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Technical Note 1883

THERMODYNAMIC CHARTS FOR INTERNAL-COMBUSTION-ENGINE FLUIDS

By W. J. McCann
(July 1943)

Revised by L. R. Turner
and Emory A. Bauer

Lewis Flight Propulsion Laboratory
Cleveland, Ohio

Washington
July 1949

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SUMMARY

Thermodynamic properties of the products of combustion of five different mixtures of air with typical aircraft-engine fuel have been calculated from the most reliable thermodynamic data available in 1943. The calculations are presented in five charts of internal energy plotted against entropy with values of temperature, specific volume, pressure, and enthalpy indicated corresponding to 80, 90, 100, 110, and 120 percent of the fuel-air ratio for perfect combustion. Each chart is based upon the use of 1 pound of original air plus the corresponding amount of fuel.

These charts represent a considerable improvement in accuracy and range over those previously available.

INTRODUCTION

The increasing use of thermodynamic-property charts for the solution of problems involving internal-combustion-engine fluids has brought out a number of weaknesses in the charts previously available. The charts of Hershey, Eberhardt, and Hottel (reference 1), though based on accurate thermodynamic data, were not calculated with the numerical care desirable in standard reference charts. Furthermore, those charts covered only three fuel-air ratios, 85, 100, and 110 percent of theoretical air. The Lutz-Wolf charts (reference 2), although purporting to cover all ranges of fuel composition and fuel-air ratio, actually make use of a roughly approximate allowance for disassociation phenomena and, consequently, are useful only up to temperatures where disassociation is a minor correction factor. The shortcomings of other thermodynamic-property charts are discussed in reference 1.

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*The original version of this report was issued as NACA RB 3G28, which was adapted from material prepared by H. C. Hottel of the Massachusetts Institute of Technology. The present revision is issued in response to a continuing demand for this information.

Accordingly, the National Advisory Committee for Aeronautics entered into a contract with the Massachusetts Institute of Technology for the preparation of a series of charts presenting the properties of mixtures of a typical aircraft-engine fuel and air both before and after combustion. The properties of combustion products were to be based upon chemical equilibrium of the fuel burned with air in various proportions. The completed charts on the thermodynamic properties after combustion of five mixtures of air with a typical aircraft-engine fuel, CH_2 or 85.62 percent C by weight, are presented. Companion charts for 1 mole quantity of unburned mixture are presented in reference 3.

A method of use of these charts for calculation of combustion temperature and of pressure during combustion, which was devised by the staff of the NACA Lewis laboratory, is also included.

FUNDAMENTAL DATA

The material basis of the charts is 1 pound of original dry air (1/28.95 lb - moles) plus an amount of original fuel of composition CH_2 corresponding to 80, 90, 100, 110, and 120 percent of the theoretical fuel.

The amounts of fuel and air with which the charts are concerned are summarized in the following table:

Percent of theoretical fuel	80	90	100	110	120
Percent of theoretical air	125.00	111.11	100.00	90.91	83.33
Pounds fuel per pound air	0.05420	0.06098	0.06775	0.07453	0.08130
Moles CH_2 per mole air	.11195	.12594	.13993	.15393	.16792

The composition of air was taken as 20.99 percent O_2 and 79.01 percent air-N_2 (atmospheric nitrogen including argon and other rare gases). The composition of air-N_2 is considered to be 98.76 percent N_2, 1.19 percent A, 0.04 percent CO_2, and 0.01 percent H_2. The air-nitrogen was treated as nitrogen in calculations of chemical equilibrium, which affects NO formation to a slight extent, but correct values of energy and entropy were used for air-N_2.

1102

Although the temperature base has no special significance in problems involving widely varying atmospheric conditions, as in aircraft engines, the temperature base used in computing these charts was 100° F and the charts are so labeled.

One physical chemical practice is to assign zero values for energy and entropy to the elements in their normal state at 1 atmosphere. For chese charts, it was considered easier to visualize zero values in the production of complete combustion; namely, CO_2, H_2O (vapor), O_2, and air-N_2 at 1 atmosphere. Accordingly, zero values were assigned to entropies and internal energies of these four gases at the base temperature (100° F) and at 1 atmosphere.

The assumption of chemical equilibrium in gaseous systems at the temperature attained in flames is, of course, inexact, and direct experimentation to determine how far a mixture departs from equilibrium is very difficult. However, agreement between calculated and measured pressures attained in constant-volume bomb explosions and between calculated and measured temperatures in Meker burner flames substantiate the belief that at engine temperatures the true composition does not differ greatly from calculated values. Consequently, calculations of engine performance, based on assumptions of equilibrium, will parallel true performance with sufficient accuracy.

DESCRIPTION OF CHARTS

The coordinates of the charts are internal energy and entropy. Arguments exist for the use of other coordinates. In the Otto cycle, idealized combustion is a constant internal-energy process. Consideration of gas-turbine cycles would involve trial-and-error use of the charts if H had to be obtained from the relation $H = E + pv$; consequently, lines of constant H have been superimposed. Interpolation between these lines is accomplished by use of an interpolation scale provided in the upper left margin of each plot; a strip of paper may be used to transfer the interpolation.

Lines of constant temperature appear at 200° intervals. Interpolation is substantially linear. Lines at constant pressure (dotted) and constant volume (solid) also appear.

Certain problems encountered in engine-cycle studies involve the mixing (without further chemical change) of a mixture

corresponding to a point on a chart, with a cold gas. For such calculations, it is convenient to know the internal energy exclusive of chemical contributions to it.

In the consideration of an equilibrium mixture at temperature T, its energy E can be evaluated along any path that finally arrives at the base state. That path, the legs of which have special utility, is the cooling, at the constant volume and without chemical change, of the equilibrium mixture to the base temperature (thereby evolving what will be termed the "sensible" internal energy E_s), followed by isothermal combustion at the base temperature and at constant volume to produce only CO_2, H_2O, O_2, and air-N_2 (thereby evolving energy that will be designated Q_v). Then $E = E_s + Q_v$. At temperatures below 1600° K (2800° R) where equilibrium is frozen, the composition, and therefore the value of Q_v, depend only on the entropy the mixture had the instant it passed that temperature in its cooling. These values of Q_v appear at the margin on the right of the charts for use in the range where frozen equilibrium is assumed. For higher temperatures where Q_v varies both with T and S, a scale of E_s is provided with curved divisions to allow for the small dependence of E_s on S. In order to read this scale, move horizontally to the right from E to the correct S-value on the E_s-scale, then up parallel to the curved scale division to the scale on the extreme right.

