COMPRESSION OF AN IDEAL GAS WITH TEMPERATURE-DEPENDENT SPECIFIC HEAT CAPACITIES

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Abstract

A computer model of the isentropic compression of a gas with temperature-dependent specific heat capacities is presented. Both tabulated data and curve-fits are used to describe the temperature variation of the thermodynamic properties, and a bracketing–bisection algorithm is used to determine the temperature of the air after compression. Students are provided with an example computer code from which to begin. Thus, the approach as described in this study reinforces programming concepts from previous computer courses, without requiring too much effort by the students. Three exercises are presented that make use of this computer model at different levels in the curriculum.

Introduction

The compression of gas in a steady-state, steady-flow (SSSF) compressor is an important topic that is addressed in virtually all engineering thermodynamics courses. A typical situation encountered is when the gas inlet conditions, temperature and pressure, are known and the compressor discharge pressure is specified. The traditional instructional approach is to make certain assumptions about the compression process and about the gas itself. For example, a special case often considered is that the compression process is reversible and adiabatic, i.e. isentropic. The gas is usually considered to be ideal, i.e. $Pv = RT$ applies, with either constant or temperature-dependent specific heat capacities. The constant specific heat capacity assumption allows for direct computation of the discharge temperature, while the temperature-dependent specific heat assumption does not.

In this paper, a MATLAB computer model of the compression process is presented. The substance being compressed is air which is considered to be an ideal gas with temperature-dependent specific heat capacities. Two approaches are presented to describe the temperature-dependent properties of air. The first approach is to use the ideal gas table data from Ref. [1] with a look-up interpolation scheme. The second approach is to use a curve fit with the NASA Lewis coefficients [2,3]. The computer model developed makes use of a bracketing–bisection algorithm [4] to determine the temperature of the air after compression. This computer code is supplied to the students and discussed after the students have performed a detailed hand calculation. Then, students are required to modify the supplied computer program to solve additional problems.

The instructional approach outlined in this paper accomplishes several objectives. First, this computer work serves as a connection between first-year, computer-tools courses and engineering science courses. At Indiana University-Purdue University Fort Wayne, students take a two-credit hour computer tools course in which they learn MATLAB and then take a two-credit hour programming course in which they learn C/C++ with an engineering emphasis. After completion of the courses, students are often eager to apply their skills to engineering problems. Unfortunately, the opportunities to utilize these skills are limited and students often question why they are required to take the computer classes. More exercises need to be developed to utilize and reinforce the computer skills. Second, the computer implementation allows students to easily vary the thermodynamic parameters so that students can develop an appreciation of the

limitations associated with thermodynamic assumptions such as the constant specific heat approximation. Third, the flexibility of the model allows for realistic extensions to the original problem, such as the incorporation of heat loss from the compressor and compressor efficiency. As students modify the provided computer code they develop additional insight and familiarity with thermodynamic equations and concepts. Finally, in later courses, the computer model can be modified to investigate more complicated situations, such as multistage compression with intercooling [5] or the gas turbine cycle [6]. Examples of how these objectives are achieved are provided and discussed.

Governing Equations

In this section, the relevant equations to describe the compression of an ideal gas are summarized. A similar presentation can be found in most undergraduate thermodynamics texts, e.g. Refs. [1,7,8]. The equation development is included here for completeness.

Work of Compression

For steady-state, steady-flow through an adiabatic compressor with one inlet and one outlet, the compression work per unit mass is given by the First Law of Thermodynamics as

$$w_{comp} = h_2 - h_1 \; , \qquad (1)$$

where the subscripts 1 and 2 denote the inlet and outlet and changes in kinetic and potential energy have been neglected. Note that the work of compression in Eq. (1) is defined to be positive.

