AC 2011-799: A STUDENT-BUILT INTERNAL COMBUSTION ENGINE SIMULATION USING EXCEL

Robert McMasters, Virginia Military Institute

Robert L. McMasters was born in Ferndale, Michigan, in 1956. He graduated from the U.S. Naval Academy, Annapolis Md, in June 1978 and completed Naval Nuclear Propulsion Training in August 1979. He subsequently served as a division officer on the USS Will Rogers (SSBN 659) until 1982. Following a 2 year tour as an instructor at the S1W prototype of the Nautilus, the worlds first nuclear powered ship, he resigned his commission as a Naval Officer and began working as a design engineer at K.I. Sawyer Air Force Base near Marquette Michigan and later at Michigan State University in East Lansing Michigan. He completed the Ph.D. at Michigan State University in 1997 and continued to serve there as a Visiting Assistant Professor until 2004 when he accepted an Associate Professor position at the Virginia Military Institute (VMI) in Lexington, Va. He currently serves as a Professor of Mechanical Engineering at VMI.

A Student-Built Internal Combustion Engine Simulation Using Excel

Abstract

A numerical model for an internal combustion engine has been developed for use in a senior elective course on internal combustion engines. The numerical model for the simulation is built in an Excel file which includes previously-developed functions for obtaining thermal properties for ideal gases. The properties include enthalpy, internal energy and the specific entropy at a pressure of one atmosphere. Prior to the use of the functions in the internal combustion engine class, mechanical engineering students enrolled in an undergraduate thermodynamics section were offered the Excel ideal gas computer file for use in completing homework assignments. Additionally, they were offered a Mathcad file programmed with ideal gas properties for air in a very similar fashion. The students were offered the option of using either of these programs on any homework or on examinations involving ideal gas problems. They were also offered a choice of using neither of these programs, interpolating ideal gas data out of the textbook instead. Records of the student selections and preferences are presented as part of this research.

The numerical internal combustion engine model uses one degree of crankshaft rotation as its differential element size, so there are 360 steps in a complete rotation of the model. Students build the model on their own by following the example presented in class. In each step, the combustion chamber volume is computed using the global input values for bore, stroke, piston rod length and crankshaft angle. Using these volume values, the cylinder pressure is calculated by using the ideal gas law and the given quantity of air and vaporized fuel in the combustion chamber, based on an assumed temperature. A converged solution for the temperature is next found through an energy balance equation where the work of compression or expansion, from one crank angle increment to the next, is set equal to the change in the internal energy of the mixture of gasses in the cylinder as a function of temperature. By using a solver routine, custom-programmed as a macro in Excel, the temperature at each crank angle increment is solved for sequentially for all 360 increments. The ignition timing for a spark ignition engine, or the fuel injection timing for a compression ignition engine, can be selected by the student. Additionally, this ignition or injection point can be optimized using a custom-programmed optimization macro in the Excel file.

With pressure and temperature calculated as functions of crank angle for an entire rotation of the crankshaft, the net power produced by the engine can be calculated using the engine RPM value, which is selected by the students. As the engine speed is varied, the students can see the changes in power produced, engine efficiency, and optimum ignition timing angle. Homework assignments involving these calculations allow the students to get direct experience with these concepts. The addition of the engine numerical simulation segment of the course was extremely well received by the students and comments from a student survey on the subject were very positive.

Introduction

Finding thermodynamic properties for various substances has traditionally been accomplished by using thermodynamic tables. Interpolation between established values is normally required when the desired values of the properties do not exactly match the tabulated values. This can be a time-consuming process, particularly when iterative calculations requiring thermodynamic properties are involved. A Microsoft Excel add-in that is available per Reference [1] includes thermodynamic properties for air and for flue gasses. To provide the versatility needed for a wide variety of fuels and their combustion products, the thermodynamic tables from Reference [2] were written into Visual Basic Applications (VBA) in a Microsoft Excel file as part of the present research. Although thermodynamic functions in Mathcad have been developed by McClain [3], the layout offered by Microsoft Excel with its compact display arrangement is better suited for the numerical modeling of an internal combustion engine than is Mathcad. Therefore, the new VBA functions were written as part of the present research. The functions given in Reference [2] are absolute values which include the heat of formation of the substances. Therefore, these functions can be used for finding properties of mixtures of burned and unburned gasses in the combustion chamber quite readily. These functions also extend to extremely high temperatures, 5000K, which makes them well suited for internal combustion engine use.