The "sensible" enthalpy H_s, which is analogous to E_s, is defined by the equation

$$H_s = E_s + pv$$

By definition,

$$H = E + pv$$

therefore

$$H = E + pv = E_s + Q_v + pv = H_s + Q_v$$

As a consequence of choosing $E = 0$ at the base temperature of 100° F, the value of E, as read from the chart, is the change in internal energy in going from a particular state to the dead state (o); but the change in enthalpy in going to the dead state is

$$H_1 - H_o = H_1 - (H_{s,o} + Q_v)$$

where $H_{s,o}$ and Q_v may be read from the extreme right and left ordinates of the charts, respectively.

The units used in the charts are as follows:

Temperature - degrees Rankin (degrees Fahrenheit plus 459.7)

Pressure - pounds per square inch absolute

Volume - cubic feet

Energy - British thermal units, 777.75 foot-pounds

APPLICATION OF CHARTS TO STEADY-FLOW COMBUSTION CALCULATIONS

Corrections of base for steady-flow combustion. - Calculations of the ideal combustion temperature and momentum pressure drop in ram jets and in other steady-flow heat engines can be made with the aid of these charts; because the charts were originally designed for calculations at constant volume, zero values were assigned to the internal energies of the completely burned phases (CO_2, H_2O, and N_2) at 100° F. For calculations at constant pressure, it is necessary to apply an additive correction to the enthalpy that depends only on the fuel-air ratio. It is more convenient to compute the quantity H that must be used to enter the charts than to correct chart readings to a standard base. The chart enthalpy H may be found from the equation

$$H = h_a \Big]_{540}^{T_a} - f\,h_c + h'_{540} - \frac{u_b^2\,(1+f)}{2gJ} - Q \qquad (1)$$

where

f fuel-air ratio

g acceleration due to gravity, 32.174 (lb/slug)

h_a enthalpy of air, (Btu/lb air)

h_c lower enthalpy of combustion of fuel, (Btu/lb fuel)

h'_{540} chart value of enthalpy of completely burned mixture at 540° R, (Btu/lb air)

J mechanical equivalent of heat, 777.97 (ft-lb/Btu)

Q heat loss from mixture to external sinks, (usually negligible), (Btu/lb air)

T_a inlet-air total temperature, °R

u_b velocity of burned mixture, (ft/sec)

For commercial fuels with a composition CH_2 injected as liquids, the average lower enthalpy of combustion at 540° R is approximately -18,590 Btu per pound of fuel. (See reference 4.)

The values of h' and h' + 18,590 f are given in the following table:

Percent of theoretical fuel	Fuel-air ratio	h' (Btu)	h' + 18,590 f (Btu)
80	0.05420	33.7	1041
90	.06098	34.7	1168
100	.06775	35.6	1295
110	.07453	36.6	1422
120	.08130	37.6	1549

Calculation of temperature and momentum pressure drop. - The pressure drop corresponding to fluid acceleration during combustion may be computed for constant-area ducts or near constant-area ducts by assuming that the momentum is conserved. The momentum of the burned mixture $P + \rho_b u_b^2$ is equal to the net momentum of the inlet-air - fuel mixture

$$P_a + \rho_a u_a(u_a + f\ u_f) - D$$

where

D drag of flame holders and other obstructions, (lb/sq in. flow area)

P pressure of burned gases, (lb/sq in.)

p_a pressure of inlet air, (lb/sq in.)

R_a gas constant for air, 53.35 (ft-lb/(lb)($^{\circ}$R))

u_a velocity of inlet air before fuel addition, (ft/sec)

u_f component of mean velocity of fuel injection parallel to u_a and u_b, (ft/sec)

ρ_a density of inlet air, $\rho_a = \dfrac{144\ p_a}{gR_aT_a}$

ρ_b density of burned gases, $\rho_b = (1 + f)/Vg$

The equations reduce to the working form

$$P = p_a \left\{1 - \frac{u_a\left[(1 + f)\ u_b - u_a\right]}{1716.5\ T_a}\right\} + \rho_a\ u_a\ f\ u_f - D \qquad (2)$$

and

$$u_b = 2.699\ \frac{p_a\ u_a}{T_a}\ V \qquad (3)$$

where

V specific volume of burned gas, (cu ft/lb air)

The enthalpy of the burned mixture H and its velocity u_b may be found by solving equations (1), (2), and (3); during the solution, the value of V is read from the chart corresponding to the fuel-air ratio f and to the values of P and H computed from equations (1) and (2).

The following procedure may be used to compute the velocity u_b and pressure P of the burned mixture. The sequence of approximate answers converges to the correct solution if the inlet velocity u_a is less than or equal to the critical value for choke and fails to converge if the inlet velocity is greater than the critical value for choke.

Step 1. Given u_a, p_a, T_a, f, and D, assume a trial value $u_{b,1}$ for u_b; compute a trial value H_1 from equation (1)

and a trial value P_1 from equation (2). An initial estimate of $u_{b,1}$ may be obtained from figure 1. Figure 1(a) corresponds to 80 percent of theoretical fuel; figure 1(b) corresponds to 90 percent; and figure 1(c) corresponds to 100, 110, and 120 percent.

Step 2. Find a trial value V_1 from the chart corresponding to f by a double interpolation between enthalpy H and pressure P lines and compute $u_{b,2}$ (a second approximation of u_b) from equation (3).

Step 3. If $u_{b,1}$ and $u_{b,2}$ are appreciably different, improve the precision of the estimate of velocity of the burned gas u_b by computing $u_{b,3}$ from equation (4):

$$u_{b,3} = u_{b,1} + \frac{\dfrac{u_{b,2} - u_{b,1}}{2}}{1 - \dfrac{u_{b,2}}{5800\ PV}} \tag{4}$$

Step 4. Repeat steps 1, 2, and 3 using $u_{b,3}$ (or $u_{b,2}$) in place of $u_{b,1}$ as an estimate of u_b. This process is continued until $u_{b,2}$ agrees with $u_{b,1}$ within the desired accuracy, or until further repetition fails to bring $u_{b,2}$ into closer agreement with $u_{b,1}$, or until it becomes clear that the process does not converge. In the case of nonconvergence, the assumed flow is physically impossible. The values given in figure 1 are not exact for any case and are to be used only for the first trial through steps 1, 2, and 3.

Step 5. When a satisfactory set of values of u_b, P, and H are found, determine T from the chart. An approximate value of the total combustion temperature T_{total} and total pressure P_{total} may be found by reading the chart at

$$H_{total} = h_a \Big]_{540}^{T_a} - f\,h_c + h' - Q$$

at a value of the entropy corresponding to final values of P and V.

