

AIR-STANDARD ANALYSIS WITH MATHCAD AN IMPROVED HEAT CAPACITY CORRELATION

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Introduction

An earlier article[1] presented an electronic version of the familiar table for thermodynamic properties of air. That version was based on a polynomial expression for the heat capacity at constant pressure that can be found in thermodynamics textbooks such as Moran[2]. Unfortunately, this polynomial expression is strictly valid only up to 1000 K (1800 R). Although it is reasonably accurate for several hundred degrees above that, there are many problems involving Otto and Diesel cycles where peak temperatures reach above 4000 R and the polynomial expression is not accurate.

The purpose of this article is to present an improved heat capacity model that is strictly valid up to 2000 K (3600 R) and reasonably accurate to about 5000 R. Mathcad software is used for this model, as it was used for the previous one. Instead of fitting a single polynomial to established heat capacity data, this model makes use of Mathcad's ability to perform cubic spline curve fitting. The spline fit is applied to heat capacity values produced by REFPROP[3] software created by the National Institute for Standards and Technology (NIST) and based on NIST Standard Database 12 Version 5.2.

Because the cubic spline process fits a series of polynomials rather than a single polynomial, it can provide an accurate fit over a very large temperature range. This makes it possible to double the temperature range of the single polynomial approach. The calculations involved in spline fitting are somewhat tedious. Fortunately, Mathcad has this capability built in.

The New Heat Capacity Model

The first step was to create two Mathcad arrays. The first contains a series of temperatures ranging from 400 R to 3600 R in 100 degree increments, and the second contains the corresponding values of heat capacity at constant pressure obtained from REFPROP. These arrays are not shown in the figures below because they occupy a large amount of space.

Once the arrays had been created, Mathcad's **cspline** command was used to generate the required constants for the spline fit. The syntax is

$$vs:=cspline(Temp,C_p)$$

where "vs" is the name of the array of spline constants, "Temp" is the array of temperature values, and "C_p" is the array of heat capacity values. A continuous function for C_p was then created by means of Mathcad's **interp** function. This syntax is

$$C_p(T):=interp(vs,Temp,C_p,T).$$

This function can be used to produce accurate heat capacity values at any temperature within its range of validity. It can also be used in integral expressions to produce values of enthalpy, relative pressure, and relative volume.

Several validity tests were performed. It is characteristic of the spline method that input data points are matched exactly. Therefore it was verified that the C_p function yielded values that exactly matched the original values that were used to produce it. Because the ultimate purpose of the function is to calculate values of h, s⁰, P_r, and v_r, these values were calculated and

compared with values from a standard Air Table[4]. In the interest of brevity, only the enthalpy validation is shown below, but similar accuracy was evident in the other parameters. This is to be expected, because all parameters are calculated from the C_p function. In Table 1, the C_p function is used to calculate enthalpy changes between arbitrarily chosen temperatures. Those values are shown in the third column. The fourth column shows enthalpy changes calculated directly from enthalpy values in the Air Table.

Excellent agreement is evident in the table. The maximum error, 0.4%, appears twice: once when the end temperature is 5000 R (well above the expected range of accuracy), and once over the range 600 R to 700 R.

The New Electronic Air Table

It is a simple matter to replace the single polynomial model for C_p with the new model in the existing Air Table worksheet. The new electronic Air Table is shown in Figures 1 and 2. To save space, the arrays “Temp” and “ C_p ” that were used to create the spline fit are not shown in the figures.

Conclusion

A new heat capacity model has been developed and incorporated into an existing electronic Air Table. The new model extends the validity of the electronic Air Table to 3600 R with certainty, and to about 5000 R with reasonable accuracy. Extending the temperature range facilitates the analysis of Otto and Diesel cycles where peak temperatures may be above 4000 R. In addition to the model described above, a parallel model in SI units has been developed. The author will email copies of the Mathcad files upon request. Please address requests to ewiggins@webb-institute.edu.