These functions have also been used in conventional thermodynamics classes on projects when solving large applied thermodynamic problems. In such cases, the time expended on interpolation can quite easily constitute the majority of the time required for solving the problems. The students can easily spend more time interpolating than in learning how to apply thermodynamic principles. Therefore, once students have shown mastery of the skills needed to interpolate tables to obtain properties for substances, more knowledge of thermodynamic principles can potentially be assimilated if the interpolation steps associated with homework problems, projects and examinations were automated. Historically, in order to avoid excessive time expenditure on interpolation, some instructors have allowed students to approximate interpolation steps on examinations. This allows the instructor to test more of the students' knowledge of thermodynamic principles, since more of the examination period can be devoted to the principles instead of interpolation. This approach is somewhat of a compromise between speed and accuracy. The reduction in accuracy, of course, can make examinations and homework assignments difficult to grade, since all of the final answers are different, even when correctly solved. This is particularly true in assigned problems where there are subtleties which may make small differences in final answers. For example, if an isentropic compressor or turbine efficiency is used in a problem, the outlet temperature of the device may only differ by a few degrees from the purely isentropic case. If students are estimating thermodynamic properties, the correct or incorrect use of the efficiency calculation can easily be obscured.

Program Development

The data tables used for the interpolation scheme in this research were scanned using optical character recognition. The files were then adapted to a Microsoft Excel worksheet, which required some manual separation of rows and columns, due to errors committed by the optical character recognition program. However, the vast majority of the data scanned correctly. Residual isolated errors were detected by graphing the data. Since ideal gas properties are functions of temperature only, each of the properties was graphed as a function of temperature and visually checked for smoothness. In this way, additional scanning errors, such as missing decimal places became obvious anomalies in the graphs, which aided in error detection and rectification.

With the property tables in place, on a dedicated worksheet called "Data", the property functions could be developed. These property functions were written using the Visual Basic Add-In feature provided as a standard feature with Excel. This ad-in allows the Visual Basic language to be used to construct built in functions for the Excel Worksheet, which are otherwise transparent to the user. These functions can then be accessed by the user, just as trigonometric functions or logarithmic functions are in the standard Excel software package. Table 1 shows the functions which were added as part of this research, allowing thermal property recovery using Excel.

Table 1: Substances for which functions were developed for thermodynamic properties and their associated chemical symbols.

Gasses Included	**Chemical Composition**	**Fuels Included**	**Chemical Composition**
Hydrogen	H_2	Methane	CH_4
Carbon Monoxide	CO	Propane	C_3H_8
Carbon Dioxide	CO_2	Butane	C_6H_6
Water Vapor	H_2O	Toluene	C_7H_8
Nitrous Oxide	Ar	n-Heptane	C_7H_{16}
Argon	OH	iso-Octane	C_8H_{18}
Monatomic Oxygen	O	Cetane	$C_{16}H_{34}$
Monatomic Hydrogen	H	n-Methylnaphlalene	$C_{10}H_7CH$
		Methanol	CH_3OH
		Ethanol	C_2H_5OH
		Nitromethane	CH_3NO_2

For each of these chemical species, the absolute molar enthalpy, the absolute molar internal energy and the molar entropy based on zero Kelvin is included. The inverse functions are required for each thermodynamic property in order to find the temperature when the property is known. Since the property values in the tables are not tabulated in uniform increments, as the temperatures are, the inverse functions were more difficult to program. In finding the direct functions, the correct row in the table could easily be located in the program by dividing by the appropriate temperature increment. The proper row in the inverse case was found by making polynomial approximations of the temperatures as functions of the properties. This method was found to locate the correct table row within a tolerance of plus or minus one row. Therefore, once the assumed correct row was initially identified, the program automatically checked the row above and below for verification. From there, the interpolation could be easily performed.