The steps involved in the calculation of u_b, P, V, and T are shown in the following table for the cases:

Static pressure, p_a, (lb/sq in.) 10
Total temperature, T_a, $^{\circ}R$ 700
Percent of theoretical fuel 100
Fuel velocity, u_f, (ft/sec) 0
Heat loss, Q, (Btu/lb air) 0
Burner drag, D 0
Inlet-air velocity, u_a, (ft/sec) 100,225,250

u_a	p_a	h_{total}	T_a	$u_{b,1}$	H	P	V	$u_{b,2}$	$u_{b,3}$	T	T_{total}
100	10	1334	700	660[a]	1325	9.498	174	671	672		
				672	1324	9.486	175	675	675		
				675	1324	9.484	175	675		4080	4100
225	10	1334	700	2200[a]	1231	6.02	263	2280	2385		
				2385	1213	5.65	275	2390	2399		
				2399	1211	5.63	277	2402	2407		
				2407	1213	5.61	277	2402	2394		
				2394	1212	5.63	278	2410	2438	3870	4080
250	10	1334	700	2930[a]	1151	4.02	375	3615	1560		
				1560	1286	7.06	232	2240	4370		
				4370	928	.8	Off chart				

[a]Obtained from figure 1(c).

The convergence of the process of calculation is rapid and definite for a u_a value of 100 feet per second in which the initial and final Mach numbers are much less than 1.

In the case of a value of u_a of 225 feet per second, the final Mach number is only slightly less than 1 and more steps are required. The accuracy is limited by the ability to read the charts and even in this case the approximation was not improved in the fourth and fifth tries, in which $u_{b,3}$ was computed and used as the next trial value of $u_{b,1}$.

When a value of u_a of 250 feet per second is used, the processes of calculation diverge in an alternating manner. In this case, the initial velocity is so large that no physically significant solution exists.

Lewis Flight Propulsion Laboratory,
National Advisory Committee for Aeronautics,
Cleveland, Ohio, March 9, 1949.

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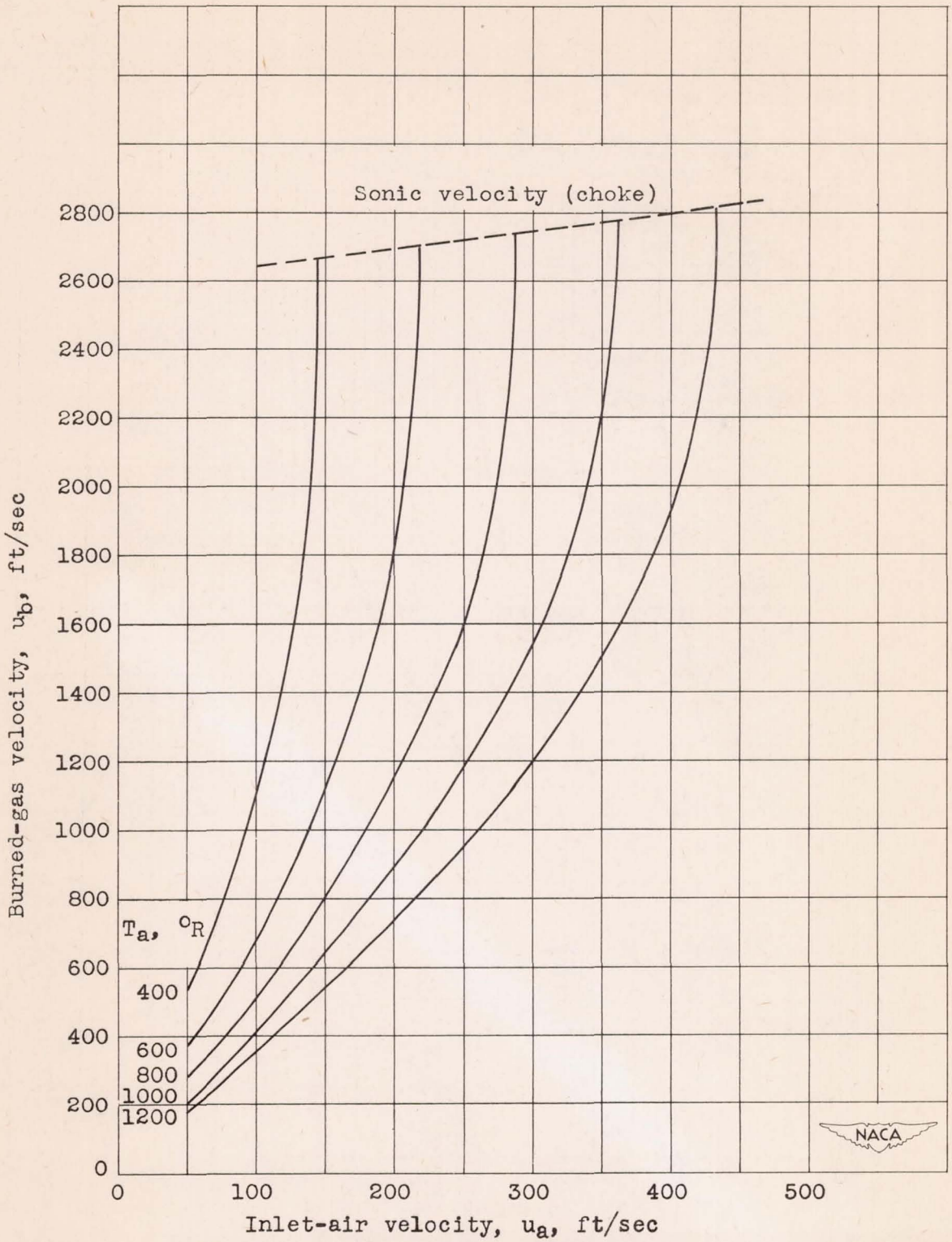
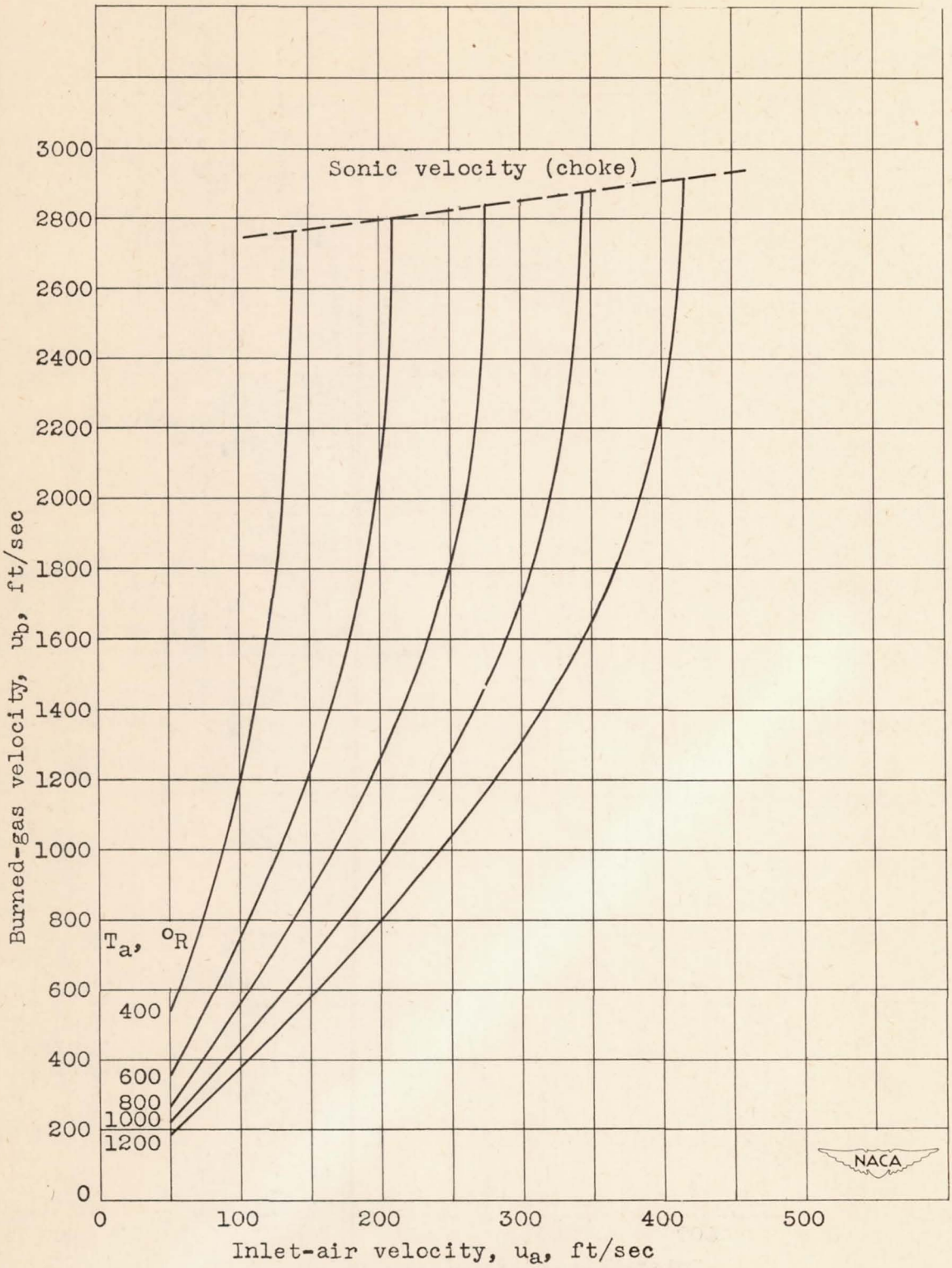
4. Turner, L. Richard, and Lord, Albert M.: Thermodynamic Charts for the Computation of Combustion and Mixture Temperatures at Constant Pressure. NACA TN 1086, 1946.



