TECHNICAL NOTE

Blending geometry with numerical computation: Charts for the enthalpy, absolute entropy, and flow exergy of 12 gases at low pressures

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This note contains a set of charts for the enthalpy change function $\Delta\bar{h}(T)$, the absolute entropy at atmospheric pressure $\bar{s}^\circ(T)$, and the flow exergy at atmospheric pressure $\bar{e}_x^\circ(T)$ of 12 gases in the ideal-gas limit. The gases considered are CO, CO_2, H, H_2, H_2O, N, N_2, NO, NO_2, O, O_2 and OH. These charts and the ideal-gas model can be used to calculate the enthalpy $\bar{h}(T)$, absolute entropy $\bar{s}(T, P)$ and flow exergy $\bar{e}_x(T, P)$ of the same gases.

Keywords: thermodynamic charts; enthalpy; entropy; exergy; ideal gases

In today's thermal engineering we are asked more and more frequently to rely on personal or minicomputers to carry out some of the more traditional and routine calculations. This trend is particularly visible in applied thermodynamics, where tables of properties that not long ago occupied an entire book[1,2] are now condensed in one diskette in an envelope or at the back of the undergraduate thermodynamics textbook[3-5].

Any "improved" tool is a good thing in the hands of the individual who knows what to do with it. To the beginner, however, the computerization of the once tabulated properties may do more harm than good, if this act of "condensation" is not accompanied by an equally creative effort of presenting a bird's-eye view of the now hidden information. Furthermore, to those beginners who do not use tables and charts simultaneously, even the tabulated properties appear confusing, despite the fact that a two-dimensional cartesian tabulation alone can offer a bird's-eye view if held sufficiently far away from the eye.

There is more at stake here than simply the loss of clarity and efficiency in learning thermodynamics. Note that the analytical results (the formulas) that serve as backbone for the thermodynamic tables are in themselves an important lesson—a legitimate chapter–in classical thermodynamics. The same can be said about all the charts and the technological reasons that triggered their invention (e.g., the Mollier chart vis-à-vis the steam turbine cycle). It is not difficult to see the culture that will be lost if the once-charted and tabulated information is allowed to be displaced *fully* by the tiny black boxes that, today, are correctly marketed as nothing more than computational "aids."

Rapid access to the needed bird's-eye view can be gained through the use of geometry and creative graphics. Now, geometry and classical thermodynamics have mixed very well from the beginning: recall, for example, Gibbs' treatment of multiphase equilibria[6] or Maxwell's original derivation of his reciprocal relations[7]. The objective of this note is to disseminate three graphic aids that the author has found useful for carrying out flow combustion calculations.

Figures 1 and 2 show the enthalpy and absolute entropy values of low-pressure gases, which traditionally appear in tabular form. The construction of these graphs is based on the numerical values listed in the text by Sonntag and Van Wylen[8], the original source of that information being the JANAF tables[9]. The enthalpy $\Delta\bar{h}$ measured on the ordinate of Figure 1 is shorthand for

$$\Delta\bar{h}(T)=\bar{h}(T)-\bar{h}_f^\circ \tag{1}$$

where $\bar{h}_f^\circ$ is the enthalpy of formation at $T_0=298.15\,K$ (25°C) and $P_0=0.101325$ MPa (1 atm). In writing Equation 1, we assume that the pressure is sufficiently low so that $\bar{h}$ and $\Delta\bar{h}$ are functions of T only (in other words, the gas approaches the ideal-gas limit).

In addition to presenting in one glance the information usually contained in 12 pages of textbook[8], Figure 1 shows the user in what temperature ranges the enthalpy change $\Delta\bar{h}$ may be approximated as a linear function of temperature, and that monatomic gases such as H, O, and N have practically the same $\Delta h(T)$ function, which is a straight line. This visual discovery invites the user to cross mentally the bridge between the routine handling of thermodynamic property "numbers" and items learned in the study of kinetic theory. Finally, Figure 1 draws attention to the issue of numerical "accuracy." The six-significant-digit numbers listed in the textbook tables[8] falsely suggest a degree of accuracy that is far in excess of the experimental errors mentioned in the original source[9]. It seems that only three or, at best, four significant digits reflect the proper accuracy of the experimental data: it is this level of precision that is approached by Figure 1 (and later, Figures 2 and 3), especially at high temperatures.