The output of the functions were all checked against each other on an Excel sheet by making a column of temperatures and a column for each of the corresponding properties. Additional temperature columns were made for each of the inverse functions as they computed the temperatures corresponding to each property. The temperatures found by the inverse functions could easily be checked against the original temperature column to assess the accuracy of the functions.

Since the Excel functions use exactly the same tables as the textbook, the students who interpolate the tables arrive at exactly the same properties as the Excel functions. This is one advantage of using the interpolation functions as opposed to using polynomial approximations for the thermodynamic properties. Not only are the steps in homework problems more uniform between students as they check their solutions against one another, the assignments are easier to grade because all of the results should be identical if the problems are done correctly. The Excel functions were written using the thermodynamic tables in SI units.

For the use of the program in the internal combustion engine class, Figure 1 shows the "blank" Excel page as it is provided to the students for downloading from the class web page. As can be seen on this form, the header of the sheet is divided into "engine Input Data" and "Calculated Parameters." The input data section of the form has dummy values inserted and the students can change these values to conform to particular homework assignments. The students are then responsible for generating the calculated parameters. The engine displacement is calculated from the bore, stroke and number of cylinders provided in the engine input data section. Likewise, the crank arm length is calculated by dividing the stroke by 2 and the piston rod length is normally assigned a value of three times the crank arm length. Students can change the crank arm length if desired in order to examine the effect on engine performance. The number of moles of the fuel/air mixture is computed using the ideal gas law at ambient temperature and pressure for the volume of the combustion chamber with the piston at bottom dead center. Torque and power are computed after the rows of the table are filled in below, which are the actual elements of the numerical solution. The "Calculate" button and the "Optimize" button are used in executing the numerical solution.

The first row of the numerical solution portion of the program corresponds to a crank angle of -180^o which is the bottom dead center position with the piston ready to begin the compression phase of the cycle. So the "volume" cell in this row is filled in by computing the bottom dead center volume from the displacement and compression ratio information. Subsequent values of volume are computed using Equation (1) which is derived from the crank arm and piston rod information.

$$V(\theta) = V_c + N_c A_c \left\{ r + l - r\cos\theta - l\cos\left[\sin^{-1}\left(\frac{r\sin\theta}{l}\right)\right]\right\} \tag{1}$$

where $V(\theta)$ is the volume in the combustion chamber as a function of crank angle, V_c is the clearance volume, N_c is the number of cylinders, A_c is the cross sectional area of one cylinder, r is the crank arm length and l is the piston rod length. The next column, the cylinder pressure, is calculated by using the ideal gas law. The initial pressure value at a crank arm position of -180^o is assumed to be atmospheric pressure. For subsequent pressure calculations, the pressure, temperature and volume from the previous step are combined with the volume and temperature from the current step to compute the new pressure. Specifically,

Engine Input Data					**Calculated Parameters**			
Bore		8	cm		Displacement			Liter
Stroke		9.5	cm		Crank Arm Length			cm
Compression Ratio		8			Piston Rod Length			cm
Intake Temperature		300	K		Moles of Air & Fuel			kmoles
Intake Pressure		100	kPa		Torque			ft-lb
Number of Cylinders		4			Power			HP
Engine Speed		2000	RPM					
Ignition Timing		-16.7	Degrees					
					Calculate Temperatures		Calculate	
					Optimize Ignition Timing		Optimize	
Degree-by-Degree Model								
Crank Angle	Volume	Pressure	Temperature	f(t)	U_{calc}	U(T)	Work	U_{error}^2
-180								
-179								
-178								
-177								
-176								
-175								
-174								
-173								
-172								

Figure 1. The “blank” Excel sheet given to students.