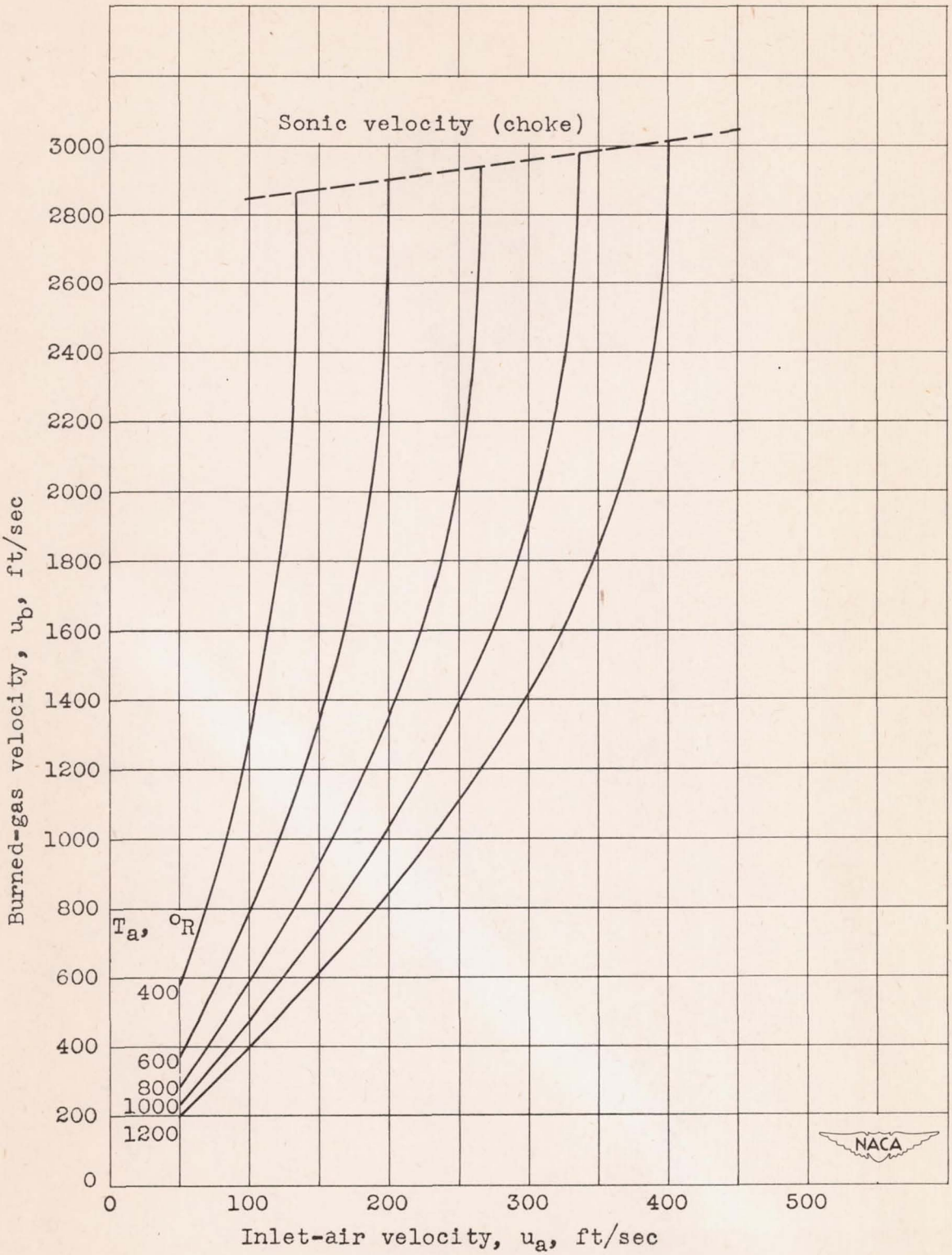
(a) 80-percent theoretical fuel.

