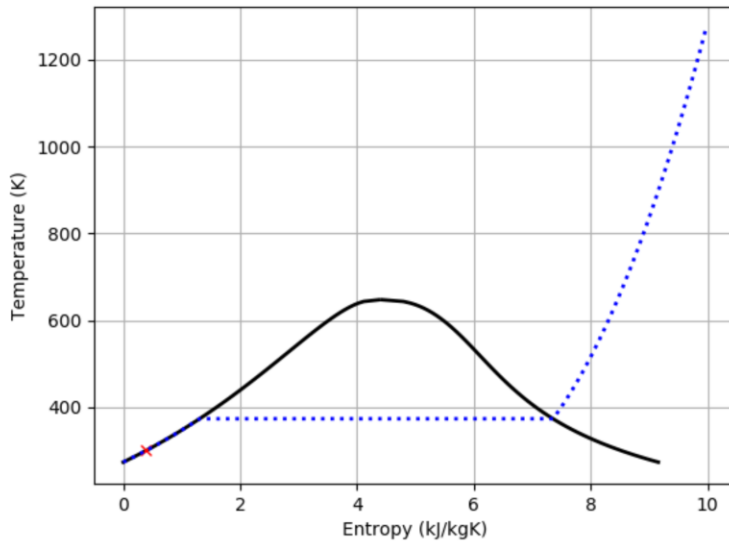


Fig. 2 - Example T-s diagram for the state shown.

#### 4. Survey

We implemented these PYroMat based calculators in a single undergraduate engineering thermodynamics course as a pilot test and gathered usability data to help guide future tool design. Students in the course were trained using both traditional table methods and the online tool, and were asked to use the tool for completion of their homework assignments throughout the semester. A total of eight homeworks were assigned, in addition to a single Rankine Cycle Design project. Student reaction to the tool was measured using the website version of the System Usability Scale (SUS) [9], a survey instrument designed to measure website usability, and that has been validated in the literature [10]. The survey contained ten questions rated on a 1-5 Likert scale from strongly disagree (1) to strongly agree (5). The questions for the SUS are listed here:

1. I think that I would like to use this website frequently
2. I found the website unnecessarily complex
3. I thought the website was easy to use
4. I think that I would need the support of a technical person to be able to use this website
5. I found the various functions in this website were well integrated
6. I thought there was too much inconsistency in this website
7. I would imagine that most people would learn to use this website very quickly
8. I found the website very cumbersome to use
9. I felt very confident using the website
10. I needed to learn a lot of things before I could get going with this website

Students were also asked to respond to the added statement on the same scale:

11. I used the website to explore what happened when property values were varied.

Results of the survey were tabulated and are presented in Table 1. The data collected are based upon a relatively small number of participants (6 students), limiting the generalizability of conclusions, however these early usability results are promising.

**Table 1: Usability Survey Results**

<b>Survey Question</b>	<b>Min</b>	<b>Avg</b>	<b>Max</b>	<b>Interpretation</b>
I think that I would like to use this website frequently	3	3.2	4	Neutral
I found the website unnecessarily complex	1	1.5	3	Disagree
I thought the website was easy to use	3	4.3	5	Agree
I think that I would need the support of a technical person to be able to use this website	1	1.8	3	Disagree
I found the various functions in this website were well integrated	3	4.2	5	Agree
I thought there was too much inconsistency in this website	1	2.0	3	Disagree
I would imagine that most people would learn to use this website very quickly	2	3.8	5	Agree
I found the website very cumbersome to use	1	2.2	5	Disagree
I felt very confident using the website	2	4.0	5	Agree
I needed to learn a lot of things before I could get going with this website	2	2.7	4	Neutral
I used the website to explore what happened when property values were varied.	4	4.8	5	Strongly Agree

*All responses were on a 5-point Likert scale from 1 (Strongly Disagree) to 5 (Strongly Agree)*

Of note in the results, no single measure of usability was worse than the neutral response (for even questions, noted in white rows, lower averages denotes higher usability). On average, student responses showed a bias of 0.9 points in the direction of favorable usability. There is certainly room for improvement, but these are reasonable results for a tool at this stage.

Also of note are the responses to the last question, which was related to the pedagogical motivation of the project. Since one of the main reasons to go from data table lookups to an automated tool such as this is to encourage students to explore the impact of various inputs, it's very encouraging to see that students were in fact exploring the impact of various input

conditions. Additionally, this supports the notion that property lookup tools can be an enabling technology to foster higher level thinking in thermodynamics courses, and justifies continued development and improvement of the tool's usability.

In terms of areas for improvement, in the open response section of the survey two of the six students mentioned frustration with needing to refresh the page and start over with invalid or out of bounds inputs. This obviously breaks the flow of exploration and is a new target for improvement. Other requests included the addition of more substances and the inclusion of a mobile app for students that want to access the tool via their phone.

## **5. Conclusions and Future Work**

The open-source PYroMat library has served as a suitable property lookup tool for an undergraduate thermodynamics course. Several webpages were created to provide an interface to PYroMat calculations, eliminating the need for students to create their own Python code to perform the calculations. Students were surveyed about use of the tool for their homework in the course, with results reported in the preceding section. In general, the results indicated agreement with the usefulness of the tool, and showed support for the stated goal that PYroMat can enable student exploration in the classroom. Generalizability of survey results was limited by a small sample size, so further research may be warranted to further validate these results. From a faculty perspective, we are hopeful about the potential of this tool to continue to facilitate exploration of thermodynamic properties by students, and to expand the range of assignment types that can feasibly be implemented by students.

Several key areas of further work are planned to improve the quality of the both the PYroMat backend and the web interface:

- Standardize the property access interface (in the Python backend) across both multiphase substances and ideal gases.
- Improve the numerical convergence of the inverse property algorithms (required for some property combinations, e.g.  $p$  and  $s$  or  $T$  and  $s$ ).
- Add more cycles to the toolkit.
- Expand the documentation on the PYroMat website to facilitate new users (note that documentation IS present in the open source code).
- Create additional live modules and improve their interface.
- Reduce or eliminate the need to refresh the page after invalid inputs.

After further tool expansion, refinement, and usability analysis, there is also room to examine student learning behavior with the tool. As stated earlier, the tool is designed to encourage student exploration. A larger sample size of students will be necessary, but work in this area also represents an interesting path for future research.



Other faculty interested in applying this tool in their classes, or in tracking its ongoing development, may find the online calculators freely available at [www.pyromat.org](http://www.pyromat.org).

## Acknowledgement

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