$$P_i = \frac{P_{i-1} V_{i-1} T_i}{T_{i-1} V_i} \qquad (2)$$

In this equation, the *i* subscript refers to the current crank arm position and the *i*-1 subscript refers to the crank arm position one degree prior to the current position. With the pressure calculated, the net work between steps can be calculated by

$$W_i = P_{ave}(V_i - V_{i-1}) \qquad (3)$$

Where P_{ave} is the average between P_i and P_{i-1}. With the work calculated, the temperature can be computed by an energy balance. The combustion chamber is assumed to be adiabatic due to the short overall time duration of each stroke. The heat which increases the temperature of the charge comes from the chemical reaction of the fuel and air, so the accounting for this energy is taken care of through the term for internal energy of the products and reactants. The energy balance equation is then

$$\left[1-f(t)\right]\left[u_{\text{reactants}}(T)\right]-f(t)\left[u_{\text{products}}(T)\right]=-w_i \qquad (4)$$

In this equation, the *u* values are internal energy for both products and reactants, as identified by the subscripts. Each of these is a function of temperature. The $f(t)$ values are a function programmed into a VBA function which represents the normalized fraction of the completion of combustion. Figure 2 shows a plot of this function with respect to time. As can be seen in Figure 2, the combustion is essentially complete within 6 milliseconds of the onset of combustion.

With this information in place, Equation 4 is next solved for temperature numerically, time step by time step. Rather than attempt to solve the 360 temperature values simultaneously, they are solved sequentially by a VBA function made just for that purpose, since no built-in feature in Excel lends itself directly to this application. The VBA solver is activated by pressing the "calculate" button on the "blank" Excel page. The sequential solver operates much more quickly than attempting a simultaneous solution, since no iteration is required after an individual line is calculated. Once the temperatures are calculated for each degree of crank arm rotation, the Pressure-volume (P-v) diagram can be plotted as shown in Figure 3. The students can examine the effects of the input parameters on this graph, including engine speed, compression ratio, ignition timing, piston rod length, etc.

Once the initial P-v diagram has been established, and students experiment with changing engine parameters, the ignition timing optimization feature of the program can be implemented. This is initiated by pressing the "optimize" button of the Excel sheet. The optimize routine executes the "calculate" function at three different settings of ignition timing. The engine power output is calculated for each of these three settings and the optimized ignition timing angle is found by an iterative process with a convergence criterion of 0.1 degree between iterations. At this point, the calculation stops and the optimum ignition timing angle is displayed in the appropriate cell and all other parameters, including the P-v diagram, are displayed for the optimized condition. In an additional class session, the students applied a turbocharger to the numerical engine model. Once again, engine parameters could be changed and the effects of these changes on engine performance could be examined, including ignition timing optimization. Table 2 summarizes the steps used in the internal combustion engine calculation.

Results

In addition to being used in an internal combustion engine elective course, the program was utilized in Thermodynamics II, an applied thermodynamics course covering applications such as vapor cycles, gas cycles, refrigeration cycles, gas mixtures, combustion and dissociation. The segment of the course covering gas cycles was the primary area where the thermodynamic property program had applicability. The students in the class were offered both of the Excel files, in English and SI units, with the thermodynamic property functions imbedded, as well as the Mathcad file developed in reference [3] which also has imbedded functions. All of these files were placed on the course web site to be downloaded as desired. The school offers copies

Table 2: Summary of steps by students in developing the internal combustion engine model.

Quantity or Property Calculated	**Procedure Used**
Displacement	Displacement = $\pi \frac{D^2}{2} Nr$
Crank Arm Length	r = Stroke/2
Piston Rod Length	l = 3r
Moles of Air and Fuel (n)	$n = \frac{PV}{\bar{R}T}$
Torque	$T = \frac{\dot{W}}{2\pi(RPM)}$
Power	$\dot{W} = \frac{\sum_{i=1}^{360} W_i}{2(RPM)}$
Volume	$V(\theta) = V_c + N_c A_c \left\{ r + l - r\cos\theta - l\cos\left[\sin^{-1}\left(\frac{r\sin\theta}{l} \right) \right] \right\}$
Pressure	$P_i = \frac{P_{i-1}V_{i-1}T_i}{T_{i-1}V_i}$
Temperature	Found by an iterative process by a pre-programmed routine to match U_{calc} and U(T)
Time	$t = \frac{\theta}{360(RPM)}$
q	Normalized combustion function of time shown in Figure 2.
U_{calc}	Internal energy of the fuel/air/exhaust mixture from the previous step minus the work from the previous step.
U(T)	Internal energy of the fuel/air/exhaust mixture as a function of temperature at the current step
W	$W_i = P_{ave}(V_i - V_{i-1})$
U_{error}	U_{calc} - U(T)