Figure 1. - Initial estimate of burned-gas velocity.



(b) 90-percent theoretical fuel.

Figure 1. - Continued. Initial estimate of burned-gas velocity.



(c) 100, 110, and 120-percent theoretical fuel.

Figure 1. - Concluded. Initial estimate of burned-gas velocity.

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E = INTERNAL ENERGY, B. T. U., ABOVE CO_2, H_2O (VAPOR), O_2, AND AIR – N_2 AT 100°F

Q_v = INT. ENERGY OF COMBUSTION, AT 100°F, OF UNBURNED FUEL IN THE EQUILIBRIUM MIXTURE AT T. WHEN T ≤ 2880°R., Q_v = 2.0, 2.5, 4.0, AT S = 0.4, 0.6, 0.8, RESPECTIVELY

$E_s = E - Q_v$

H = ENTHALPY, E + J(PV)

$H_s = E_s + J(PV)$ [$\therefore H = H_s + Q_v$]

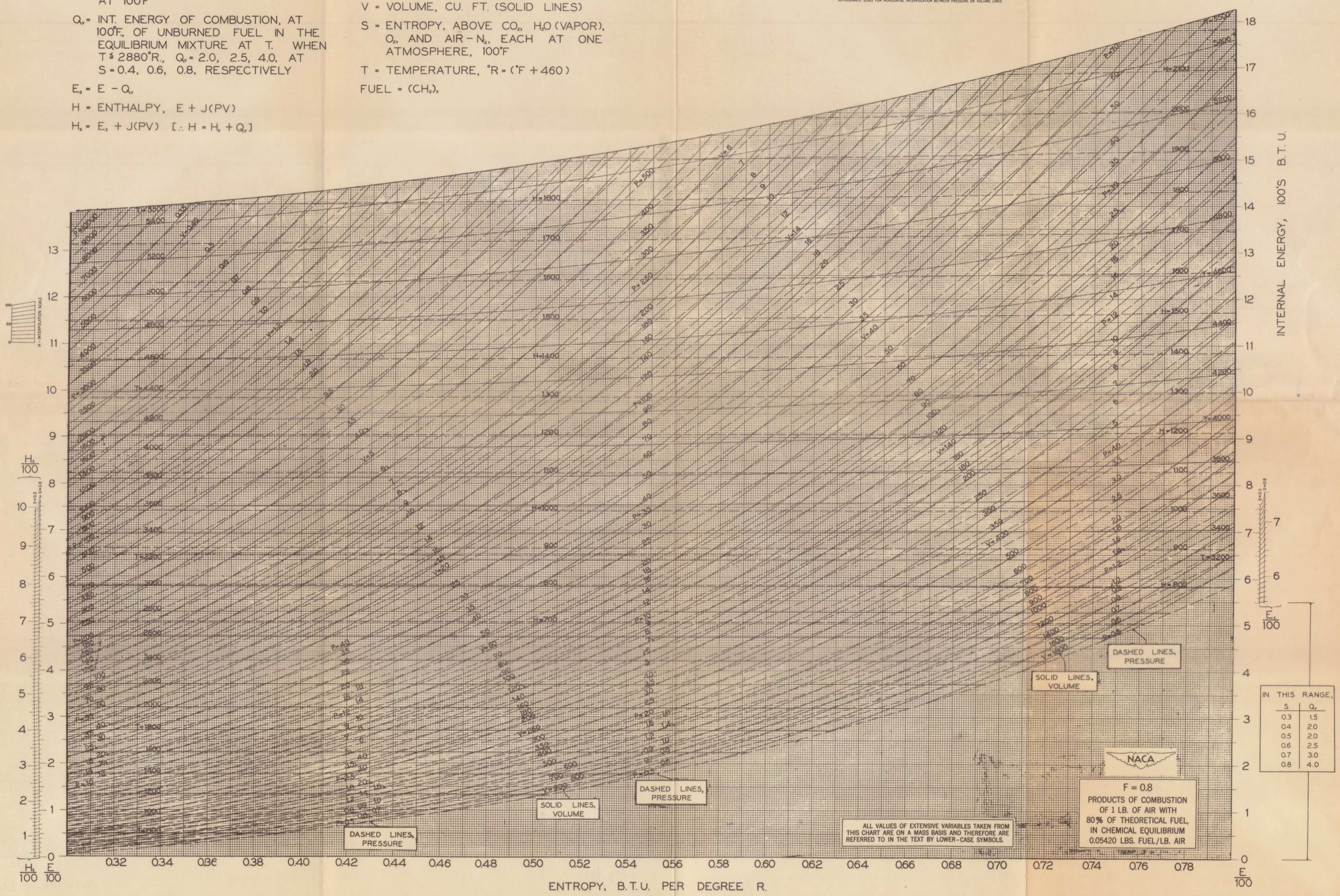
P = PRESSURE, LBS./SQ. IN. (DASHED LINES)

V = VOLUME, CU. FT. (SOLID LINES)

S = ENTROPY, ABOVE CO_2, H_2O (VAPOR), O_2, AND AIR – N_2, EACH AT ONE ATMOSPHERE, 100°F

T = TEMPERATURE, °R = (°F + 460)

FUEL = $(CH_2)_x$



IN THIS RANGE,

S	Q_v
0.3	1.5
0.4	2.0
0.5	2.0
0.6	2.5
0.7	3.0
0.8	4.0

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E = INTERNAL ENERGY, B. T. U., ABOVE CO_2, H_2O (VAPOR), O_2, AND AIR-N_2 AT 100°F

Q_v = INT. ENERGY OF COMBUSTION, AT 100°F, OF UNBURNED FUEL IN THE EQUILIBRIUM MIXTURE AT T. WHEN T ≤ 2880°R, Q_v = 1.5, 2.0, 3.0, AT S = 0.4, 0.6, 0.8, RESPECTIVELY

$E_s = E - Q_v$

H = ENTHALPY, E + J(PV)

$H_s = E_s + J(PV)$ [· $H = H_s + Q_v$]

