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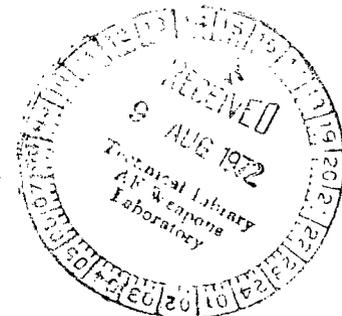
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POLYNOMIAL APPROXIMATIONS
OF THERMODYNAMIC PROPERTIES
OF ARBITRARY GAS MIXTURES OVER
WIDE PRESSURE AND DENSITY RANGES

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SUMMARY

Computer programs for flow fields around planetary entry vehicles require real-gas equilibrium thermodynamic properties in a simple form which can be evaluated quickly. To fill this need, polynomial approximations were found for thermodynamic properties of air and model planetary atmospheres. A coefficient-averaging technique was used for curve fitting in lieu of the usual least-squares method. The polynomials consist of terms up to the ninth degree in each of two variables (essentially pressure and density) including all cross terms. Four of these polynomials can be joined to cover, for example, a range of about 1000 to 11 000 K and 10^{-5} to 10^0 atmosphere ($1 \text{ atm} = 1.0133 \times 10^5 \text{ N/m}^2$) for a given thermodynamic property. Relative errors of less than 1 percent are found over most of the applicable range.

INTRODUCTION

Computer programs used to analyze the flow field around a vehicle traveling at planetary entry velocities require real-gas equilibrium thermodynamic properties in a simple form which can be evaluated quickly. In the preliminary design studies for such vehicles, thermodynamic properties are needed for chemically reacting gas mixtures similar in complexity to air. However, the elemental compositions of other planetary atmospheres are not yet known, and the proposed models change as new discoveries are made. Furthermore, the flow fields around blunt body shapes, which are being considered for entry vehicles, require the thermodynamic properties over wide ranges of pressure and density. A simple and versatile means of handling the thermodynamic properties consistent with the above considerations is needed.

One approach is to read large tables of properties into the computer memory for interpolation purposes. However, the storage required by such tables can be prohibitive in view of the number of other variables which must be carried in the high-speed memory for a detailed flow-field calculation, especially in three-dimensional problems. Another approach is to represent the tables by two-dimensional approximate functions. (For such

a problem, see ref. 1.) For air, Grabau (ref. 2) determined approximate functions by constructing two-dimensional continuous equations from straight-line segments, transition functions, and eighth-degree polynomials. However, Grabau's approach requires tedious hand calculations which would have to be carried out for each model planetary atmosphere. Another approach, the one-dimensional spline fit (ref. 3), was used in reference 4 but is not easily adaptable to two independent variables such as pressure and density (ref. 5). Also, in references 2 and 4 approximate functions are determined for first-order properties only and are differentiated to obtain second-order properties. (Second-order properties are those which depend on the partial derivatives of the species concentrations, for example, heat capacity and speed of sound. (See ref. 6.))

The present two-dimensional curve-fit procedure is designed to convert thermodynamic properties to a simple form suitable for automatic computation for various model planetary atmospheres. This procedure employs a 100-term polynomial of ninth degree in each of two variables to approximate any thermodynamic property. Since the input data (refs. 6 and 7) are not experimental, the type of smoothing of the least-squares method (which is discussed in ref. 8, for example) is not appropriate in determining the polynomial coefficients. That is, many thermodynamic properties are characterized by large variations due primarily to chemical reactions; a least-squares curve fit tends to smooth out variations in computed data just as it smooths out scatter in experimental data. In an attempt to preserve the variations but to smooth out oscillations which may occur between input data points, the coefficients are determined by taking the average of polynomials which exactly reproduce alternate points of an input data array. No error criterion is met uniformly over the entire range of input data. Instead, large errors are concentrated on the edges of the range, and good accuracy is found throughout the central area. The central areas of several polynomials can be joined to accurately cover wide pressure and density ranges. Curve fits of the present type have been applied in the calculation of a blunt-body flow field in reference 9.

SYMBOLS

Because of the lack of lower case letters and subscripts on the computer, some of the symbols in the figures are different from those in the text. These symbols are indicated in parentheses in the symbol list.

a (A) speed of sound

a_0 (AO) reference speed of sound, $\left(1.4 \frac{p_0}{\rho_0}\right)^{1/2}$

$A_n(x)$ polynomial coefficients (see eq. (2))

$A_n'(x), A_n''(x)$ coefficients whose average is $A_n(x)$

$B_{m,n}$ polynomial coefficients (see eq. (3))

c_p (CP) heat capacity at constant pressure per mole of undissociated mixture

h (H) enthalpy of mixture per mole of undissociated mixture

i (IX) index

j (IW) index

M_U molecular weight of undissociated mixture

p pressure

p_0 reference pressure, 1.0133×10^5 N/m² (1 atm)

R universal gas constant, 8314.3 J/kmole-K

s (S) entropy of mixture per mole of undissociated mixture

T absolute temperature

T_0 reference temperature, 273.15 K

w normalized W , $\frac{W - W_1}{W_{20} - W_1} - \frac{1}{2}$

$$W = \log_{10} \left(\frac{p/p_0}{\rho/\rho_0} \right)$$

W_j j th value of evenly spaced W 's (see fig. 1)

x normalized X , $\frac{X - X_1}{X_{20} - X_1} - \frac{1}{2}$

$$X = \log_{10} \left(\frac{p}{p_0} \right)$$

- X_i ith value of evenly spaced X 's (see fig. 1)
- $Y = \log_{10} T$
- Z any thermodynamic property
- $Z_{i,j}$ input thermodynamic-property value corresponding to X_i and W_j (see fig. 1)
- ρ mass density
- ρ_0 reference mass density, $\frac{M_U P_0}{RT_0}$

CURVE-FIT PROCEDURE

The analytical form of the curve-fit polynomial will be given, and will be followed by a discussion of some numerical studies used to determine parameters which give useful results. The problem is to find a procedure which gives accurate results over fairly wide ranges of two independent variables and which can be programmed so that as model atmospheres are updated, the new versions can be treated automatically.

The input thermodynamic properties can be obtained from a number of sources, and therefore, the calculation of these properties is not described herein. The properties for all the curve fits in this report were computed by use of the methods in references 6 and 7.

Analytical Form

The basic curve-fit polynomial for any thermodynamic property Z is of ninth degree in each of two variables x and w , that is,

$$Z(x,w) = \sum_{n=0}^9 \sum_{m=0}^9 B_{m,n} x^m w^n \quad (1)$$

The coefficients $B_{m,n}$ are determined in two steps. First, for a fixed value of x ,

$$Z(x,w) = \sum_{n=0}^9 A_n(x) w^n \quad (2)$$

is solved for the 10 coefficients $A_n(x)$. Next,

$$A_n(x) = \sum_{m=0}^9 B_{m,n} x^m \quad (3)$$

for $n = 0, 1, \dots, 9$ is solved for the 100 coefficients $B_{m,n}$. In both of these steps, the coefficients are determined by taking the average of polynomials which exactly reproduce alternate points of an input data array. That is, the thermodynamic property $Z(x_i, w_j)$ is known for 20 evenly spaced values of x_i and w_j . For a fixed value of $x = x_i$, 10 simultaneous equations are formed by substituting $Z(x_i, w_j)$ and w_j for $j = 1, 3, \dots, 19$ into equation (2) and are solved for a set of 10 coefficients $A'_n(x_i)$. Another set, $A''_n(x_i)$, is determined for $j = 2, 4, \dots, 20$. A final set of $A_n(x_i)$ is found by simply averaging the first two sets,

$$A_n(x_i) = \frac{A'_n(x_i) + A''_n(x_i)}{2} \quad (4)$$

for $n = 0, 1, \dots, 9$. The $B_{m,n}$ are found in the same way from equation (3). The details of using the 400 input property values $Z_{i,j}$ in figure 1 to determine the 100 coefficients $B_{m,n}$ are given in the appendix. The relationship between the variables in equation (1) and those in figure 1 is

$$\left. \begin{aligned} x &= \frac{X - X_1}{X_{20} - X_1} - \frac{1}{2} \\ \text{and} \\ w &= \frac{W - W_1}{W_{20} - W_1} - \frac{1}{2} \end{aligned} \right\} \quad (5)$$

In order to assess the accuracy of the fit whose form is given by equations (1) to (5), both relative and absolute errors are monitored for each property as follows: Relative errors (percent deviation from input values) are displayed by a chart of error codes, defined in table I. A chart (fig. 2, for example) contains one error-code entry for each input $Z_{i,j}$ in figure 1. Absolute errors are checked by a series of six plots (fig. 3, for example) which compare curves from equation (1) with the input $Z_{i,j}$ values. These curves cover the range of independent variables as follows: Two of the plots cross through the center and four pass near the edges of the X and W range.

The large error codes found on the edges of a chart such as figure 2 are to be disregarded since the valid range is taken to be $X_2 \leq X \leq X_{19}$ and $W_2 \leq W \leq W_{19}$, which

excludes the outermost rows and columns. Similarly, for a series of six plots such as figure 3, the deviation of each curve from the first and 20th input data points is to be disregarded. The valid range of each curve is taken to be $2 \leq i \leq 19$ or $2 \leq j \leq 19$. Greater accuracy could be achieved by choosing a smaller valid range. When the valid ranges of polynomials are joined as in figure 4, the 19th column of one chart lies on top of the second column of the next chart. The maximum of the two error codes is given for each entry in that column.