of the Mathcad software to the students, under a site license, for $15 per computer, so most students have both Excel and Mathcad loaded on their personal machines.

The students were told at the beginning of the course that they could use Mathcad, Excel, or textbook table interpolation to find thermal properties. There would be no distinction made in terms of grading, regardless of their choice. They were free to use these programs on projects and examinations as well. They were only asked to identify, on each assignment, the method or methods they chose to use. The class was polled to see if there were any objections to the use of

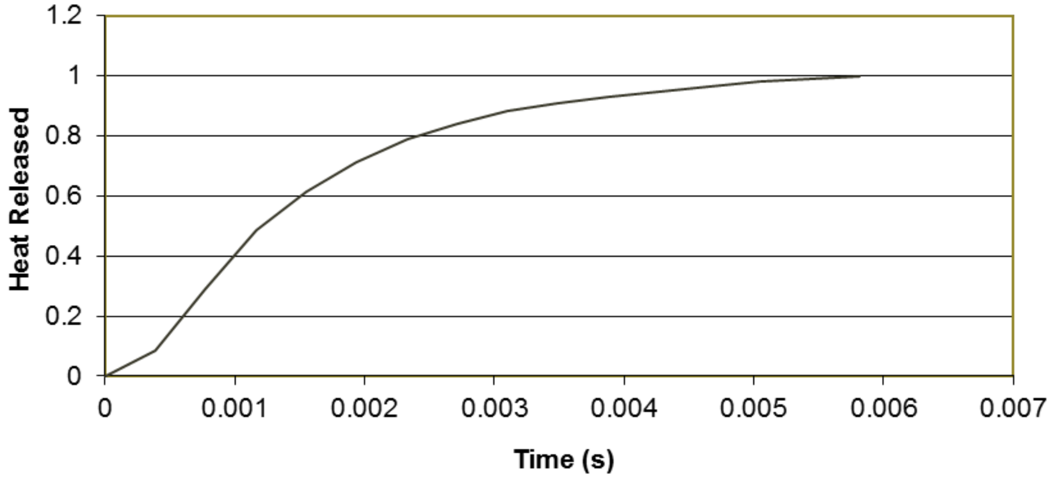

Figure 2. The normalized heat release function, providing the fraction of combustion completion as a function of time.

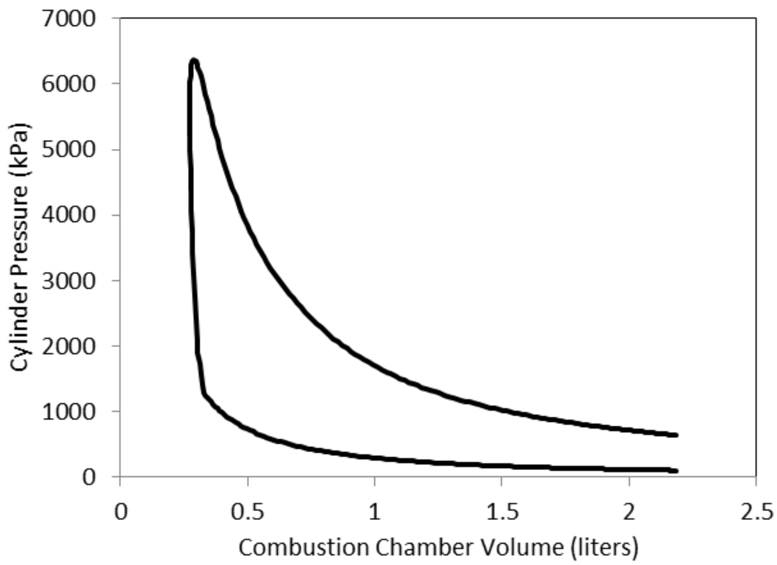

Figure 3. Pressure-volume diagram generated by the program.