For an ideal gas, the change in enthalpy for a process is related to the change in temperature by the constant pressure specific heat, i.e.

$$dh = c_p dT \; . \qquad (2)$$

In general, the specific heat capacities of gases are functions of temperature. Curve-fits of the specific heat for many gases as a function of temperature have been developed [2,3]; thus, the change in enthalpy needed to calculate the work in Eq. (1) can be found via integration, i.e.

$$h_2 - h_1 = \int_{T_1}^{T_2} c_p dT \; . \qquad (3)$$

For the case in which the specific heat capacities are constant, the change in enthalpy in Eq. (3) is simply related to the temperature difference, i.e.

$$h_2 - h_1 = c_p (T_2 - T_1). \qquad (4)$$

When the heat capacities depend on temperature, the relationship between the temperature and enthalpy is more complicated. With the use of properties of integration, Eq. (3) can be rewritten in a more convenient form, i.e.

$$h_2 - h_1 = \int_{T_0}^{T_2} c_p dT - \int_{T_0}^{T_1} c_p dT \; , \qquad (5)$$

where T_0 is a suitably chosen reference temperature. Equation (5) is more convenient than Eq. (3) because the integrals are now functions of a single temperature (and the reference temperature), and thus the integral terms can be expressed as

$$h^0 (T) \equiv \int_{T_0}^{T} c_p dT \qquad (6)$$

and tabulated as a function of temperature [1,7,8]. If the temperatures at the inlet and outlet are known, Eqs. (4) and (5) indicate that the work of compression can be calculated.

However, an important thermodynamic process is the compression of gas from a known inlet temperature T_1 and pressure P_1 to a specified outlet pressure P_2, i.e. the outlet temperature is not known. (See Fig. 1 for a schematic of the compressor and the process on

a T-s diagram.) To proceed with the analysis of this process, another thermodynamic property is required to fix the outlet temperature. For an ideal (i.e. reversible), adiabatic compressor the process is isentropic, which implies that $s_1 = s_2$. Thus, two properties, P_2 and s_2, are available to fix the outlet temperature, T_2. For the isentropic compression of a gas with constant specific heats, T_2 can be calculated directly, while for a gas with temperature-dependent specific heats a numerical solution is required.
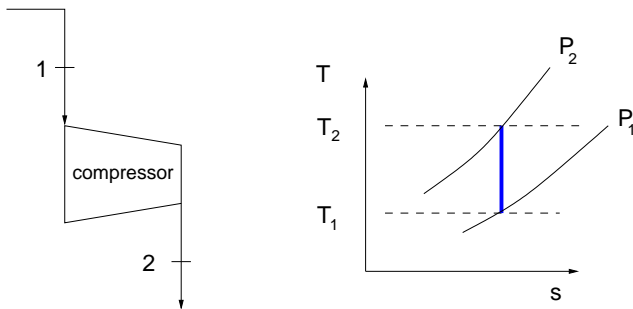

Figure 1. Schematic of the single-stage compressor and T-s diagram.

Change in Entropy

As a starting point to derive an expression for the change in entropy, recall the second Gibb's relationship, viz.

$$Tds = dh - vdP \qquad (7)$$

that is valid for all compressible substances undergoing an infinitesimal process. Equation (7) can be used to find the change in entropy for an ideal gas with division by T, substitution of $dh = c_p dT$, and application of the ideal gas equation, i.e. $v/T = R/P$, which yields

$$ds = c_p \frac{dT}{T} - R \frac{dP}{P} . \qquad (8)$$

Integration of Eq. (8) from state 1 to state 2 yields

$$s_2 - s_1 = \int_{T_1}^{T_2} c_p \frac{dT}{T} - \int_{P_1}^{P_2} R \frac{dP}{P} , \qquad (9)$$

which following an approach similar to that described above, can be rewritten in a more convenient form, viz.

$$s_2 - s_1 = \int_{T_0}^{T_2} c_p \frac{dT}{T} - \int_{T_0}^{T_1} c_p \frac{dT}{T} - R \ln(P_2/P_1) , \qquad (10)$$

where T_0 is a suitably chosen reference temperature. Equation (10) is more convenient than Eq. (9) because the integrals, denoted as

$$s^0(T) \equiv \int_{T_0}^{T} c_p \frac{dT}{T} , \qquad (11)$$

are now functions of a single temperature (and the reference temperature and pressure) and, for cases in which the variation of c_p is known, can be evaluated and tabulated.