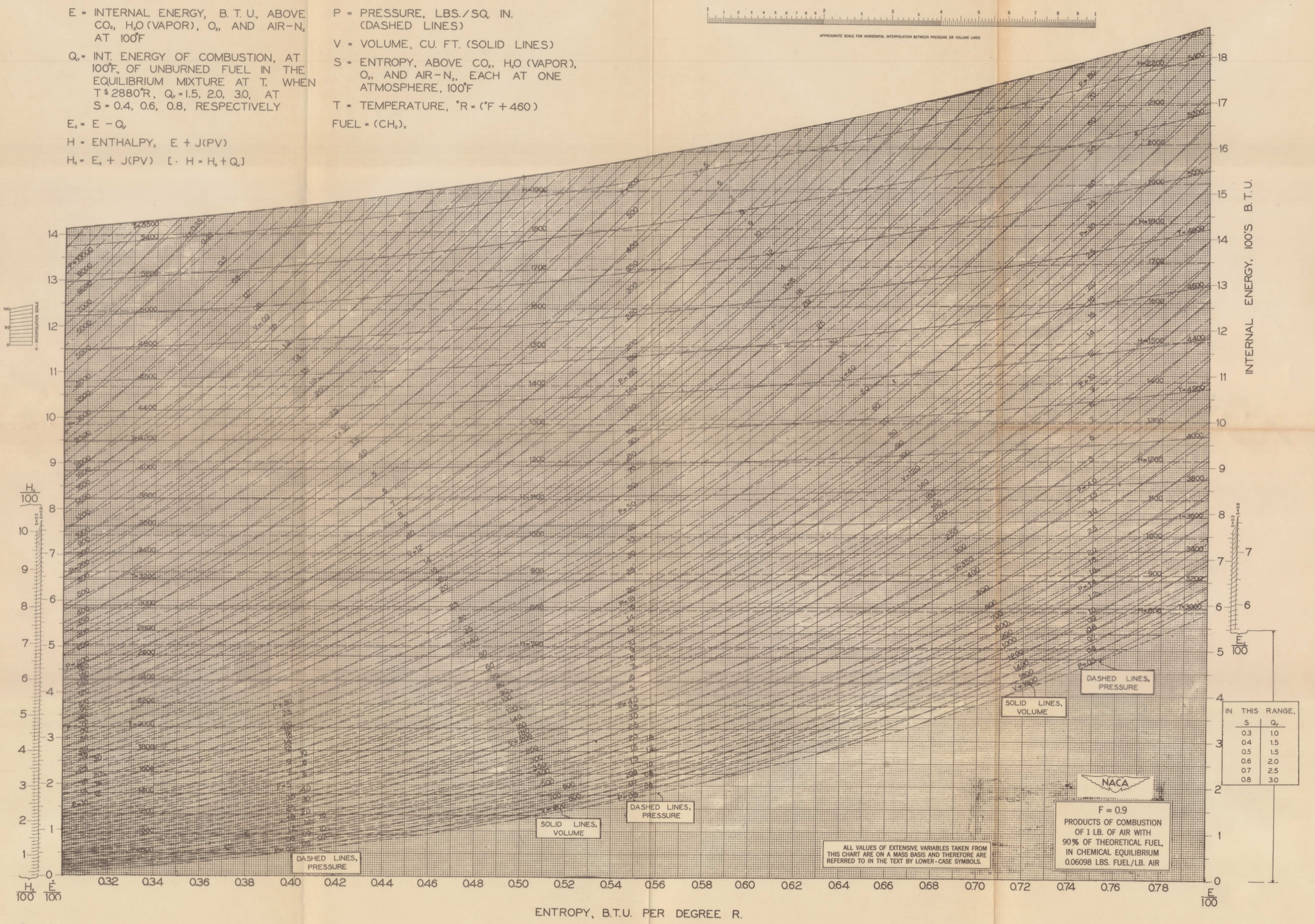
P = PRESSURE, LBS./SQ. IN. (DASHED LINES)

V = VOLUME, CU. FT. (SOLID LINES)

S = ENTROPY, ABOVE CO_2, H_2O (VAPOR), O_2, AND AIR-N_2, EACH AT ONE ATMOSPHERE, 100°F

T = TEMPERATURE, °R = (°F + 460)