Numerical Studies

Numerical studies show that the accuracy of the fit varies with choice of independent variables, degree of polynomial, coefficient averaging, and range covered by the independent variables. The present numerical studies were not exhaustive; therefore, the best combination of all these aspects may not have been found. The accuracy resulting from a good combination is illustrated in figures 4 and 5, which are for h/RT of air. The independent variables are $X = \log_{10}\left(\frac{p}{p_0}\right)$ and $W = \log_{10}\left(\frac{p/p_0}{\rho/\rho_0}\right)$, the polynomial is of ninth degree, each coefficient is an average of two coefficients, and the ranges of the variables for a given polynomial are $\Delta X \approx 5.0$ and $\Delta W \approx 0.4$. Note that these four aspects are not entirely unrelated. For example, if the range of a variable is restricted, an accurate fit can be made with a lower order polynomial. However, in several subsequent examples, three of these aspects will be kept the same as given here while one will be changed. In each of these examples, the resulting error-code chart will be compared with that in figure 4.

Independent variables.- One alternate set of independent variables which was tried is X and $Y = \log_{10} T$. Error codes for h/RT of air are given in figure 6. The X range is the same as that in figure 4, whereas the Y range is similar to that for W . A comparison of figure 6 with figure 4 shows that the errors in figure 6 are larger. This difference indicates that the independent variables X and Y are not as effective as X and W .

Degree of polynomial.- The choice of the degree of the polynomials is arbitrary; ninth-degree polynomials give accuracy comparable to that of the input thermodynamic properties (refs. 6 and 7). The use of lower order polynomials might be desirable to save computer storage space, provided that sufficient accuracy is achieved for the intended application. Figure 7 gives error codes for seventh-degree polynomials approximating h/RT of air in the same X and W ranges as in figure 4. The maximum error code is 2 in both figures 7 and 4. However, more error codes of 1 and 2 appear for seventh-degree polynomials than for ninth-degree polynomials.

Coefficient averaging.- The coefficient averaging is eliminated by using a 10 by 10 array of input data which consists of entries for every other X and every other W from the 20 by 20 array in figure 1. A ninth-degree polynomial exactly reproduces these 100 input data points; these points must therefore have zeros for error codes in figure 8, which is for h/RT of air. The remaining 300 error codes are a measure of the oscillations between the 100 input data points. Figure 8 corresponds to the second polynomial of figure 4. It can be seen that the errors are larger (particularly for $W = 0.9630$) for the case without averaging.

Range covered by a polynomial.- An attempt was made to approximate a thermodynamic property over very wide X and W ranges with one two-dimensional polynomial. An X range of $X_{19} - X_2 \approx 8$ is covered in figure 9, compared with the previous range of $X_{19} - X_2 \approx 5$ in figure 4. The range of W for the error codes of the polynomial in figure 9 is about the same as for the four polynomials combined in figure 4. The errors shown in figure 9 are judged to be much too large to justify the use of one polynomial to approximate a property over such wide ranges of variables. Although this case is extreme, it illustrates that the accuracy deteriorates rapidly as the range is increased.

For applications in which higher pressures are encountered, variations in thermodynamic properties are generally weaker and are consequently easier to approximate. Smaller errors are shown in the valid range of figure 10, which is for $-3 \lesssim X \lesssim 2$, than in the third polynomial of figure 4, which is for $-5 \lesssim X \lesssim 0$. The W range is the same in both figures.

DISCUSSION OF RESULTS

The discussion will be limited to a few sample results for several thermodynamic properties of air and carbon dioxide. For all these results, the independent variables are

$X = \log_{10} \left(\frac{p}{p_0} \right)$ and $W = \log_{10} \left(\frac{p/p_0}{\rho/\rho_0} \right)$, the polynomial is of ninth degree, each coefficient

is an average of two coefficients, and the ranges of the variables for a given polynomial are $\Delta X \approx 5.0$ and $\Delta W \approx 0.4$. Second-order properties are more difficult to approximate than first-order properties; however, some results will be given for both types. Polynomials approximating h/RT and c_p/R are generally found to contain the largest errors of the approximations for all first- and second-order properties, respectively. Therefore, results for these two properties will be emphasized.

Properties of Air

Temperature.- The polynomial approximations of thermodynamic properties are functions of pressure and density but not temperature. If, for example, properties are

needed at a given temperature and density, the polynomial for temperature can be used in an iterative process to determine the corresponding pressure. All other properties can then be evaluated from the computed pressure and known density. This process is accurate because temperature is accurately approximated, as illustrated by the typical results in figures 2 and 3. (Recall that the outermost rows and columns of an error-code chart such as figure 2 are outside the valid range of the polynomial.)

Entropy.- Entropy is also an easy property to fit. Figures 11 and 12 indicate that entropy is accurately approximated.

Enthalpy.- The approximation of h/RT of air is shown in figure 4, where the valid ranges of four polynomials have been joined to cover a wide W range (corresponding to temperatures of about 1000 to 11 000 K). The edges of each error-code chart have been omitted from figure 4. Where the 19th column of one chart coincides with the second column of the next chart, the maximum of each pair of error codes is shown. Note that most of the relative errors are less than 1 percent and none are larger than 2 percent in the valid range for h/RT . The plots in figure 5 correspond to the error-code chart of the third polynomial in figure 4, where the largest error codes are found.

Heat capacity.- Second-order properties are more difficult to approximate because they have stronger variations. Results for one such property, c_p/R , are given in figures 13 and 14. Figure 13 is constructed from error codes for the valid ranges of four polynomials in such a manner that the X and W ranges are the same as in figure 4. The plots corresponding to the third polynomial are given in figure 14 because the largest relative errors occur there. Note, for example, that the first row ($X_2 = -5.1112$) in figure 13 contains a large error code of 5 where the value of c_p/R is small at $IW = 12$ in figure 14(a). In this case, the large error code is misleading since the absolute error is small. A similar situation exists for $X_{10} = -2.7408$ for $IW = 17, 18, \text{ and } 19$. Most of the valid range contains relative errors of 1 percent or less; reasonably small absolute errors are found throughout the valid range.

Speed of sound.- The X and W range for the a/a_0 results in figures 15 and 16 is the same as that of the third polynomial in figure 13 because the largest errors in a/a_0 are found there. Most of these errors are less than 1 percent, and none are larger than 5 percent in the valid range.

Properties of CO_2

Results similar to those for air were found for the model Mars atmospheres considered in reference 9, where the present method was used. Results for those mixtures of carbon dioxide (CO_2), oxygen (O_2), and argon can be illustrated by considering 100 percent CO_2 . Actually, the dissociation of 100 percent CO_2 is more complicated (hence, curve fitting is more difficult) than that of air. This complexity is caused by the three

major dissociation processes for CO_2 ($2\text{CO}_2 \rightarrow 2\text{CO} + \text{O}_2$, $\text{O}_2 \rightarrow 2\text{O}$, and $\text{CO} \rightarrow \text{C} + \text{O}$) compared with the two for air ($\text{O}_2 \rightarrow 2\text{O}$ and $\text{N}_2 \rightarrow 2\text{N}$).

Enthalpy.- Figures 17 and 18 are for h/RT of CO_2 , which is negative at temperatures below about 3000 K. The negative values pose no problem in curve fitting except that the error code is meaningless where h/RT passes through zero. This problem has been avoided in the error codes of figure 17 by simply adding a constant to h/RT to prevent the property from passing through zero. The first polynomial approximates $h/RT + 45$; the second, $h/RT + 15$; and the last two, h/RT . The X and W ranges in figure 17 are the same as those for air in figure 4. The largest of the relative errors in the valid range is 4 percent, and most of the errors are less than 2 percent. Since the largest error codes occur in the third polynomial, plots for it are given in figure 18.

Heat capacity.- Results for c_p/R of CO_2 are given in figures 19 and 20 for the same X and W ranges as before. In figure 19, as in previous figures, the largest error codes occur in the third polynomial, for which plots are given in figure 20. These plots indicate that the value of c_p/R is small in areas where the error codes are largest. In these areas the plots in figure 20 show that the absolute errors are reasonably small.

CONCLUDING REMARKS

Ninth-degree two-dimensional polynomials can be used with a coefficient-averaging technique to approximate thermodynamic properties of air and model planetary atmospheres. For a temperature range of about 1000 to 11 000 K and a pressure range of 10^{-5} to 10^0 atmosphere ($1 \text{ atm} = 1.0133 \times 10^5 \text{ N/m}^2$), four polynomials can be joined to approximate a single thermodynamic property. These four polynomials would be stored in a computer as 400 polynomial coefficients. Relative errors of less than 1 percent are found over most of the applicable range.

Langley Research Center,
National Aeronautics and Space Administration,
Hampton, Va., June 27, 1972.

APPENDIX

DETERMINATION OF POLYNOMIAL COEFFICIENTS

The 400 values of any property Z , as illustrated in figure 1, are used to determine the 100 coefficients of the two-dimensional ninth-degree polynomial

$$Z(x,w) = \sum_{m=0}^9 \sum_{n=0}^9 B_{m,n} x^m w^n = \begin{bmatrix} 1 & x & x^2 & \dots & x^9 \end{bmatrix} \begin{bmatrix} B_{0,0} & B_{0,1} & B_{0,2} & \dots & B_{0,9} \\ B_{1,0} & B_{1,1} & B_{1,2} & \dots & B_{1,9} \\ B_{2,0} & B_{2,1} & B_{2,2} & \dots & B_{2,9} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ B_{9,0} & B_{9,1} & B_{9,2} & \dots & B_{9,9} \end{bmatrix} \begin{bmatrix} 1 \\ w \\ w^2 \\ \vdots \\ w^9 \end{bmatrix} \quad (A1)$$

where

$$\left. \begin{aligned} x &= \frac{X - X_1}{X_{20} - X_1} - \frac{1}{2} \\ \text{and} \\ w &= \frac{W - W_1}{W_{20} - W_1} - \frac{1}{2} \end{aligned} \right\} \quad (A2)$$

These variables x and w are normalized to range between -0.5 and 0.5 to avoid the possibility of ill-conditioning (ref. 10) in matrices whose elements are powers of x 's or w 's. The normalization is also numerically convenient, since the x 's and w 's always have the same values: $x_1 = w_1 = -0.5$, $x_2 = w_2 = -0.44737$, $x_3 = w_3 = -0.39474$, . . . , $x_{18} = w_{18} = 0.39474$, $x_{19} = w_{19} = 0.44737$, and $x_{20} = w_{20} = 0.5$.