In the case when the specific heat capacities are constant, the integration in Eq. (10) can be performed to yield

$$s_2 - s_1 = c_p \ln T_2 - c_p \ln T_1 - R \ln(P_2/P_1) , \qquad (12)$$

where the reference temperature has been cancelled. For an isentropic process, the change in entropy is zero which implies that $s_1 = s_2$. The ideal adiabatic compression process is isentropic. Moreover, the first step in the analysis of a non-ideal compression process is often the isentropic analysis. Therefore, isentropic compression is an important process to be modeled. For an isentropic process, Eq. (12) becomes

$$T_2/T_1 = P_2/P_1^{(k-1)/k} , \qquad (13)$$

where $k = c_p/c_v$ and the relationship $R/c_p = (k-1)/k$ was used. For the problem under consideration in this paper, T_1, P_1, and P_2 are assumed to be known. Thus, the outlet temperature T_2 can be calculated directly for a

gas with constant specific heats. For the case of temperature-dependent specific heats, Eq. (10) becomes

$$F(T_2) = 0 = s^0(T_2) - s^0(T_1) - R\ln(P_2/P_1) . \quad (14)$$

Equation (14) can be used to determine the unknown outlet temperature T_2. The appropriate value of the temperature is the value of T_2 that makes $F(T_2) = 0$. Thus, the determination of the outlet temperature can be accomplished by finding the root of a nonlinear equation.

Temperature-Dependent Specific Heat Capacities

In this work two approaches are discussed to calculate the enthaply h and entropy s for an ideal gas. The first approach is to simply use tabulated data found in standard thermodynamics texts such as Ref. [1,7,8]. The enthalpy and entropy of a gas with temperature-dependent specific heats from Ref. [1] are shown in Fig. 2. Because only differences in the properties are important, the data is plotted with a reference temperature of 298.15 K, i.e. $h^0(T) - h^0(298.15)$ and $s^0(T) - s^0(298.15)$. Also shown in Fig. 2 are the enthalpy and entropy of a gas with constant specific heats, i.e.

$$h^0(T) - h^0(298.15) = h^0 - h^0_{298.15} = c_p(T - 298.15) \quad (15)$$

and

$$s^0(T) - s^0(298.15) = s^0 - s^0_{298.15} = c_p[\ln(T) - \ln(298.15)] , \quad (16)$$

where $c_p = 1.004$ kJ/kg-K. Agreement between the temperature-dependent specific heat properties and the constant specific heat properties is best at lower temperatures. As expected all properties in Fig. 2 are zero at $T = 298.15$ K.

The second approach to describe the temperature variation of the specific heats discussed in this paper makes use of the curve fits given in Ref. [3]. The forms of the fits are

$$c_p/R = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 , \quad (17)$$

$$\frac{h^0}{RT} = -a_1 T^{-1} + a_2(\ln T)/T + a_3 + a_4 T/2 + a_5 T^2/3 + a_6 T^3/4 + a_7 T^4/5 + b_1/T \quad (18)$$
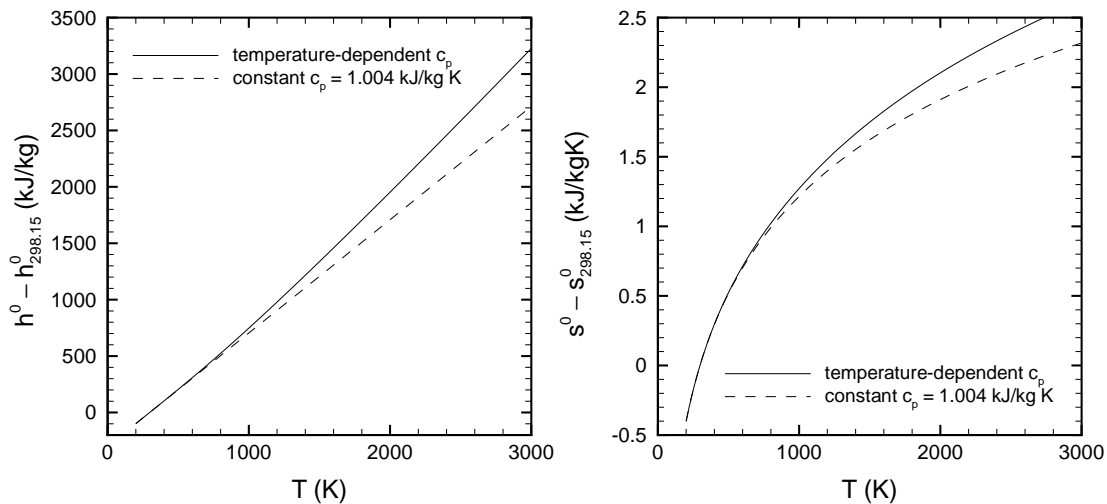
and