References

1. Wiggins, Edwin G., “Air-Standard Analysis with Mathcad,” Computers in Education Journal, Vol. XIV, no. 1, January – March 2004, p. 25.
2. Moran, Michael J. and Howard N. Shapiro, Fundamentals of Engineering Thermodynamics, 5th ed., 2004, John Wiley & Sons, Inc., p. 845.
3. NIST Standard Reference Database 12 Version 5.2, 2005.
4. Moran, Michael J. and Howard N. Shapiro, Fundamentals of Engineering Thermodynamics, 5th ed., 2004, John Wiley & Sons, Inc., p. 846-847.

Biographical Information

Edwin G. Wiggins holds BS, MS, and Ph.D. degrees in chemical, nuclear, and mechanical engineering respectively from Purdue University. He is the Mandell and Lester Rosenblatt Professor of Marine Engineering at Webb Institute in Glen Cove, NY. Ed is a past chairman of the New York Metropolitan Section of the Society of Naval Architects and Marine Engineers (SNAME) and a past regional vice president of SNAME. A Centennial Medallion and a Distinguished Service Award recognize his service to SNAME. As a representative of SNAME, Ed Wiggins serves on the Board of Directors of the Accreditation Board for Engineering and Technology (ABET).

Table 1
Enthalpy Validity Test

Start Temperature (R)	End Temperature (R)	Δh from Function (BTU/lb)	Δh from Air Table (BTU/lb)	Difference %
400	5000	1302.9	1297.4	0.4
500	1000	121.8	121.5	0.2
600	700	24.2	24.1	0.4
700	1700	255.4	255.0	0.2
800	3000	599.3	598.9	0.1
900	1200	75.1	75.0	0.1

Figure 1
Abbreviated Mathcad Worksheet
(Large Arrays Omitted)

This Mathcad worksheet contains the equations that replicate the values in the air table. Thus it can be used as the basis for air standard analysis.

Specific heat ratio for air $k := 1.4$

Specific heat of air - Note that the heat capacity function developed below represents a spline curve fit over the range 400 R to 3600 R. Use outside that range is not recommended, however it appears to be within about 2% up to 5000 R.

$$R_{\text{air}} := \frac{1.986 \frac{\text{BTU}}{\text{mol}\cdot\text{R}}}{28.97 \frac{\text{lb}}{\text{mol}}} \quad R_{\text{air}} = 0.06855 \frac{\text{BTU}}{\text{lb}\cdot\text{R}}$$

The following arrays contain temperatures and the corresponding values of the specific heat of air at constant pressure as calculated from NIST 12.

(Temp and Cp arrays omitted here)

Figure 2 (Mathcad worksheet continued)

The *cspline* command produces an array, which is given the name *vs*, that contains the constants for a cubic spline that is fitted to the data above.

$$vs := cspline(Temp, Cp)$$

A continuous function for heat capacity is defined in terms of the spline constants by means of the *interp* function.

$$C_p(T) := interp(vs, Temp, Cp, T)$$

$$C_v(T) := C_p(T) - R_{air}$$

$$s_0(T) := \int_{45R}^T \frac{C_p(T)}{T} dT \quad s^0 \text{ function}$$

$$P_r(T) := \frac{e^{\frac{s_0(T)}{R_{air}}}}{4750} \quad \text{relative pressure function}$$

$$v_r(T) := \frac{T}{P_r(T) \cdot 2.694R} \quad \text{relative volume function}$$

$$h(T) := \int_{7.32R}^T C_p(T) dT \quad \text{enthalpy function}$$

$$u(T) := \int_{7.32R}^T C_v(T) dT \quad \text{internal energy function}$$

The Valid function below tests for validity of the results. **It should be applied to every calculated temperature**

$$Valid(T) := \begin{cases} \text{"Okay"} & \text{if } T \leq 3600R \\ \text{"Too high. functions may be inaccurate"} & \text{otherwise} \end{cases}$$