The solution for the 100 coefficients $B_{m,n}$ of equation (A1) begins by determining two "exact" one-dimensional polynomials for each given x value, with w as the variable. (An "exact" polynomial is referred to as a polynomial interpolating function in chapter 3 of reference 11. It passes through every point.) One polynomial is required to exactly reproduce the first, third, . . . , and the 19th property values while the other exactly reproduces the second, fourth, . . . , and 20th values. For the i th x value, one of these polynomials is found by solving

APPENDIX – Continued

$$\begin{bmatrix} Z_{1,1} & Z_{1,3} & Z_{1,5} & \dots & Z_{1,19} \\ Z_{2,1} & Z_{2,3} & Z_{2,5} & \dots & Z_{2,19} \\ Z_{3,1} & Z_{3,3} & Z_{3,5} & \dots & Z_{3,19} \\ Z_{4,1} & Z_{4,3} & Z_{4,5} & \dots & Z_{4,19} \\ Z_{5,1} & Z_{5,3} & Z_{5,5} & \dots & Z_{5,19} \\ Z_{6,1} & Z_{6,3} & Z_{6,5} & \dots & Z_{6,19} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ Z_{20,1} & Z_{20,3} & Z_{20,5} & \dots & Z_{20,19} \end{bmatrix} = \begin{bmatrix} a_{1,0} & a_{1,1} & a_{1,2} & \dots & a_{1,9} \\ a_{2,0} & a_{2,1} & a_{2,2} & \dots & a_{2,9} \\ a_{3,0} & a_{3,1} & a_{3,2} & \dots & a_{3,9} \\ a_{4,0} & a_{4,1} & a_{4,2} & \dots & a_{4,9} \\ a_{5,0} & a_{5,1} & a_{5,2} & \dots & a_{5,9} \\ a_{6,0} & a_{6,1} & a_{6,2} & \dots & a_{6,9} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_{20,0} & a_{20,1} & a_{20,2} & \dots & a_{20,9} \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ w_1 & w_3 & w_5 & \dots & w_{19} \\ w_1^2 & w_3^2 & w_5^2 & \dots & w_{19}^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ w_1^9 & w_3^9 & w_5^9 & \dots & w_{19}^9 \end{bmatrix} \quad (A3)$$

for the i th row of $a_{i,n}$ and the other by solving

$$\begin{bmatrix} Z_{1,2} & Z_{1,4} & Z_{1,6} & \dots & Z_{1,20} \\ Z_{2,2} & Z_{2,4} & Z_{2,6} & \dots & Z_{2,20} \\ Z_{3,2} & Z_{3,4} & Z_{3,6} & \dots & Z_{3,20} \\ Z_{4,2} & Z_{4,4} & Z_{4,6} & \dots & Z_{4,20} \\ Z_{5,2} & Z_{5,4} & Z_{5,6} & \dots & Z_{5,20} \\ Z_{6,2} & Z_{6,4} & Z_{6,6} & \dots & Z_{6,20} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ Z_{20,2} & Z_{20,4} & Z_{20,6} & \dots & Z_{20,20} \end{bmatrix} = \begin{bmatrix} b_{1,0} & b_{1,1} & b_{1,2} & \dots & b_{1,9} \\ b_{2,0} & b_{2,1} & b_{2,2} & \dots & b_{2,9} \\ b_{3,0} & b_{3,1} & b_{3,2} & \dots & b_{3,9} \\ b_{4,0} & b_{4,1} & b_{4,2} & \dots & b_{4,9} \\ b_{5,0} & b_{5,1} & b_{5,2} & \dots & b_{5,9} \\ b_{6,0} & b_{6,1} & b_{6,2} & \dots & b_{6,9} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ b_{20,0} & b_{20,1} & b_{20,2} & \dots & b_{20,9} \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ w_2 & w_4 & w_6 & \dots & w_{20} \\ w_2^2 & w_4^2 & w_6^2 & \dots & w_{20}^2 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ w_2^9 & w_4^9 & w_6^9 & \dots & w_{20}^9 \end{bmatrix} \quad (A4)$$

for the i th row of $b_{i,n}$. The left-hand side of equation (A3) is formed from the odd-numbered columns of figure 1; the left-hand side of equation (A4) is formed from the even-numbered columns. The two polynomials are then averaged to obtain one polynomial given by the i th row of equation (A5),

$$\begin{bmatrix} Z(x_1,w) \\ Z(x_2,w) \\ Z(x_3,w) \\ Z(x_4,w) \\ Z(x_5,w) \\ Z(x_6,w) \\ \vdots \\ \vdots \\ \vdots \\ Z(x_{20},w) \end{bmatrix} = \begin{bmatrix} A_{1,0} & A_{1,1} & A_{1,2} & \dots & A_{1,9} \\ A_{2,0} & A_{2,1} & A_{2,2} & \dots & A_{2,9} \\ A_{3,0} & A_{3,1} & A_{3,2} & \dots & A_{3,9} \\ A_{4,0} & A_{4,1} & A_{4,2} & \dots & A_{4,9} \\ A_{5,0} & A_{5,1} & A_{5,2} & \dots & A_{5,9} \\ A_{6,0} & A_{6,1} & A_{6,2} & \dots & A_{6,9} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{20,0} & A_{20,1} & A_{20,2} & \dots & A_{20,9} \end{bmatrix} \begin{bmatrix} 1 \\ w \\ w^2 \\ \vdots \\ \vdots \\ \vdots \\ w^9 \end{bmatrix} \quad (A5)$$

where $A_{i,n} = \frac{a_{i,n} + b_{i,n}}{2}$ for $i = 1, 2, \dots, 20$ and $n = 0, 1, \dots, 9$.

APPENDIX – Continued

At this point, the i th row of $Z_{i,j}$ is approximated by a polynomial such that

$$Z(x_i, w) \approx \sum_{n=0}^9 A_{i,n} w^n$$

for $i = 1, 2, 3, \dots, 20$. Now the n th column of $A_{i,n}$ is to be approximated by a polynomial function of x . Two "exact" polynomials are formed for the n th column of $A_{i,n}$ by first solving

$$\begin{bmatrix} A_{1,0} & A_{1,1} & A_{1,2} & \dots & A_{1,9} \\ A_{3,0} & A_{3,1} & A_{3,2} & \dots & A_{3,9} \\ A_{5,0} & A_{5,1} & A_{5,2} & \dots & A_{5,9} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{19,0} & A_{19,1} & A_{19,2} & \dots & A_{19,9} \end{bmatrix} = \begin{bmatrix} 1 & x_1 & x_1^2 & \dots & x_1^9 \\ 1 & x_3 & x_3^2 & \dots & x_3^9 \\ 1 & x_5 & x_5^2 & \dots & x_5^9 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{19} & x_{19}^2 & \dots & x_{19}^9 \end{bmatrix} \begin{bmatrix} c_{0,0} & c_{0,1} & c_{0,2} & \dots & c_{0,9} \\ c_{1,0} & c_{1,1} & c_{1,2} & \dots & c_{1,9} \\ c_{2,0} & c_{2,1} & c_{2,2} & \dots & c_{2,9} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ c_{9,0} & c_{9,1} & c_{9,2} & \dots & c_{9,9} \end{bmatrix} \quad (A6)$$

for the n th column of $c_{m,n}$ and then solving

$$\begin{bmatrix} A_{2,0} & A_{2,1} & A_{2,2} & \dots & A_{2,9} \\ A_{4,0} & A_{4,1} & A_{4,2} & \dots & A_{4,9} \\ A_{6,0} & A_{6,1} & A_{6,2} & \dots & A_{6,9} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{20,0} & A_{20,1} & A_{20,2} & \dots & A_{20,9} \end{bmatrix} = \begin{bmatrix} 1 & x_2 & x_2^2 & x_2^3 & \dots & x_2^9 \\ 1 & x_4 & x_4^2 & x_4^3 & \dots & x_4^9 \\ 1 & x_6 & x_6^2 & x_6^3 & \dots & x_6^9 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & x_{20} & x_{20}^2 & x_{20}^3 & \dots & x_{20}^9 \end{bmatrix} \begin{bmatrix} d_{0,0} & d_{0,1} & d_{0,2} & \dots & d_{0,9} \\ d_{1,0} & d_{1,1} & d_{1,2} & \dots & d_{1,9} \\ d_{2,0} & d_{2,1} & d_{2,2} & \dots & d_{2,9} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ d_{9,0} & d_{9,1} & d_{9,2} & \dots & d_{9,9} \end{bmatrix} \quad (A7)$$

for the n th column of $d_{m,n}$. The left-hand side of equation (A6) is formed from the odd-numbered rows of $A_{i,n}$ of equation (A5); the left-hand side of equation (A7) is formed from the even-numbered rows. The two polynomials are then averaged to obtain one polynomial given by the n th column of equation (A8),

$$\begin{bmatrix} A_0(x) & A_1(x) & A_2(x) & \dots & A_9(x) \end{bmatrix} = \begin{bmatrix} 1 & x & x^2 & \dots & x^9 \end{bmatrix} \begin{bmatrix} B_{0,0} & B_{0,1} & B_{0,2} & \dots & B_{0,9} \\ B_{1,0} & B_{1,1} & B_{1,2} & \dots & B_{1,9} \\ B_{2,0} & B_{2,1} & B_{2,2} & \dots & B_{2,9} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ B_{9,0} & B_{9,1} & B_{9,2} & \dots & B_{9,9} \end{bmatrix}$$

(A8)

APPENDIX - Continued

where

$$B_{m,n} = \frac{c_{m,n} + d_{m,n}}{2} \tag{A9}$$

for $m, n = 0, 1, \dots, 9$. The two-dimensional polynomial approximation is finally formed by substituting $B_{m,n}$ of equation (A9) into equation (A1).