computers on examinations, since all students may not have had access to laptop machines. They were told that, should they have any objections, they were to e-mail the instructor to make their concerns known. In such a case, no computers would then be used on examinations and their names would not be revealed. The class was told that each student, in effect, had "veto power" over the use of computers on examinations. There were no objections.

The students were asked why they chose to use the tools they used. Students who used Mathcad said that they liked the presentation that Mathcad provided, allowing the user to see the equations rather than having them hidden in the Worksheet. Users of Excel cited the user friendliness of the program and their distaste for the peculiarities of Mathcad. Some students found themselves having to re-type equations from scratch after having made typographical errors in Mathcad as they get pulled into a spiral of compounded cut-and-paste entanglements. Users of textbook interpolation said that they did not think interpolation was very taxing and preferred not to bother with a computer.

The choices of methods used for property determination for ideal gas problems on homework assignments, the course project, and examinations were as follows: Excel 59%, Mathcad 15% and manual table interpolation 31%. Figure 4 shows a graphical breakdown of the usage of each property evaluation tool for each of the 10 homework assignments involving air as an ideal gas during the course. This plot shows that the popularity of Mathcad grew over the semester, but the predominant choice among the students was Excel.

Table 2 shows a breakdown of homework and examination usage of property evaluation tools. As this table shows, Mathcad was somewhat more popular for use on homework than on examinations. This is likely due to the fact that students typically have more time available on homework than on examinations and Mathcad produces a more detailed record of the process in solving the problems. The speed with which Excel operates is most likely the reason for its popularity on examinations. Since there is less overhead in Excel, it launches more quickly and typing the functions is quicker. It should be noted that, on the hourly examination, the ideal gas problem was posed such that there was no interpolation required. This accounts for the large number of students using manual interpolation of the tables.

The course project assigned for the thermodynamics course involved evaluating an air standard Brayton cycle using two turbines with constant pressure reheat between turbines. The maximum allowed inlet temperature for each turbine was 1500K, based on the material limitations of the turbine blades. The compressor inlet conditions for this cycle were 300K and 100 kPa. Both the turbines and the compressor in this system performed with isentropic efficiencies of 85%. Using air as a working fluid and assuming variable specific heats, the students were to find the optimum inlet pressures for each of the two turbines for the maximum net power output of this system. This assignment was intended to cause the students to use the computer in evaluating the optimum case. Since the alternative to using a computer would be trial and error calculations, in this two-degree of freedom case, none of the students chose to use manual interpolation on the project. In terms of the breakdown of the students' choices between Mathcad and Excel on the project, 42% of the students chose to use only Excel, 8% chose to use only Mathcad and 50% chose to use both. The high percentage of Mathcad users on this project can be attributed to the fact that the instructor worked most of the project in class on the