FUEL = $(CH_2)_x$



IN THIS RANGE,

S	Q_v
0.3	1.0
0.4	1.5
0.5	1.5
0.6	2.0
0.7	2.5
0.8	3.0

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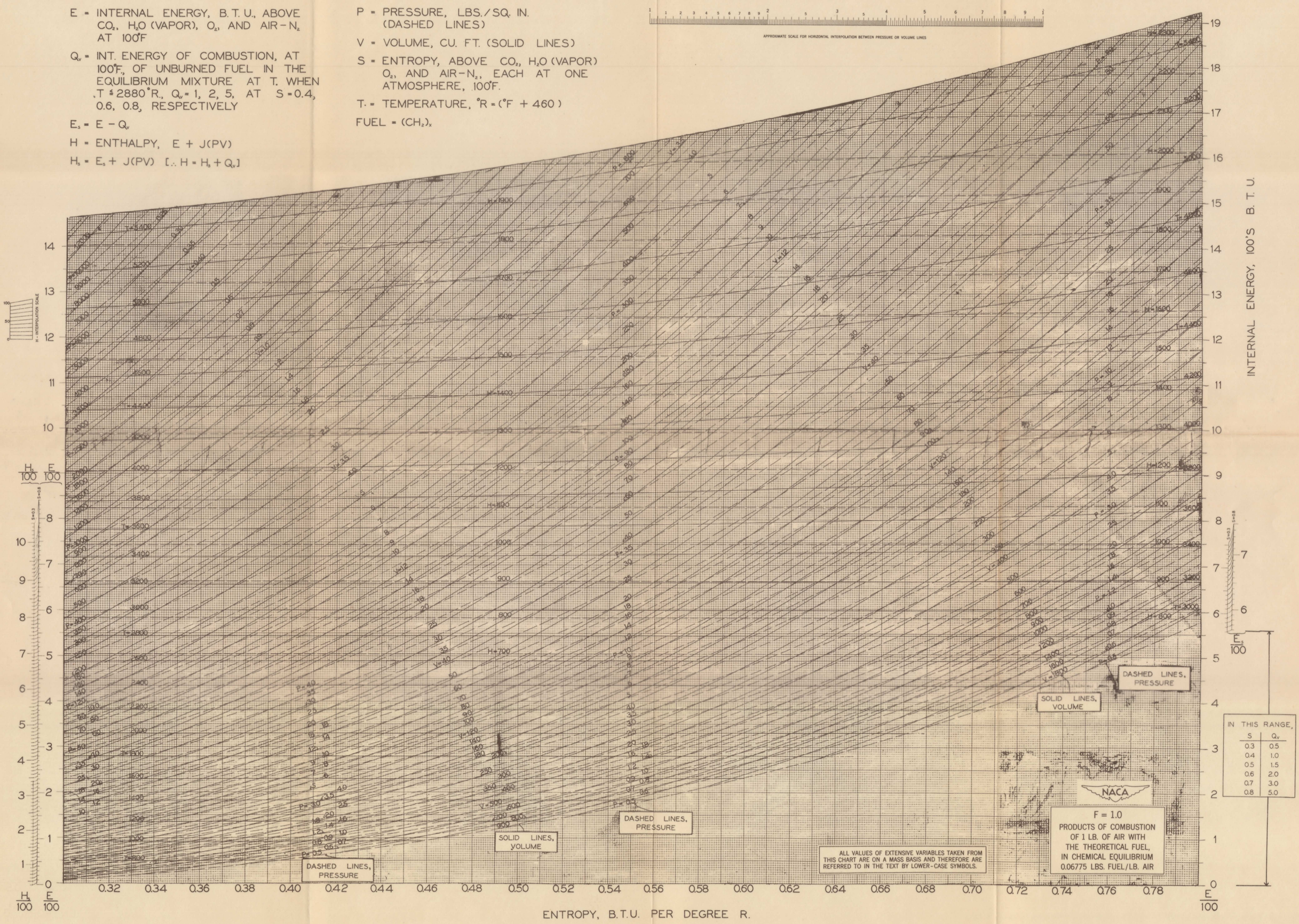
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Q_v = INT. ENERGY OF COMBUSTION, AT 100°F., OF UNBURNED FUEL IN THE EQUILIBRIUM MIXTURE AT T. WHEN T = 2880°R., Q_v = 1, 2, 5, AT S = 0.4, 0.6, 0.8, RESPECTIVELY
E_s = E − Q_v
H = ENTHALPY, E + J(PV)
H_s = E_s + J(PV) [∴ H = H_s + Q_v]
P = PRESSURE, LBS./SQ. IN. (DASHED LINES)
V = VOLUME, CU. FT. (SOLID LINES)
S = ENTROPY, ABOVE CO_2, H_2O (VAPOR) O_2, AND AIR-N_2, EACH AT ONE ATMOSPHERE, 100°F.
T = TEMPERATURE, °R = (°F + 460)
FUEL = $(CH_2)_x$
APPROXIMATE SCALE FOR HORIZONTAL INTERPOLATION BETWEEN PRESSURE OR VOLUME LINES
H - INTERPOLATION SCALE
INTERNAL ENERGY, 100'S B. T. U.
ENTROPY, B.T.U. PER DEGREE R.
DASHED LINES, PRESSURE
SOLID LINES, VOLUME
DASHED LINES, PRESSURE
SOLID LINES, VOLUME
DASHED LINES, PRESSURE
ALL VALUES OF EXTENSIVE VARIABLES TAKEN FROM THIS CHART ARE ON A MASS BASIS AND THEREFORE ARE REFERRED TO IN THE TEXT BY LOWER-CASE SYMBOLS.
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F = 1.0
PRODUCTS OF COMBUSTION OF 1 LB. OF AIR WITH THE THEORETICAL FUEL, IN CHEMICAL EQUILIBRIUM 0.06775 LBS. FUEL/LB. AIR
IN THIS RANGE,
S | Q_v
0.3 | 0.5
0.4 | 1.0
0.5 | 1.5
0.6 | 2.0
0.7 | 3.0
0.8 | 5.0

E = INTERNAL ENERGY, B.T.U., ABOVE CO_2, H_2O (VAPOR), O_2, AND AIR-N_2 AT 100°F.

Q_v = INT. ENERGY OF COMBUSTION, AT 100°F., OF UNBURNED FUEL IN THE EQUILIBRIUM MIXTURE AT T. WHEN T = 2880°R., Q_v = 169.

$E_s = E - Q_v$

H = ENTHALPY, E + J(PV)

$H_s = E_s + J(PV)$ [$\therefore H = H_s + Q_v$]

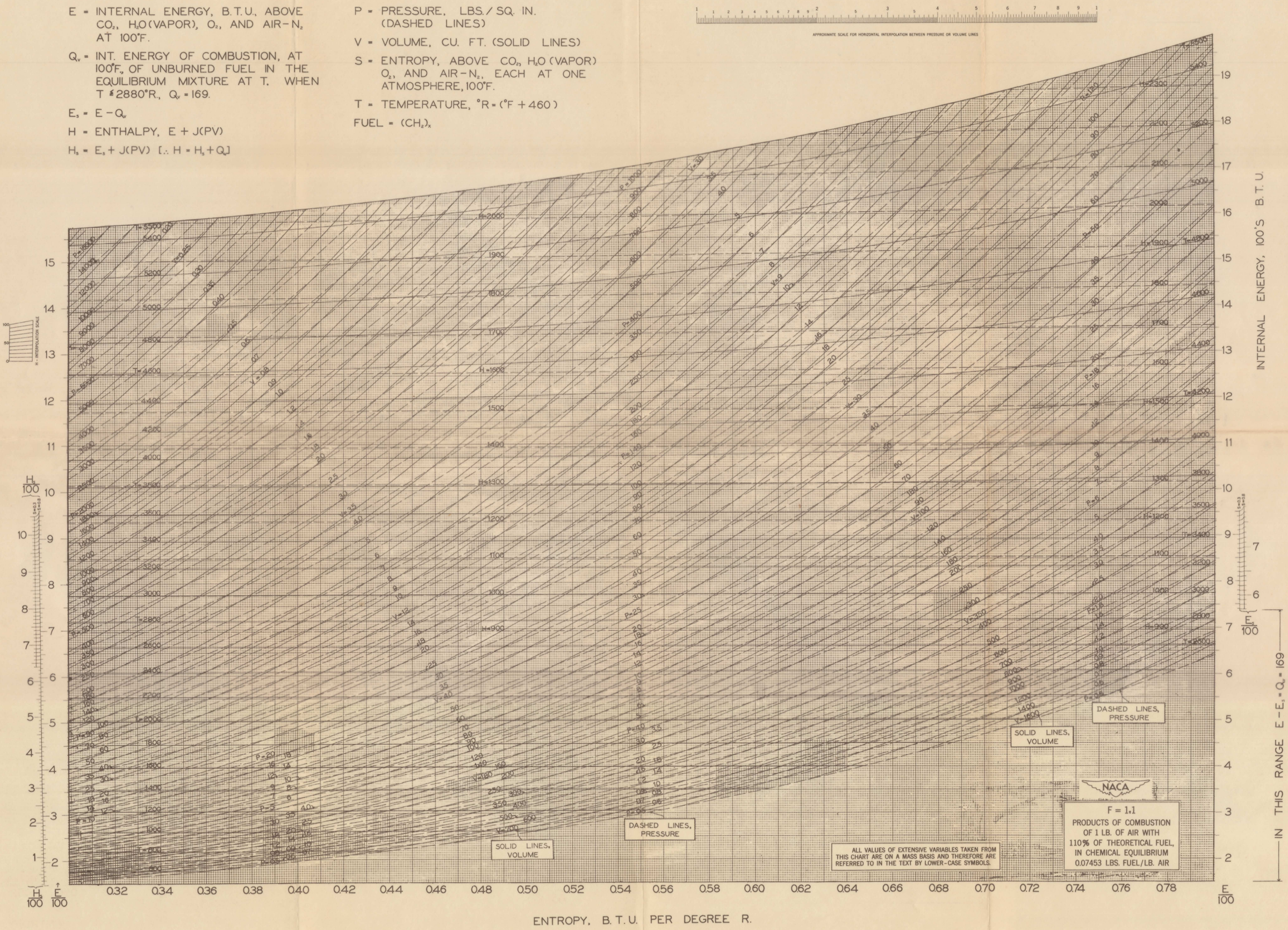
P = PRESSURE, LBS./SQ. IN. (DASHED LINES)