The set of $B_{m,n}$ and X_1 , X_{20} , W_1 , and W_{20} for the third polynomial of figure 4 for h/RT of air are given here, and a sample evaluation of the polynomial is given. The $B_{m,n}$ are ordered as follows:

$B_{0,0}$	$B_{0,1}$	$B_{0,2}$	$B_{0,3}$	$B_{0,4}$
$B_{0,5}$	$B_{0,6}$	$B_{0,7}$	$B_{0,8}$	$B_{0,9}$
.
.
.
$B_{9,5}$	$B_{9,6}$	$B_{9,7}$	$B_{9,8}$	$B_{9,9}$

The integer following the E is a power of 10; for example, $1.2081E+03 = 1.2081 \times 10^3$.

m = 0:	1.8842E+01	1.8724E+01	-1.9274E+01	-7.4597E+01	-1.4161E+02
	2.2529E+01	1.2081E+03	1.8045E+03	-2.4644E+03	-5.0926E+03
m = 1:	-1.9223E+01	5.9860E+00	1.4767E+02	4.5817E+02	1.2088E+02
	-4.9694E+03	-8.4302E+03	1.5751E+04	2.7259E+04	-1.3093E+04
m = 2:	5.7650E-01	-7.9885E+01	-4.7190E+02	-1.2060E+03	7.5502E+03
	4.0263E+04	-3.0717E+04	-2.8412E+05	2.8112E+04	6.0981E+05
m = 3:	1.5838E+01	1.7215E+02	7.5910E+02	-3.2372E+03	-3.7724E+04
	-3.8374E+04	3.4992E+05	6.2886E+05	-9.1143E+05	-1.8723E+06
m = 4:	-2.3310E+01	-2.6170E+02	1.8817E+03	3.1578E+04	1.0701E+04
	-5.8825E+05	-4.4625E+05	3.6933E+06	1.7799E+06	-7.4600E+06
m = 5:	1.8278E+01	-2.6375E+02	-1.0231E+04	-4.6790E+04	2.9272E+05
	1.5589E+06	-2.3791E+06	-1.3535E+07	5.7175E+06	3.4212E+07
m = 6:	3.1957E+01	1.7667E+03	5.0661E+03	-1.4085E+05	-4.1131E+05
	2.3622E+06	5.3044E+06	-1.3483E+07	-1.7221E+07	2.4399E+07
m = 7:	-5.9066E+01	-1.0437E+03	2.9512E+04	3.4704E+05	-6.6843E+05
	-9.2474E+06	4.2249E+06	7.5263E+07	-7.1884E+06	-1.8508E+08
m = 8:	1.1476E+01	-2.6431E+03	-2.1784E+04	1.9858E+05	1.1113E+06
	-2.9386E+06	-1.3065E+07	1.3530E+07	4.1034E+07	-1.6564E+07
m = 9:	-2.2317E+01	2.1902E+03	-2.5838E+04	-6.5313E+05	2.5673E+05
	1.6827E+07	1.6364E+06	-1.3486E+08	-1.3248E+07	3.2885E+08

For these values of $B_{m,n}$, the X_1 , X_{20} , W_1 , and W_{20} are

$$\begin{aligned}
 X_1 &= -5.4075 & X_{20} &= 0.2222 \\
 W_1 &= 1.3310 & W_{20} &= 1.7680
 \end{aligned}$$

APPENDIX - Concluded

This polynomial for h/RT can only be used in the valid range as shown in figure 4, $-5.1112 \leq X \leq -0.0741$ and $1.3540 \leq W \leq 1.7450$. If, for example, h/RT is desired at the point $X = -3.0$ and $W = 1.5$, equation (A2) is used to find that $x = -0.07236$ and $w = -0.11327$. These normalized variables and $B_{m,n}$ are then substituted into equation (A1) to evaluate $h/RT = Z(x,w) = 17.9$.

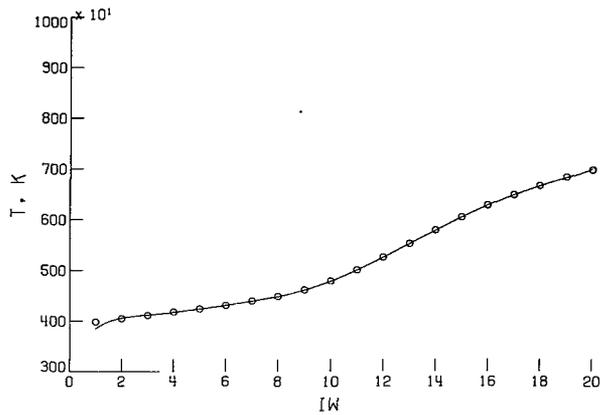
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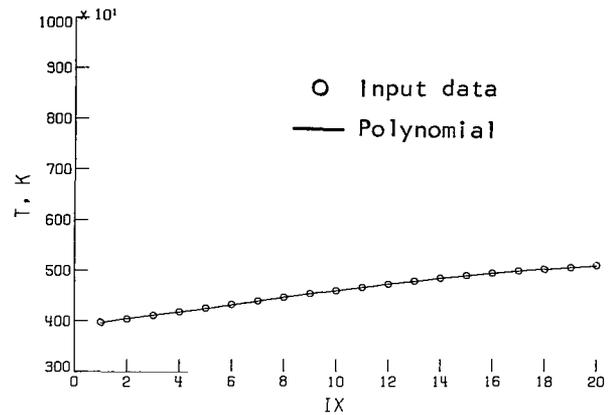
TABLE I.- DEFINITION OF ERROR CODES

Error code	Percent error ^a
0	0.0 to 0.1
1	0.1 to 1.0
2	1.0 to 2.0
3	2.0 to 3.0
4	3.0 to 4.0
5	4.0 to 5.0
6	5.0 to 7.0
7	7.0 to 10.0
8	10.0 to 15.0
9	15.0 to 20.0
*	20.0 to ∞

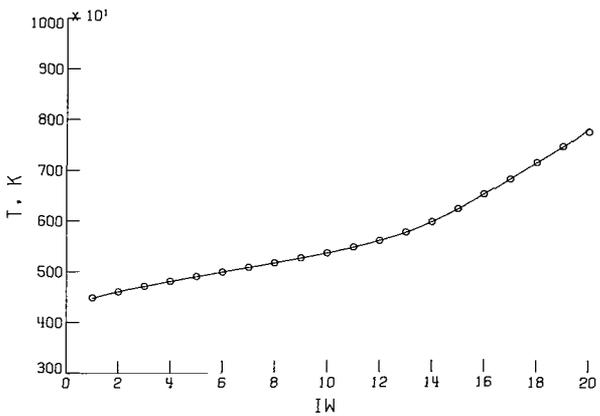
$$^a (\text{Percent error})_{i,j} = 100 \left| \frac{Z_{i,j} - Z(x_i, w_j)}{Z_{i,j}} \right|.$$



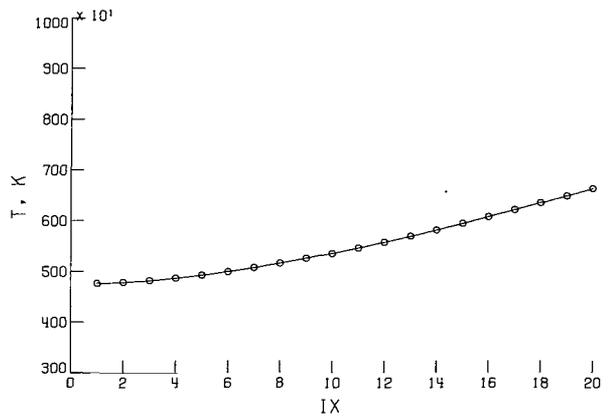
(A) $IX \square 2$ ($X \square -5.1112$).



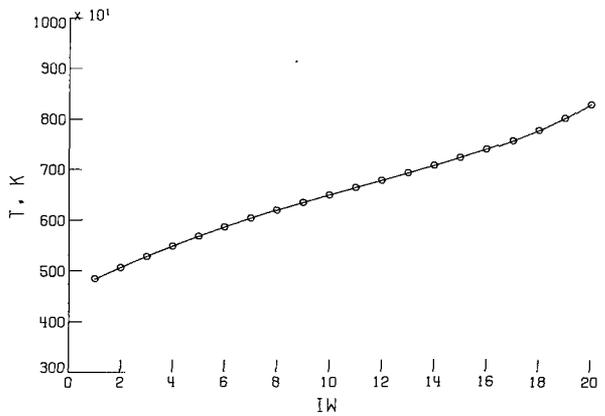
(D) $IW \square 2$ ($W \square 1.3540$).



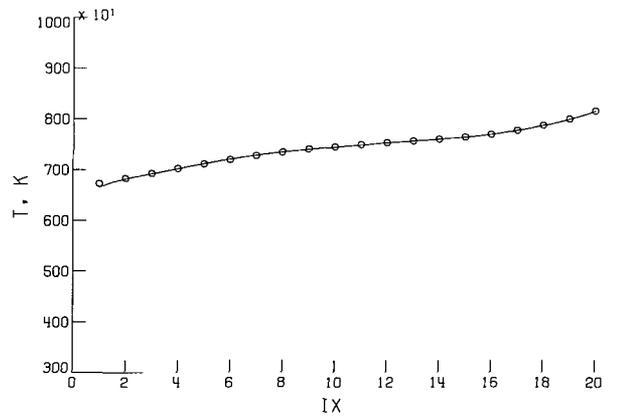
(B) $IX \square 10$ ($X \square -2.7408$).