Figure 2. Effect of the temperature on $h^0(T) - h^0(298.15)$ and $s^0(T) - s^0(298.15)$.

$$\frac{s^0}{R} = -a_1 T^{-2}/2 + a_2/T + a_3 \ln T + a_4 T + a_5 T^2/2 + \tag{19}$$
$$a_6 T^3/3 + a_7 T^4/4 + b_2$$

where the coefficients are given in Ref. [3] (and in the subroutine in Appendix B). One set of coefficients is valid for $0 < T < 1000$ K, and one set is valid for $1000 < T < 6000$ K. There is no noticeable difference when Eqs. (18) and (19) are plotted in the same form as in Fig. 2. In fact, the percent error between the tabulated values and the curve fit is less than 0.1% over the range $0 < T < 3000$ K.

Bracketing/Bisection Routine

In this section, a modified version of the bracketing–bisection routine of Ref. [4] is discussed. This routine is dependent on the physical situation of the problem considered, i.e. compression of a gas and the form of the function considered is shown in Fig. 3. If the physical situation differs, say the gas is expanding, the form of the function will change and the code must be modified accordingly.
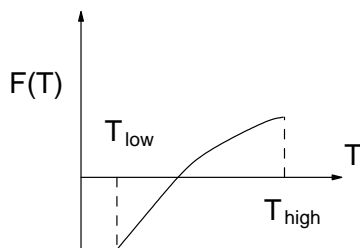

Figure 3. Graph of the type of functions considered.

Bracketing

The first step to find the solution to the equation $F(T) = 0$ is to bracket the root with two temperatures T_{low} and T_{high}. This accomplished by starting at the initial temperature $T_{low} = T_1$ and incrementing the high temperature by 100 K until the product $F(T_{low}) \times F(T_{high}) < 0$. This subroutine returns two bracketing temperatures.

Bisection

The next step to find the root is to successively halve the overall interval $T_{high} - T_{low}$ and select the half that contains the root. It can be shown [4] that to achieve an accuracy of less than $\pm \varepsilon$ in the temperature T_2 the maximum number of interval halving steps required is given by $\ln(\Delta T / \varepsilon)/\ln 2$, where $\Delta T = T_{high} - T_{low}$.

Discussion of Exercises

In this section, three typical exercises that involve the above material are presented. In the first exercise, students simply use the supplied code to solve a test problem and then make minor parameter adjustments and solve a similar problem. In the next two exercises, students modify the computer code provided in the first exercise. These three exercises were designed to be given in successive thermal science courses, but they can be used in one course if time permits.

Exercise 1: Consider the isentropic compression of air at 300 K, 100 kPa to a pressure of 1600 kPa in a SSSF device. Calculate the outlet temperature and the specific work required.