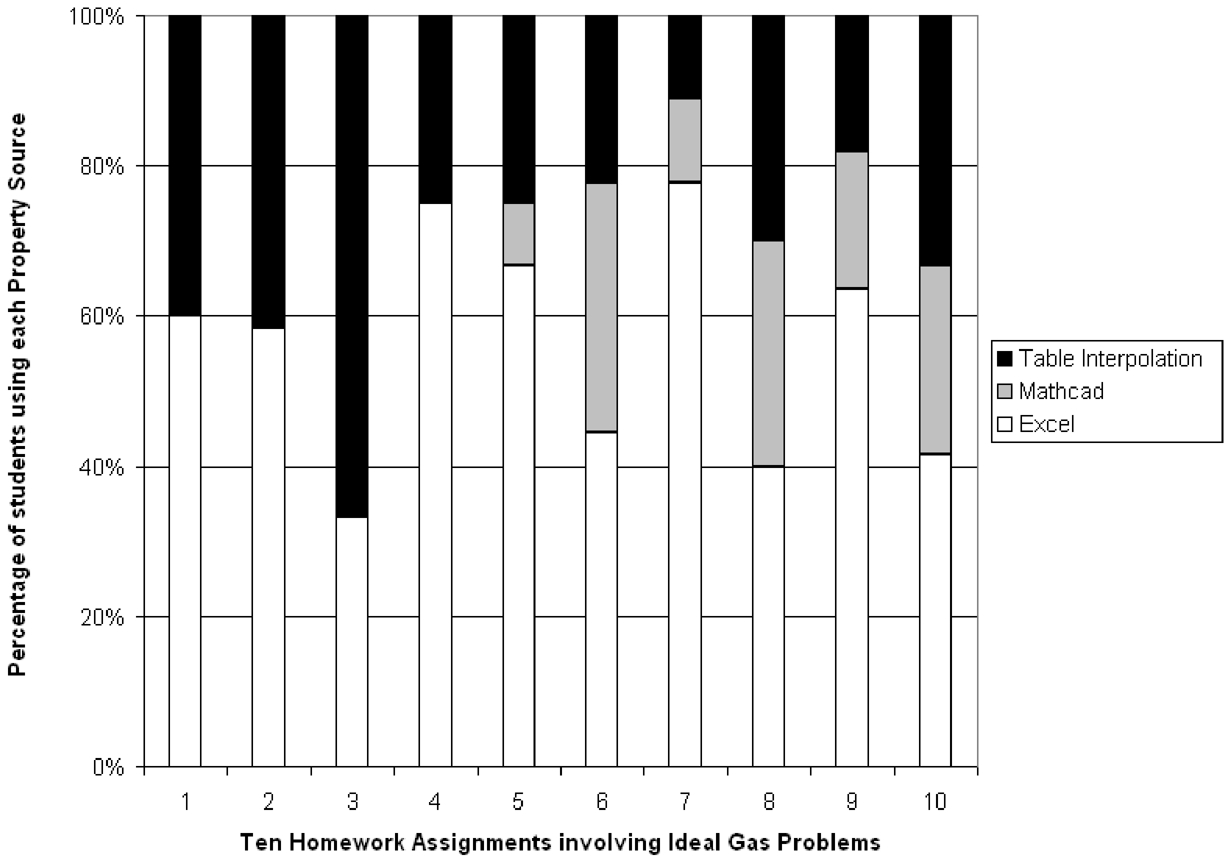

Figure 4: Graphical record of the percentage of students using the various methods of thermodynamic property evaluation for each of the 10 homework assignments involving air as an ideal gas in the course.

Table 3: Percentage of students using various methods of thermodynamic property evaluation by assignment type

Method	Homework	Hourly Exam	Final Exam
Excel	57	50	58
Mathcad	12	0	8
Tables	31	50	34

projection screen using Mathcad. The Mathcad sheet was not posted on the class web page in Mathcad format, but was posted as a pdf file, so that students could have a written record of what had been done in class. Therefore, many of the students chose to use Mathcad, at least to start the problem. Many of them still chose to use only Excel, even after the initial in-class start in Mathcad. Some used Excel to plot their results, since the plots in Excel presented a better appearance or were easier to generate. Plots of the results were required as part of the project, displaying system performance as a function of the two system pressures. The correct plot resembled a two-dimensional inverted parabola, with the maximum point being the optimum output point for the system as a function of the two turbine pressures.

In the internal combustion engine class, the only option available to the students was Excel, since Mathcad was effectively incapable of modeling the engine. The reactions from the students to the introduction of the internal combustion engine model were very favorable. The details of their responses are shown in the appendix, which features the questions asked on a survey form and the numbers of students who selected the various answers. As shown on this form, no negative replies were returned; all choices selected were positive or neutral.