(E) $IW \square 10$ ($W \square 1.5380$).

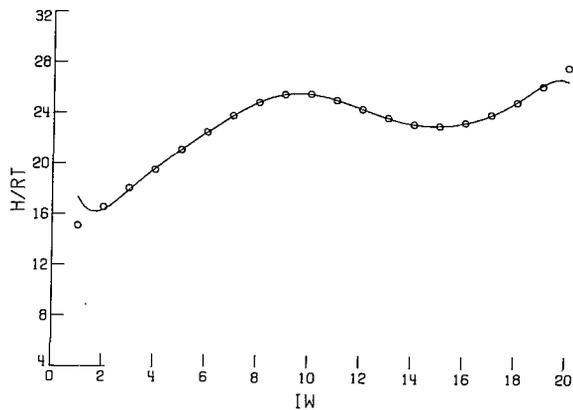


(C) $IX \square 19$ ($X \square -0.0741$).

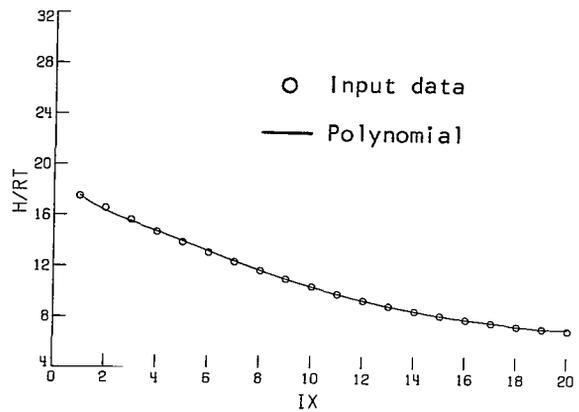


(F) $IW \square 19$ ($W \square 1.7450$).

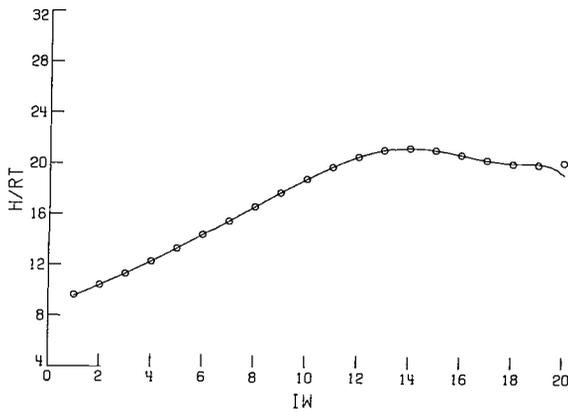
Figure 3.- Comparison of polynomial approximating T of air with input data.



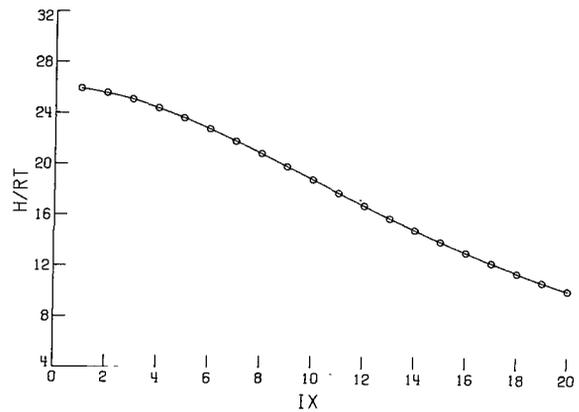
(A) $IX = 2$ ($X = -5.1112$).



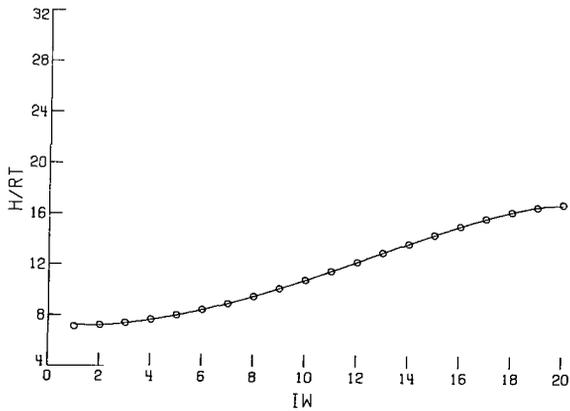
(D) $IW = 2$ ($W = 1.3540$).



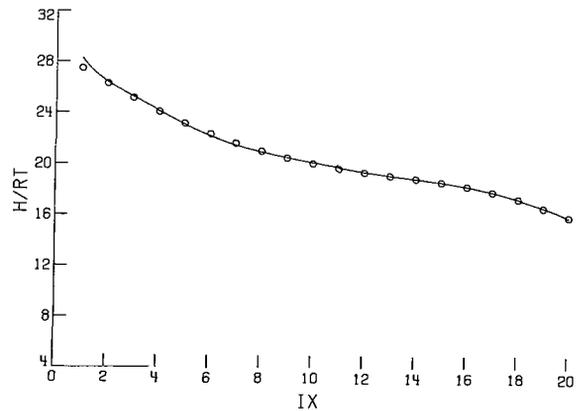
(B) $IX = 10$ ($X = -2.7408$).



(E) $IW = 10$ ($W = 1.5380$).



(C) $IX = 19$ ($X = -0.0741$).



(F) $IW = 19$ ($W = 1.7450$).

Figure 5.- Comparison of third polynomial of figure 4 approximating h/RT of air with input data.

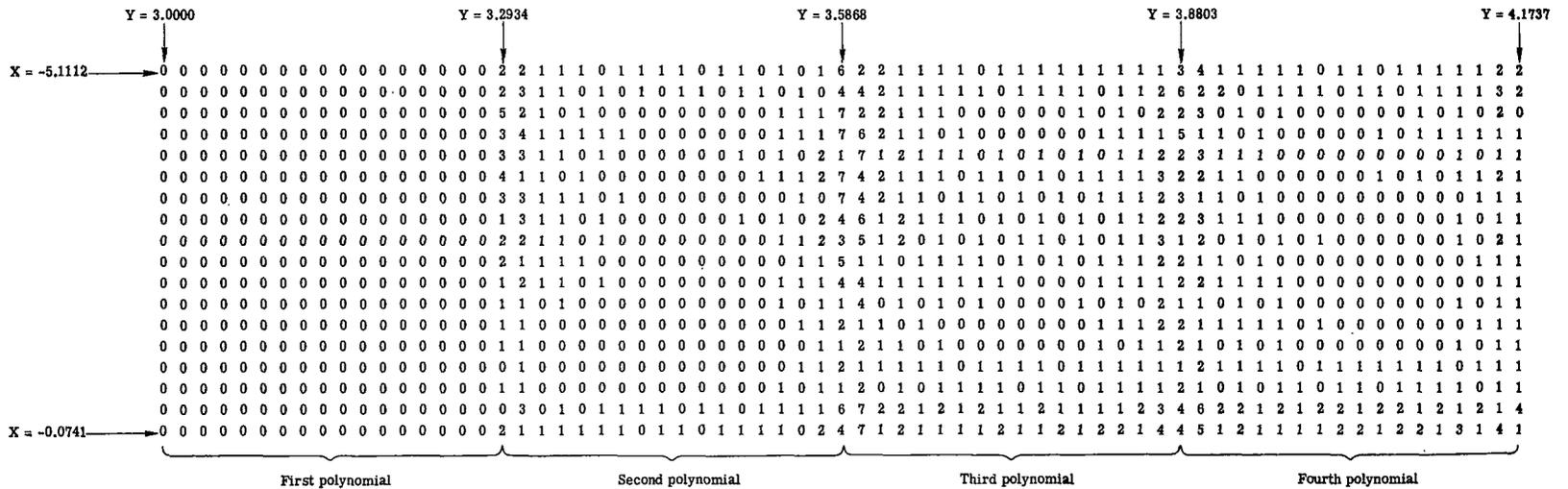


Figure 6.- Error codes for valid X and Y ranges of four polynomials joined to approximate h/RT of air.

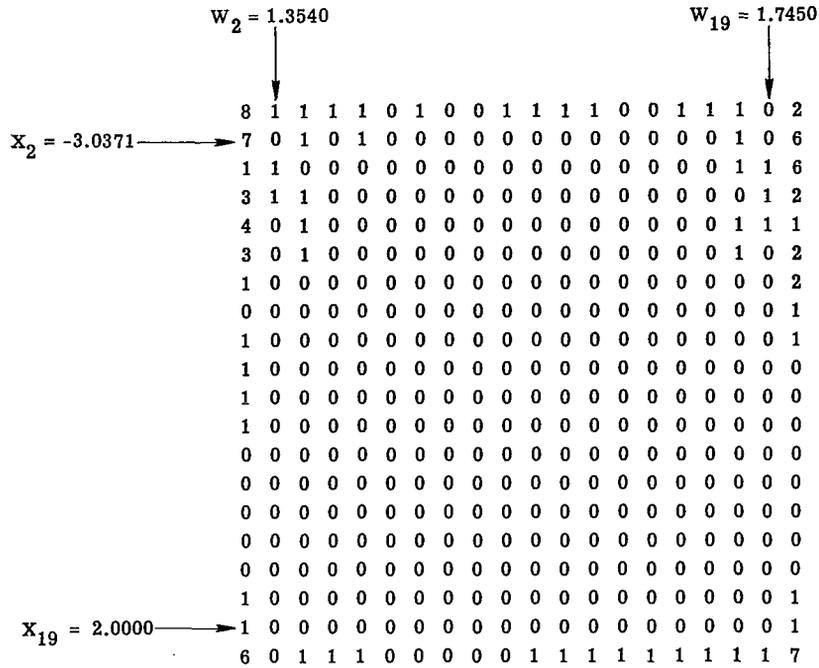


Figure 10.- Error-code chart for polynomial approximating h/RT of air in same W range as that of third polynomial of figure 4 but in a higher X range.