This first exercise is a typical problem encountered in an introductory thermodynamics course taken by sophomore students. First, this problem is solved in detail on the board with the constant specific heat assumption and tabulated data. Next, students are provided a copy of the computer code in Appendix A and the computer output as shown in Fig. 4. The computer code is carefully explained. The code in Appendix A uses table look-up and interpolation for the thermodynamic properties and bracketing–bisection to solve for the temperature after compression. The table look-up interpolation scheme is easily implemented in MATLAB using the function `interp1`. The table look-up routine can be replaced by the NASA curve-fit routines provided in Appendix B. Students are

required to type in the code, reproduce the results in Fig. 4, and then solve a similar problem with different inlet conditions as a homework assignment.

```
inlet conditions:  T1 = 300.0 K    P1 = 100.0 kPa    P2 = 1600.0 kPa


constant specific heats (k = 1.40):  T2 = 662.5 K    w = 363.9 kJ/kg


loop to demonstrate bracketing process

       T        delta_s
     -----      -------
     300.00     -0.7959
     400.00     -0.5059
     500.00     -0.2782
     600.00     -0.0888
     700.00      0.0750
     800.00      0.2200
     900.00      0.3507
    1000.00      0.4698

bracket:  T low = 300.0    T high = 700.0


bisection routine

    T_low      T_high      T_mid       delta_s
    -----      ------      -----       -------
    300.00     700.00     500.0000     -0.2782
    500.00     700.00     600.0000     -0.0888
    600.00     700.00     650.0000     -0.0043
    650.00     700.00     675.0000      0.0359
    650.00     675.00     662.5000      0.0160
    650.00     662.50     656.2500      0.0059
    650.00     656.25     653.1250      0.0008
    650.00     653.12     651.5625     -0.0018
    651.56     653.12     652.3438     -0.0005
    652.34     653.12     652.7344      0.0002
    652.34     652.73     652.5391     -0.0002
    652.54     652.73     652.6367     -0.0000

variable specific heats:  T2 = 652.6 K    w = 362.5 kJ/kg
```

Figure 4. Computer output from isentropic_ compression.m (see Appendix A) demonstrating the bracketing–bisection procedure.

Consider the isentropic compression of air in a SSSF device. Calculate the final temperature for pressure ratios from 2 to 25 using both the constant and variable specific heat model. Consider inlet temperatures of 300 K and 1000 K.

This next exercise is suitable for junior/senior students in a second thermodynamics course. In this exercise, students are provided a copy of Exercise 1 which is discussed briefly, and then they are assigned the second exercise as a homework problem/computer project.

The solution to this problem requires several modifications to the code in Appendix A. First, students are instructed to remove the bracketing demonstration loop and the print statements in the subroutines. Then, the students are briefly reminded of how to use loops and plot functions using MATLAB. Sample results from this exercise are provided in Fig. 5. The constant specific heat approximation shows better agreement with the temperature-dependent specific heat results at lower pressure ratios and at lower inlet temperatures.
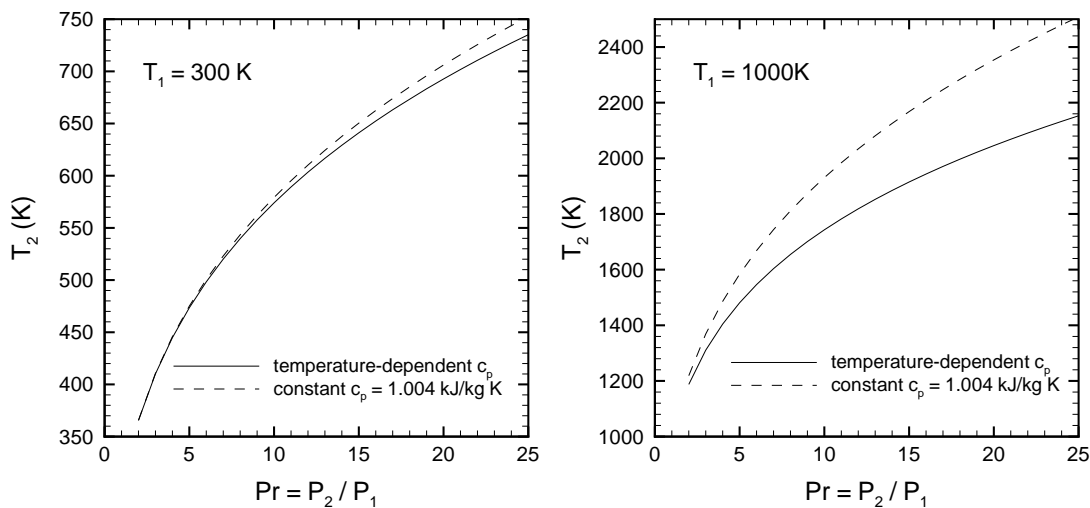