By way of assessment, as noted in the introduction, the main advantage of the program in the thermodynamics class is that it allows a larger percentage of the student examinations to be focused on the students' thermodynamics ability, rather than on interpolation. Since all of the interpolation is done automatically by the program, the students can solve more problems during a given examination period, allowing their thermodynamics knowledge to be more thoroughly assessed. In applying the program in the internal combustion engine class, the assessment covering the segment of the course in which the numerical engine model is included, evaluates the students' knowledge gained from the numerical engine model exercise. Specific questions are asked that essentially require the students to rebuild one step of the numerical engine model. This step is posed in a different way than a typical step in the numerical engine model exercise, usually involving a different fuel and sometimes decoupling the combustion chamber volume from the crank arm angle. These measures are to insure the students understand the thermodynamic relationships involved and are not simply copying their project work into their examination problems. They are typically asked to find the temperature of a second time step after the parameters in an initial time step are given. This requires them to numerically solve for the final temperature by balancing internal energy terms, solving for temperature using the numerical solver in Excel as opposed to the built-in solver provided in the template program. Most students are able to do this successfully. However, the students who simply copy equations from the in-class presentations, and do not understand the principles behind the equations in program, are unable to solve for temperature correctly.

Conclusions

A means of interpolating thermodynamic properties by use of built-in functions in an Excel worksheet was developed. This tool was used in both an intermediate thermodynamics course and a senior elective on internal combustion engines. When offered an opportunity to use any of three available methods, students chose to use the Excel program in preference to either of the other two. The Excel program for finding thermodynamic properties for air has shown to be a viable method and a very useful tool for use in thermodynamics courses, a combustion course, or an internal combustion engine course. Moreover, the use of the program in developing a numerical model for an internal combustion engine allowed students to simulate internal combustion engine performance at a level that would be prohibitive by hand. The Excel platform allows the simulation to be performed with the focus primarily on internal combustion engine principles rather than on programming.

References

[1] Tiftan Data http://www.taftan.com/thermoxl.shtml

[2] Richard Stone, *Introduction to Internal Combustion Engines, Society of Automotive Engineers*, Warrendale, Pa, 1999.

[3] Steven McClain, "Mathcad Functions for Thermodynamic Analysis of Ideal Gasses", *Proceedings of the 2005 ASEE Conference*, Portland Oregon, 2005.

[4] Steven McClain, "A Mathcad Functions Set for Solving Thermodynamic Problems", *Proceedings of the 2006 ASEE Conference*, Chicago, 2006.

[5] Michael Moran and Howard Shapiro, *Fundamentals of Engineering Thermodynamics, 5th Edition*, John Wiley and Sons, Hoboken, NJ, 2004.

Appendix: Survey on Numerical Engine Model

1.) Overall, I thought the degree-by-degree program was
   (a) Awesome! (4 students)
   (b) Good (8 students)
   (c) OK (0 students)
   (d) Bad (0 students)
   (e) Terrible (0 students)

2.) The degree-by-degree program helped me better understand what happens inside an engine.
   (a) Strongly Agree (5 students)
   (b) Agree (3 students)
   (c) Maybe (4 students)
   (d) Disagree (0 students)
   (e) Strongly Disagree (0 students)

3.) The degree-by-degree program seemed pretty realistic to me.
   (a) Strongly Agree (2 students)
   (b) Agree (8 students)
   (c) Maybe (2 students)
   (d) Disagree (0 students)
   (e) Strongly Disagree (0 students)

4.) Compared to the Powerpoint segment of the course, where we just learned stuff out of the book, the degree-by-degree program was
   (a) Way Better (7 students)
   (b) Better (4 students)
   (c) About the same (1 student)
   (d) Worse (0 students)
   (e) Way Worse (0 students)

5.) What aspect did you think was best about the degree-by-degree program?
   Responses:
   1) Adding the turbocharger to the basic engine
   2) Optimizing the ignition timing
   3) Seeing the effects of changing the input parameters

6.) What do you think could be better about the degree-by-degree program?
   Responses:
   1) Trying additional fuels
   2) Accounting for heat transfer
   3) Accounting for valve losses and the exhaust/intake stroke