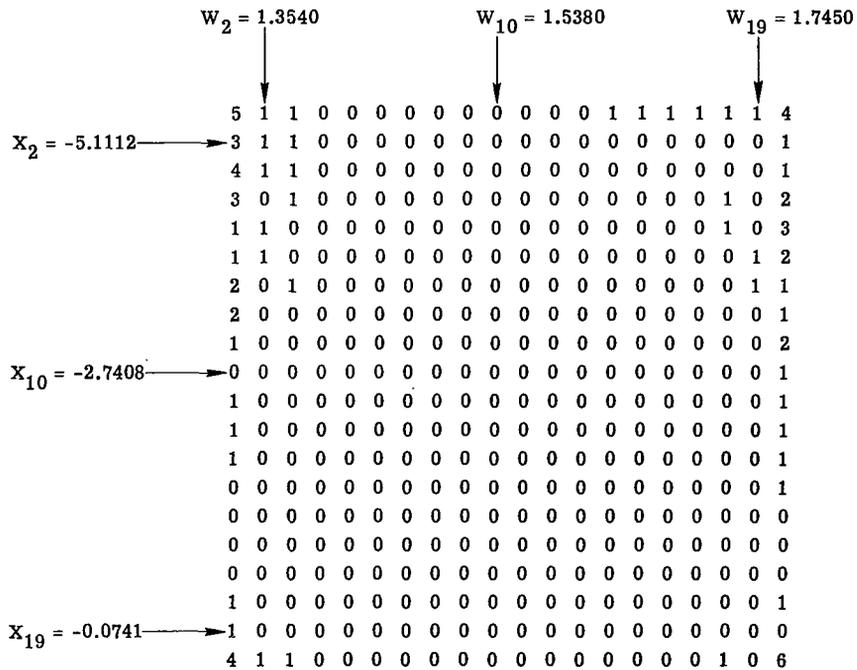
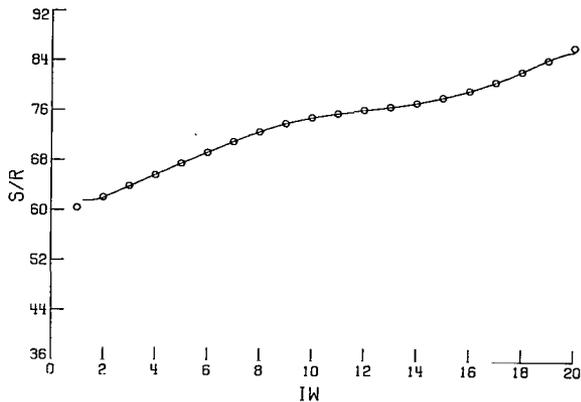
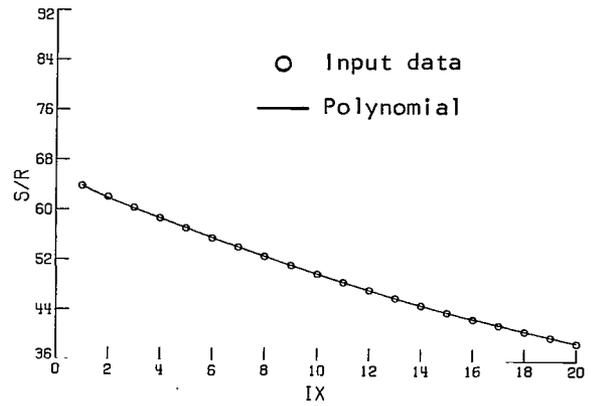


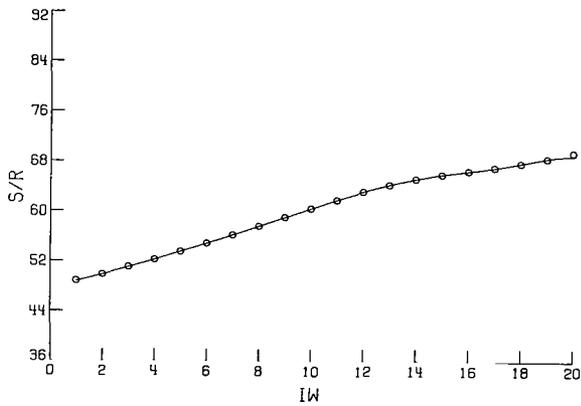
Figure 11.- Error-code chart for polynomial approximating s/R of air.



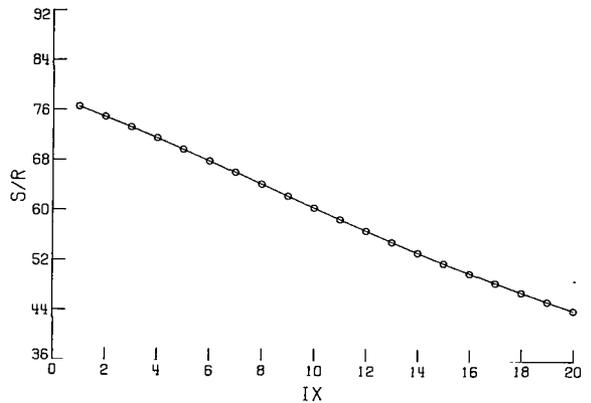
(A) $IX = 2$ ($X = -5.1112$).



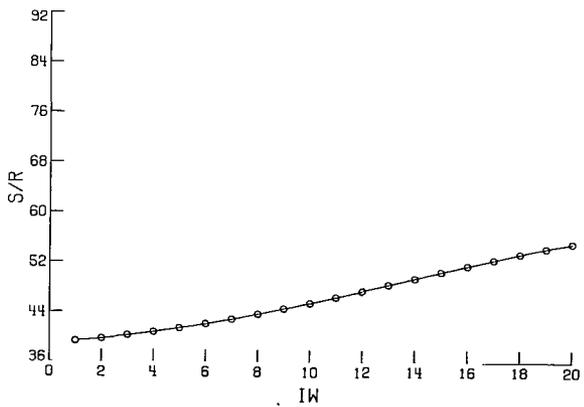
(D) $IW = 2$ ($W = 1.3540$).



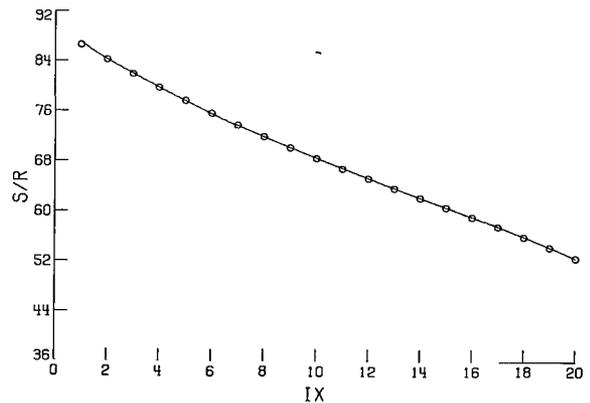
(B) $IX = 10$ ($X = -2.7408$).



(E) $IW = 10$ ($W = 1.5380$).

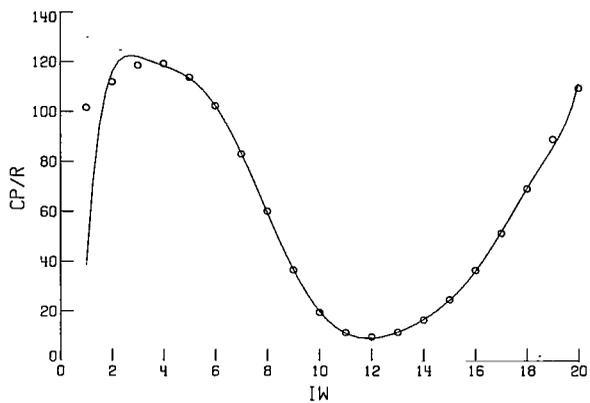


(C) $IX = 19$ ($X = -0.0741$).

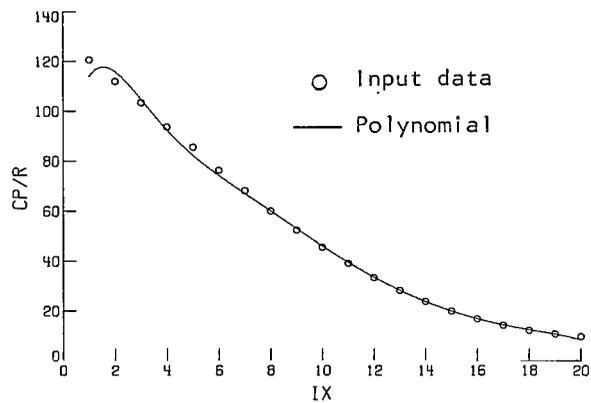


(F) $IW = 19$ ($W = 1.7450$).

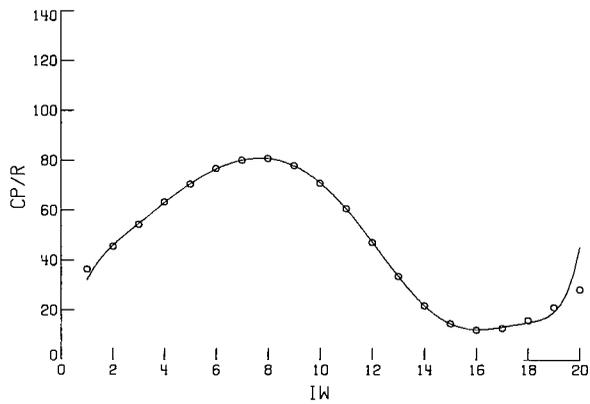
Figure 12.- Comparison of polynomial approximating s/R of air with input data.