Figure 5. Effect of the pressure ratio on outlet temperature T_2 for air with an inlet temperature of 300 K (left) and 1000 K (right).

Exercise 3: Consider the compression of air at pressure of 100 kPa to a pressure of 1600 kPa, in two-stage SSSF compressor with intercooling, as shown in Fig. 6. Determine the intermediate pressure P_x to minimize the compressor work. Consider inlet temperatures of 300 K and 1000 K.

This final exercise has been given as a project to students in a thermal science elective course entitled *Design and Optimization of Thermal Systems.* Students were first given a copy of the computer code in Appendix A, and the solution to Exercise 1 was presented in class.

A schematic of a two-stage compressor with intercooling is shown in Fig. 6. The T - s diagram for this process is also shown. The solution to Exercise 3 requires significant modification to the supplied computer code. Students must model two compressors and insert loops for the pressure ratio. One approach to solve this problem is to vary the intermediate or intercooler pressure P_x between the minimum and maximum pressures and calculate the compressor work required for each pressure.

For constant specific heat capacities, the optimum pressure to minimize the compressor

work is $P_x = \sqrt{P_1 P_2}$ [1,7,8]. Lewins[5] has shown using Lagrange multipliers that the same pressure minimizes the work for the temperature-dependent specific heat case also. Sample results are shown in Fig. 7. For the lower inlet temperature $T_1 = 300$ K, the constant and temperature dependent specific heat results are very similar and appear as one curve. For an inlet temperature of 1000 K, the constant specific heat results are higher than the temperature-dependent specific heat results. This problem presents many interesting topics for future investigation, such as the effect of compressor efficiency, intercooler effectiveness, and intercooler pressure-drop.

Concluding Remarks

In this study, a computer model of the isentropic compression of a gas with temperature-dependent specific heat capacities has been presented. The approach as described in this study reinforces programming concepts from previous computer courses, without requiring too much effort by the students. The students benefit from an example computer code from which to begin. Finally, the computer program developed is a useful tool to strengthen students' understanding of thermodynamic concepts and to use in the modeling of more complicated problems.
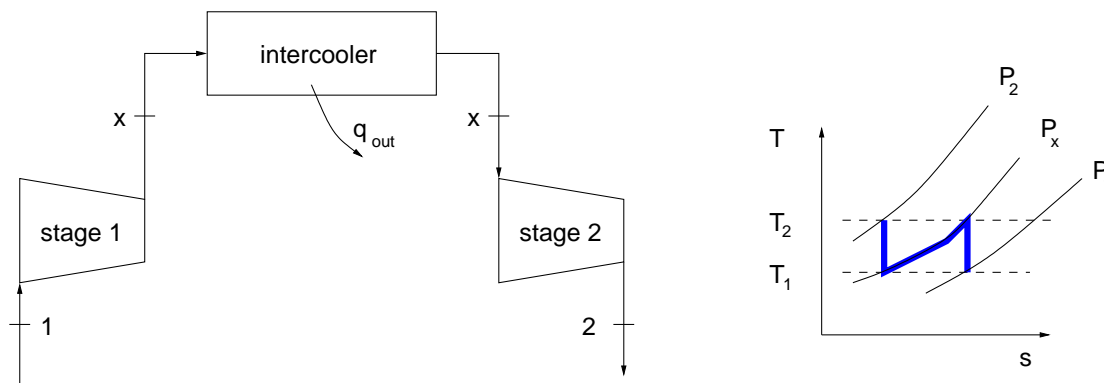