Figure 2 shows the absolute entropy at atmospheric pressure,

$$\bar{s}^\circ(T)=s(T, P_0) \tag{2}$$

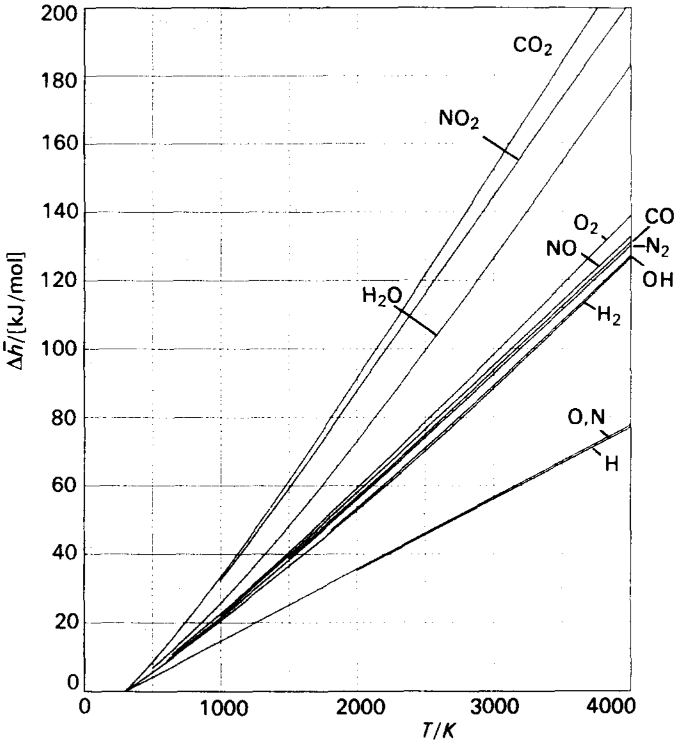

Figure 1 The enthalpy change function $\Delta\bar{h}(T)$ for several ideal gases

The observations made in the preceding paragraph apply here as well. The entropy at a state (T, P), where P is not necessarily the atmospheric pressure P_0, can be evaluated by invoking the ideal-gas model

$$\bar{s}(T,P)=\bar{s}^\circ(T)-\bar{R}\ln(P/P_0) \tag{3}$$

Finally, Figure 3 shows the flow exergy of the 12 gases at atmospheric pressure. This particular chart is even more novel than Figures 1 and 2 because tabulations of flow exergies for low-pressure gases do not exist. Figure 3 was constructed from Figures 1 and 2 by noting the general definition of flow exergy[10,11]

$$\bar{e}_x(T,P)=\bar{h}(T,P)-T_0\bar{s}(T,P)-[\bar{h}(T_0,P_0)-T_0\bar{s}(T_0,P_0)] \tag{4}$$

As notation for flow exergy, the engineering thermodynamics literature appears to be divided between using the symbol $\bar{e}_x$ and $\bar{\varepsilon}$ (more precisely, $\bar{\varepsilon}_{ph}$, for "physical" exergy[11]). Writing $\bar{e}_x^\circ$ for the $P=P_0$ version of Equation 4, we have

$$\bar{e}_x^\circ(T)=\Delta\bar{h}(T)-T_0[\bar{s}^\circ(T)-\bar{s}^\circ(T_0)] \tag{5}$$

where $T_0=298.15$ K (25°C). The right side of Equation 5 can be evaluated directly from Figures 1 and 2 or from the tables on which those figures are based. The resulting quantity, $\bar{e}_x^\circ$, is reported in Figure 3. The observations listed in the paragraph above Equation 2 apply also to Figure 3. In addition, note that each of the $\bar{e}_x^\circ$ curves has a minimum at $T=T_0$.