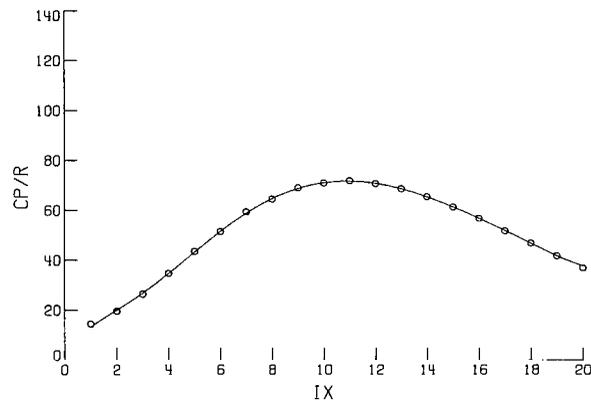
(A) $IX = 2$ ($X = -5.1112$).



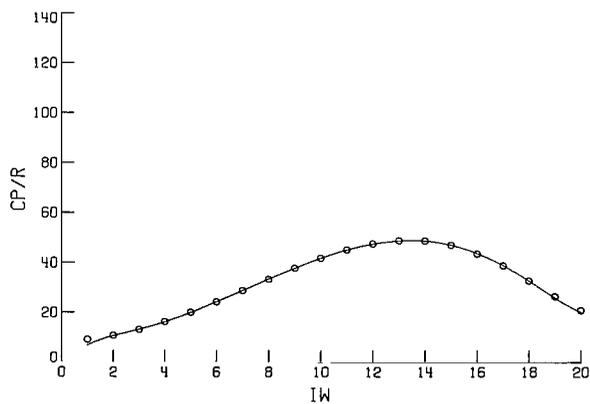
(D) $IW = 2$ ($W = 1.3540$).



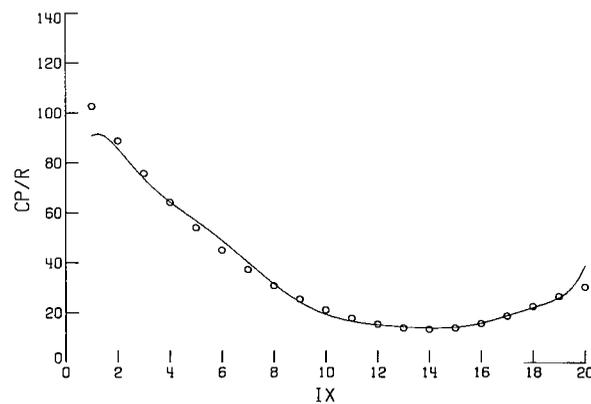
(B) $IX = 10$ ($X = -2.7408$).



(E) $IW = 10$ ($W = 1.5380$).



(C) $IX = 19$ ($X = -0.0741$).



(F) $IW = 19$ ($W = 1.7450$).

Figure 14.- Comparison of third polynomial of figure 13 approximating c_p/R of air with input data.

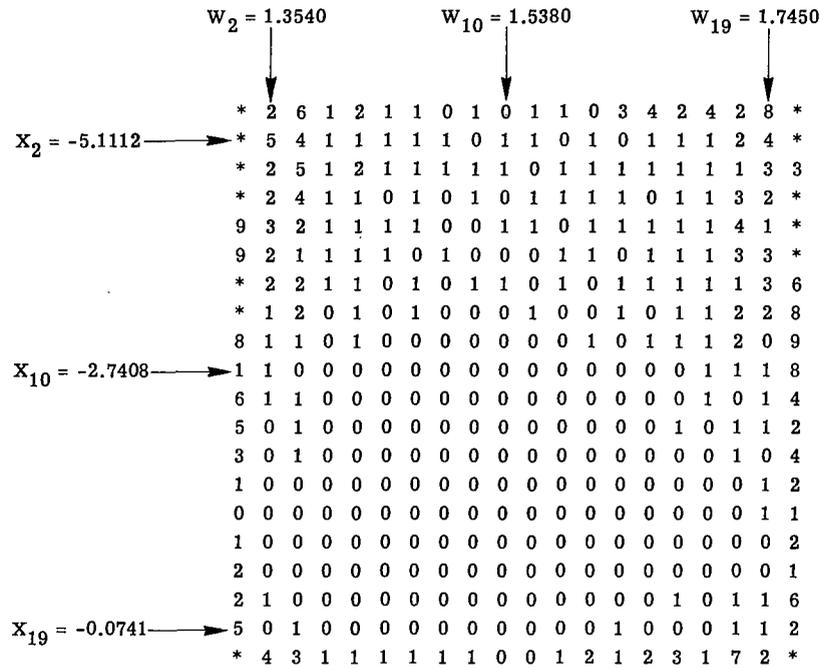
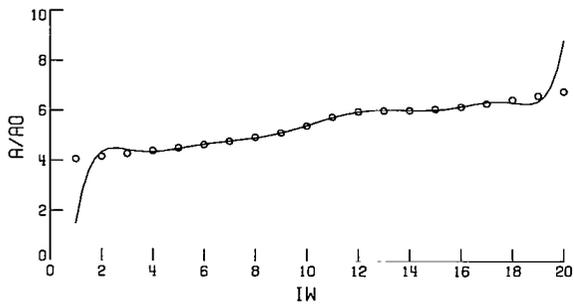
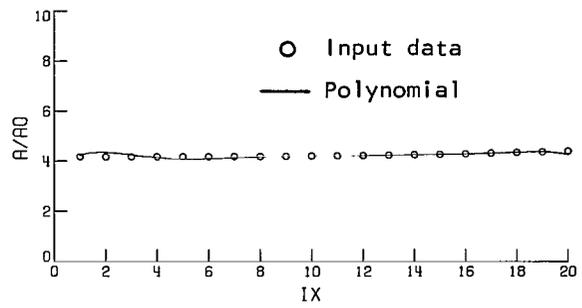


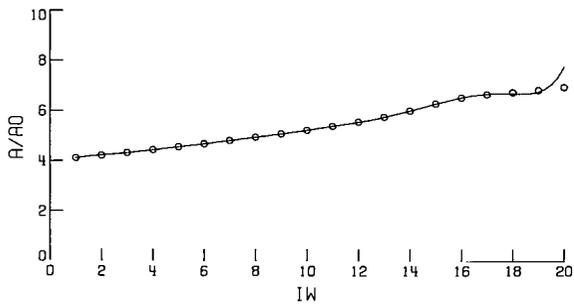
Figure 15.- Error-code chart for polynomial approximating a/a_0 of air.



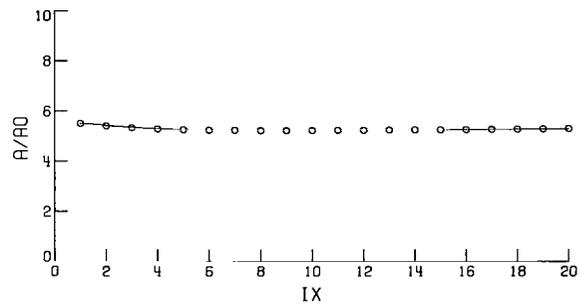
(A) $IX = 2$ ($X = -5.1112$).



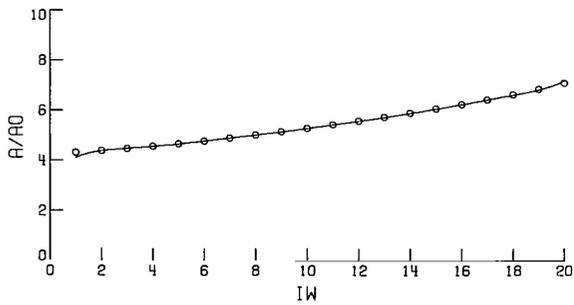
(D) $IW = 2$ ($W = 1.3540$).



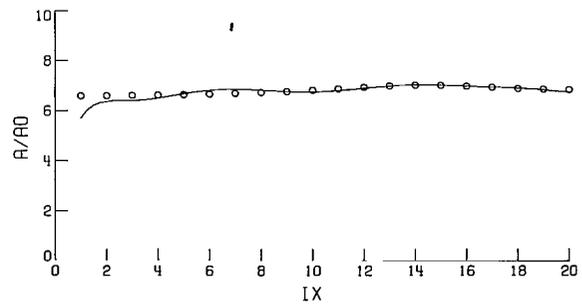
(B) $IX = 10$ ($X = -2.7408$).



(E) $IW = 10$ ($W = 1.5380$).

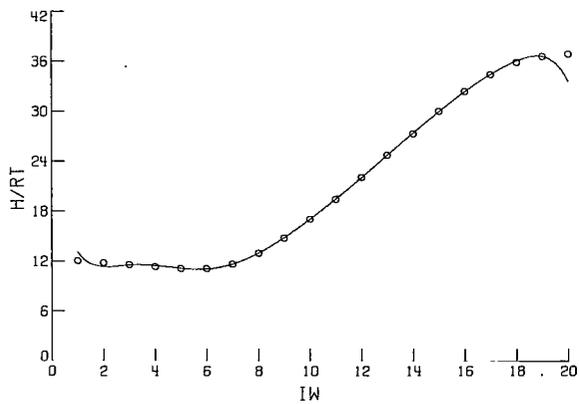


(C) $IX = 19$ ($X = -0.0741$).