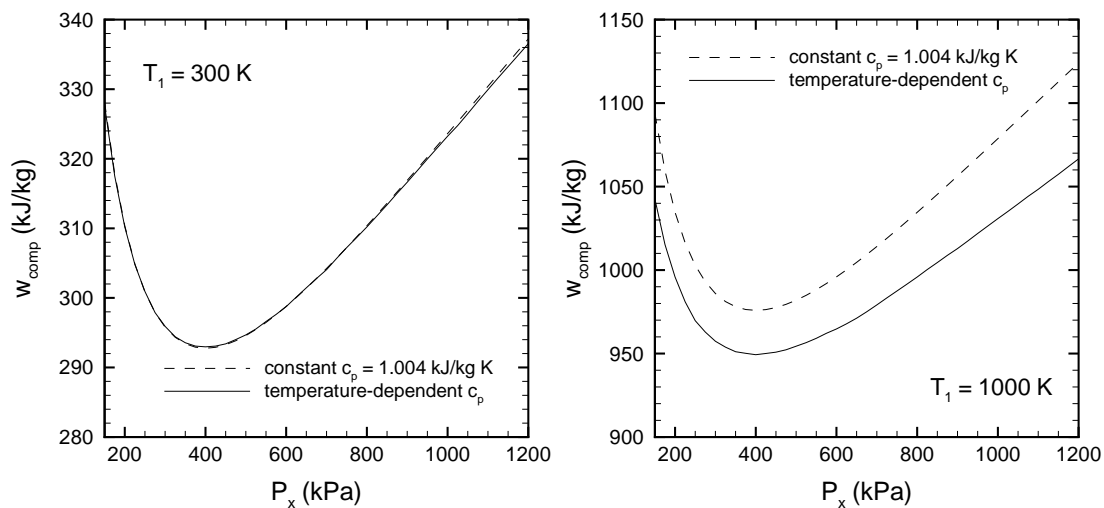Figure 6. Schematic of the two-stage compressor and T - s diagram.

Figure 7. Effect of the pressure ratio on the work required to compress air at 300 K (left) and 1000 K (right) in a two stages.

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Biographical Information

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```
function isentropic_compression
%
% read in property vectors and declare global
%
global T_vec h_vec s0_vec;
[T_vec,h_vec,s0_vec] = textread('air_thermo_props.dat','%f %f %f');
%
% inlet conditions and pressure ratio
%
T1 = 300; P1 = 100; P2 = 1600; Pr = P2/P1;
fprintf('inlet conditions:  T1 = %5.1f K  Pr = %6.2f\n',T1,Pr)
%
% constant specific heat case
%
fprintf('\n \n');
k = 1.4; cp = 1.004;  km1dk = (k-1)/k;
T2 = T1*(Pr)^km1dk; w = cp*(T2-T1);
fprintf('constant c_p (k = %4.2f):  T2 = %5.1f K   w = %5.1f kJ/kg
\n',k,T2,w)
fprintf('\n \n');
%
% temperature-dependent specific heat case
%
fprintf('loop to demonstrate bracketing process \n \n');
fprintf('      T          delta_s \n');
fprintf('    -----        ------- \n');
for i = 3:10
 T2 = i*100;
 ds = delta_s(T1,T2,Pr);
  fprintf('%10.2f  %10.4f \n',T2,ds);
end
T_bracket = bracket(T1,Pr);
fprintf('\n');
fprintf('bracket: T_low = %5.1f  T_high = %5.1f
\n',T_bracket(1),T_bracket(2));
fprintf('\n \n');

fprintf('bisection routine \n \n');
T2 = bisect(T1,T_bracket,Pr,0.1); w = delta_h(T1,T2);

fprintf('\n');
fprintf('temperature-dependent c_p:  T2 = %5.1f K   w = %5.1f kJ/kg
\n',T2,w);
%
%  subroutines
%
function T_bracket = bracket(T1,Pr)
step = 100; Tl = T1; Th = Tl + step;
dsl = delta_s(Tl,Tl,Pr); dsh = delta_s(Tl,Th,Pr);
while dsl*dsh > 0
```