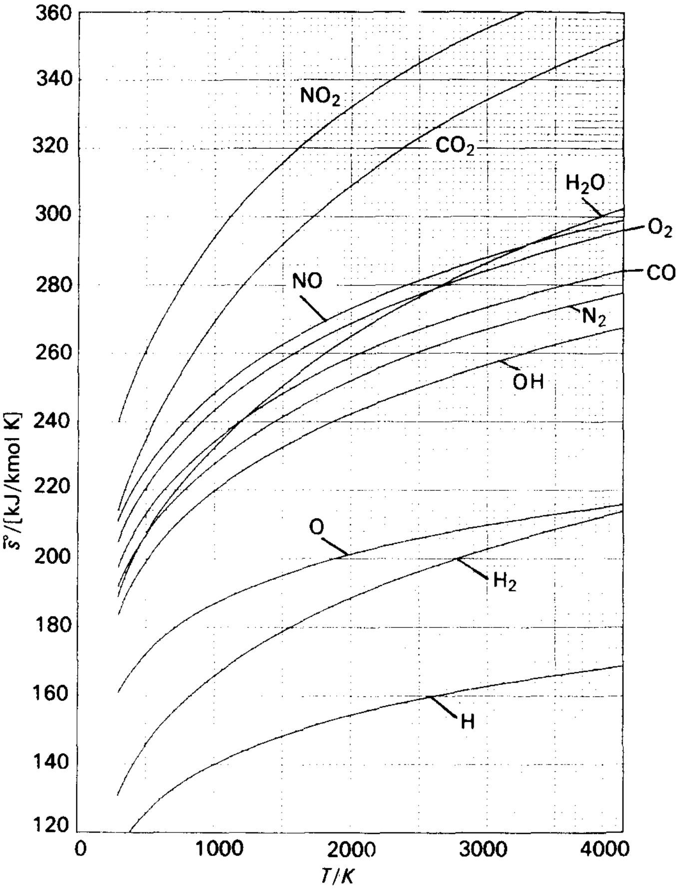

Figure 2 The absolute entropy at atmospheric pressure, $\bar{s}^\circ(T)$, for several ideal gases

The flow exergy at a low pressure that is not necessarily equal to P_0 can be deduced from Equations 3–5, that is, based on the ideal-gas model,

$$\bar{e}_x(T,P)=\bar{e}_x^\circ(T)+\bar{R}T_0\ln(P/P_0) \tag{6}$$

In conclusion, the flow exergy $\bar{e}_x(T,P)$ can be calculated by combining the reading of Figure 3 with the pressure correction Equation 6.

The charts exhibited in this note are a sample of a much more extensive effort to bring graphics and geometric reasoning back into the discipline of engineering thermodynamics. The result of that greater effort is a new graduate-level treatise[12].

Notation

$\bar{e}_x$	Flow exergy, J/mol
$\bar{e}_x^\circ$	Flow exergy at atmospheric pressure, Figure 3
$\bar{h}$	Enthalpy, J/mol
$\Delta\bar{h}$	Enthalpy change function, Figure 1
$\bar{h}_f^\circ$	Enthalpy of formation at T_0 and P_0
P	Pressure, Pa
P_0	Atmospheric pressure, 0.101325 MPa
$\bar{R}$	Universal gas constant, 8.3143 J/mol K
$\bar{s}$	Absolute entropy, J/mol K
$\bar{s}^\circ$	Absolute entropy at atmospheric pressure, Figure 2
T	Absolute (thermodynamic) temperature, K
T_0	Reference temperature, 298.15 K or 25°C

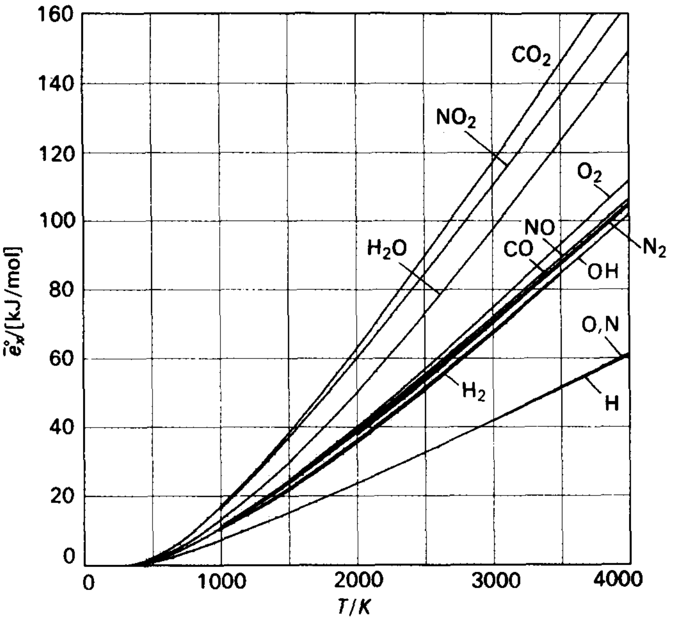

Figure 3 The flow exergy at atmospheric pressure, $\tilde{e}_x^\circ(T)$, for several ideal gases

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