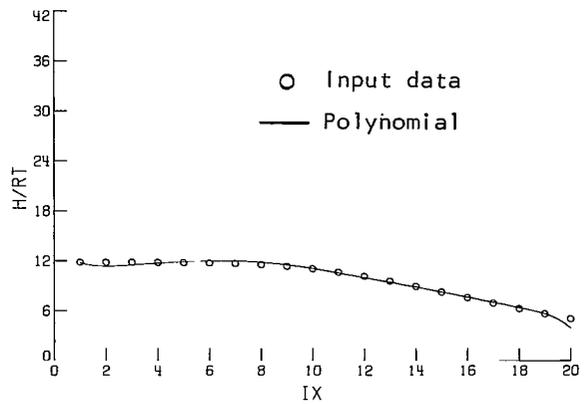


(F) $IW = 19$ ($W = 1.7450$).

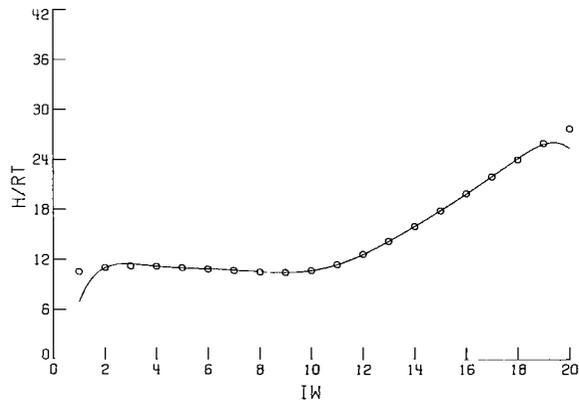
Figure 16.- Comparison of polynomial approximating a/a_0 of air with input data.



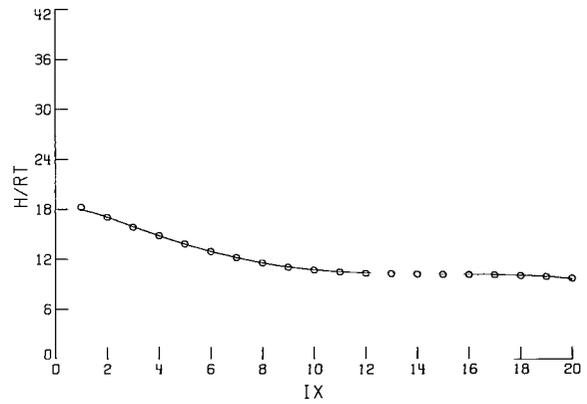
(R) $IX = 2$ ($X = -5.1112$).



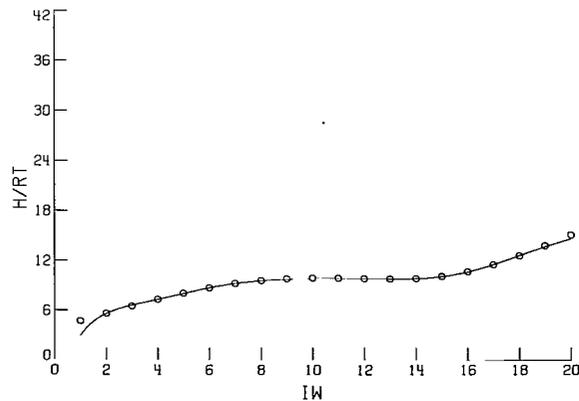
(D) $IW = 2$ ($W = 1.3540$).



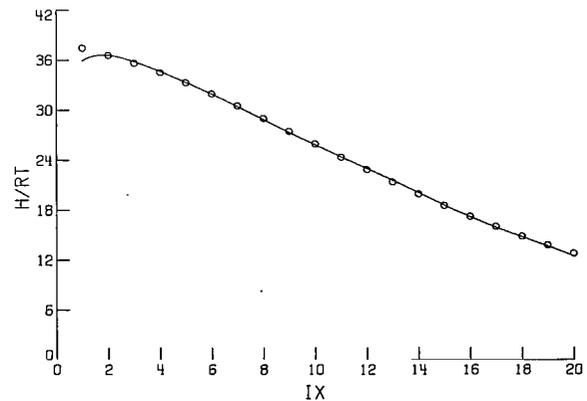
(B) $IX = 10$ ($X = -2.7408$).



(E) $IW = 10$ ($W = 1.5380$).

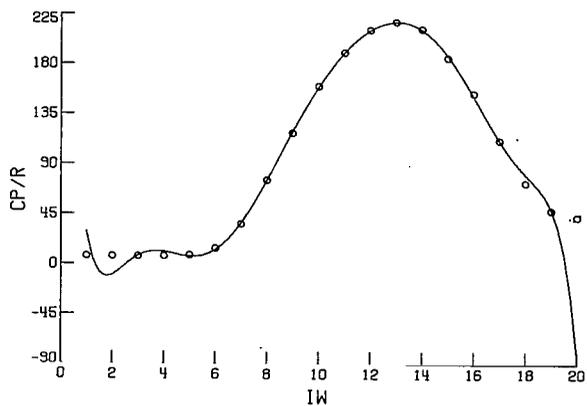


(C) $IX = 19$ ($X = -0.0741$).

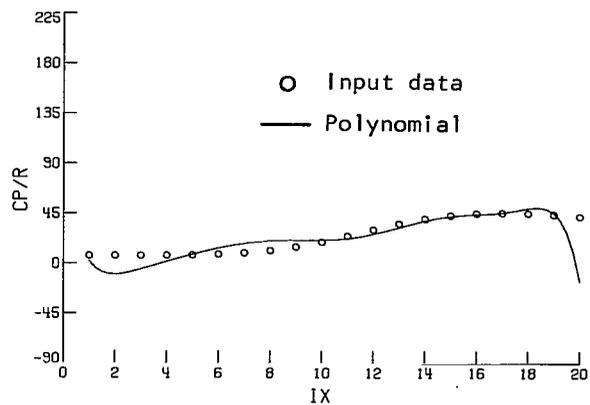


(F) $IW = 19$ ($W = 1.7450$).

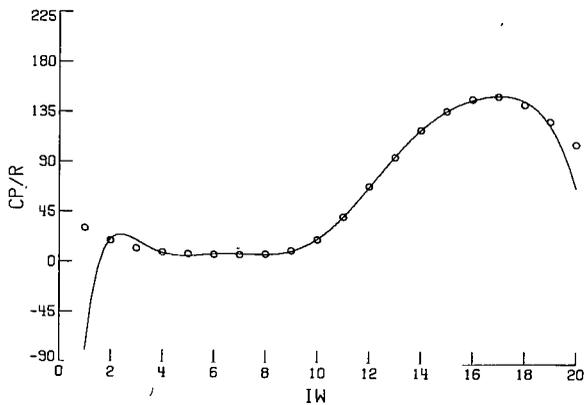
Figure 18.- Comparison of third polynomial of figure 17 approximating h/RT of CO_2 with input data.



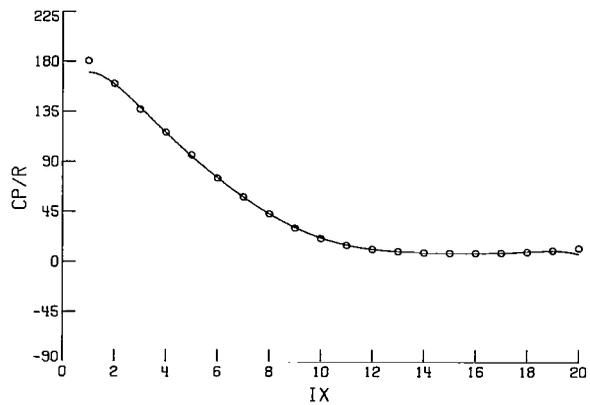
(A) $IX = 2$ ($X = -5.1112$).



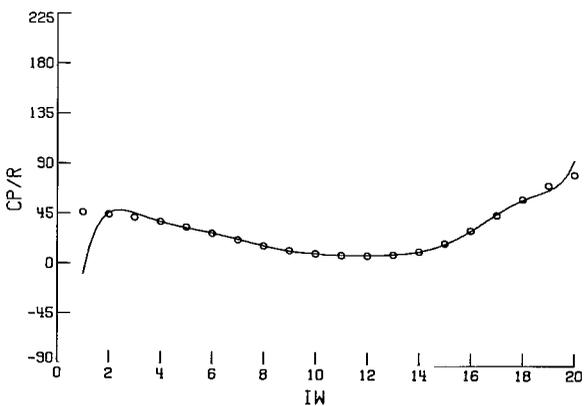
(D) $IW = 2$ ($W = 1.3540$).



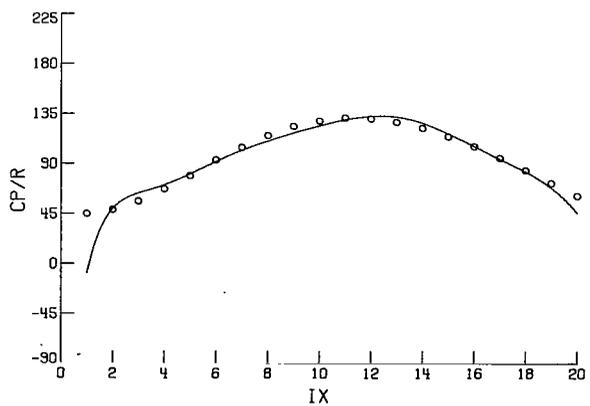
(B) $IX = 10$ ($X = -2.7408$).



(E) $IW = 10$ ($W = 1.5380$).



(C) $IX = 19$ ($X = -0.0741$).



(F) $IW = 19$ ($W = 1.7450$).

Figure 20.- Comparison of third polynomial of figure 19 approximating c_p/R of CO_2 with input data.

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