```matlab
    Th = Th + step;
    dsh = delta_s(Tl,Th,Pr);
end
T_bracket = [Tl,Th];

function T = bisect(T1,T_bracket,Pr,error)
Tl = T_bracket(1); Th = T_bracket(2);
delta_T = Th - Tl; j_max = ceil(log(delta_T/error)/log(2));
dsl = delta_s(T1,Tl,Pr); dsh = delta_s(T1,Th,Pr);
T = (Tl + Th)/2; ds = delta_s(T1,T,Pr);
fprintf('    T_low      T_high     T_mid       delta_s \n');
fprintf('    -----      ------     -----       ------- \n');
fprintf('%10.2f  %10.2f %12.4f %12.4f\n',Tl,Th,T,ds);
for j = 2:j_max
if dsl*ds > 0
    Tl = T; dsl = delta_s(T1,Tl,Pr);
else
    Th = T; dsh = delta_s(T1,Th,Pr);
end
T = (Tl + Th)/2; ds = delta_s(T1,T,Pr);
fprintf('%10.2f  %10.2f %12.4f %12.4f\n',Tl,Th,T,ds);
end

function ds = delta_s(T_1,T_2,Pr)
global T_vec h_vec s0_vec;
MW = 28.96512; R = 8.31451; R_air = R/MW;
s0_1 = interp1(T_vec,s0_vec,T_1);
s0_2 = interp1(T_vec,s0_vec,T_2);
ds = s0_2 - s0_1 - R_air*log(Pr);

function dh = delta_h(T_1,T_2)
global T_vec h_vec s0_vec;
h_1 = interp1(T_vec,h_vec,T_1);
h_2 = interp1(T_vec,h_vec,T_2);
dh = h_2 - h_1;
```

```
function ds = delta_s(T_1,T_2,Pr)
MW = 28.96512; R = 8.31451; R_air = R/MW;
[cp_1,h_1,s0_1] = air_prop(T_1);
[cp_2,h_2,s0_2] = air_prop(T_2);
ds = s0_2 - s0_1 - R_air*log(Pr);
%
%
function [cp,h,s0] = air_prop(T)
%
MW = 28.96512; R = 8.31451; R_air = R/MW;
if T < 200
    fprintf('\n Temperature not in range \n',T)
elseif T < 1000
    a1 =  1.009950160e+04;
    a2 = -1.968275610e+02;
    a3 =  5.009155110e+00;
    a4 = -5.761013730e-03;
    a5 =  1.066859930e-05;
    a6 = -7.940297970e-09;
    a7 =  2.185231910e-12;
    b1 = -1.767967310e+02;
    b2 = -3.921504225e+00;
elseif T < 6000
    a1 =  2.415214430E+05;
    a2 = -1.257874600E+03;
    a3 =  5.144558670E+00;
    a4 = -2.138541790E-04;
    a5 =  7.065227840E-08;
    a6 = -1.071483490E-11;
    a7 =  6.577800150E-16;
    b1 =  6.462263190E+03;
    b2 = -8.147411905E+00;
else
    fprintf('\n Temperature not in range \n',T)
end
cp = R_air*(a1*T^-2 + a2*T^-1 + a3 + a4*T + ...
                    a5*T^2 + a6*T^3 + a7*T^4);
h0 = R_air*T*(-a1*T^-2 + a2*T^-1*log(T) + a3 + a4*T/2 + ...
                    a5*T^2/3 + a6*T^3/4 + a7*T^4/5 + b1/T);
s0 = R_air*(-a1*T^-2/2 - a2*T^-1 + a3*log(T) + a4*T + ...
                    a5*T^2/2 + a6*T^3/3 + a7*T^4/4 + b2);
```