V = VOLUME, CU. FT. (SOLID LINES)

S = ENTROPY, ABOVE CO_2, H_2O (VAPOR) O_2, AND AIR-N_2, EACH AT ONE ATMOSPHERE, 100°F.

T = TEMPERATURE, °R = (°F + 460)

FUEL = $(CH_2)_x$



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Q_v = INT. ENERGY OF COMBUSTION, AT 100°F., OF UNBURNED FUEL IN THE EQUILIBRIUM MIXTURE AT T. WHEN T = 2880°R., Q_v = 336.

$E_s = E - Q_v$

H = ENTHALPY, E + J(PV)

$H_s = E_s + J(PV)$ [$\therefore H = H_s + Q_v$]

P = PRESSURE, LBS./SQ. IN. (DASHED LINES)

V = VOLUME, CU. FT. (SOLID LINES)

S = ENTROPY, ABOVE CO_2, H_2O (VAPOR), O_2, AND AIR-N_2, EACH AT ONE ATMOSPHERE, 100°F

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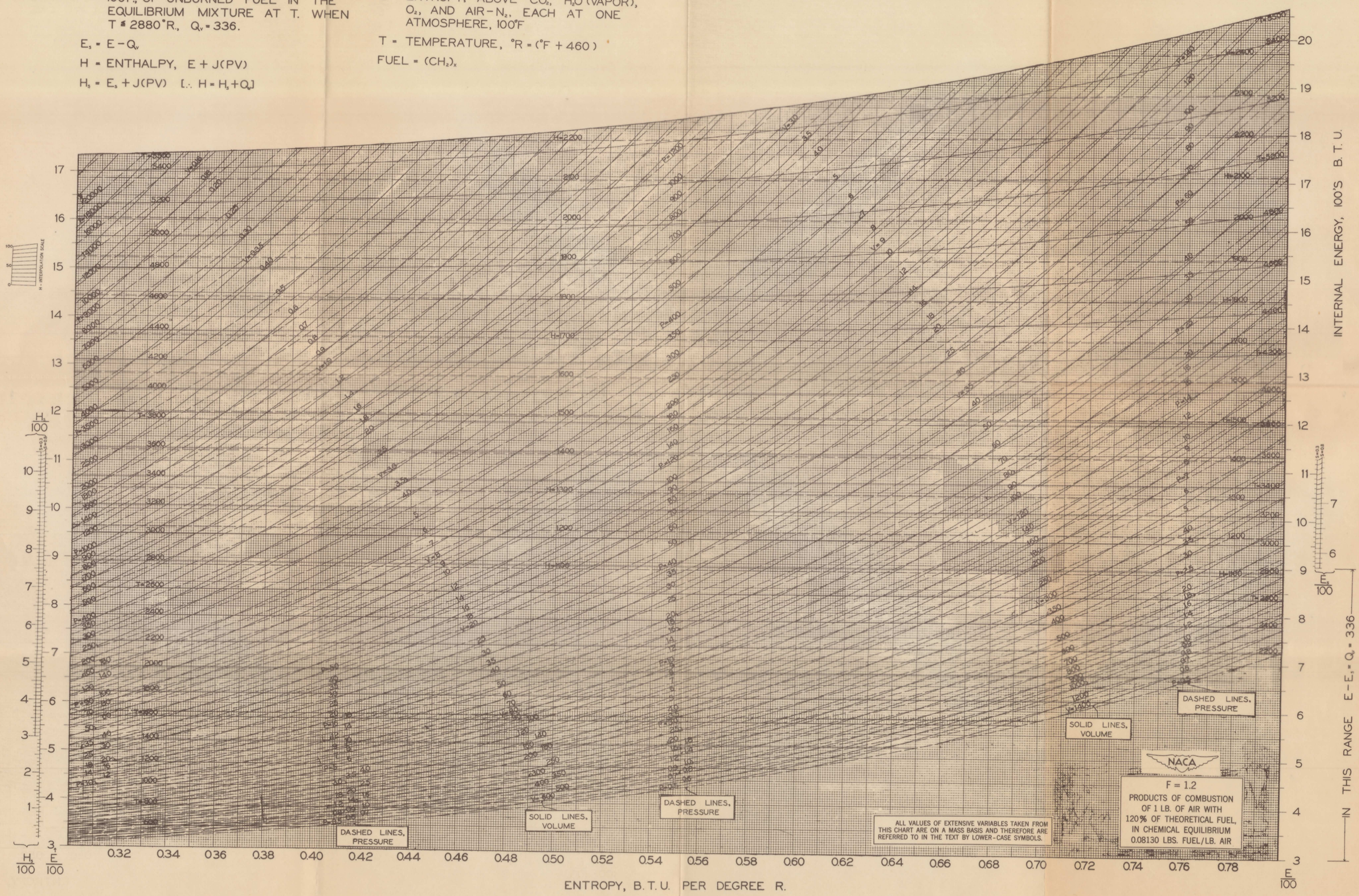
FUEL = $(CH_2)_x$



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