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WETAIR - A Computer Code for Calculating Thermodynamic and Transport Properties of Air-Water Mixtures

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for Calculating Thermodynamic
and Transport Properties
of Air-Water Mixtures

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National Aeronautics
and Space Administration

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Summary

A computer-program subroutine, WETAIR, has been developed to calculate the thermodynamic and transport properties of air-water mixtures. It determines the thermodynamic state from assigned values of temperature and density, pressure and density, temperature and pressure, pressure and entropy, or pressure and enthalpy. WETAIR calculates the properties of dry air and water (steam) by interpolating to obtain values from property tables. Then it uses simple mixing laws to calculate the properties of air-water mixtures. Properties of mixtures with water contents below 40 percent (by mass) can be calculated at temperatures from 273.2 to 1497 K and pressures to 450 MN/m². Dry-air properties can be calculated at temperatures as low as 150 K. Water properties can be calculated at temperatures to 1747 K and pressures to 100 MN/m². WETAIR is available in both SFTRAN and FORTRAN.

Introduction

In research on gas-turbine engines, measured temperatures and pressures of the working fluid are compared with the ideal temperatures and pressures that could be obtained if there were no losses. In this way, the performance of the components under test can be evaluated. Recently, there has grown a need for procedures that can more accurately calculate ideal temperatures and pressures — procedures that take into account real-gas effects.

A high-pressure facility at the Lewis Research Center will be used to test gas-turbine engine components operating in relatively humid air at pressures to 40 atmospheres. The properties of such an air-water mixture differ appreciably from those of a perfect gas. Preliminary studies have shown that, at a pressure of 10 atmospheres, errors of as much as 2 to 3 percent in measured efficiency can result if a perfect-gas approximation is used (instead of the actual air properties) to calculate no-loss temperatures and pressures. These errors are incompatible with the goal of measuring efficiencies to an accuracy of 0.5 percent.

In another Lewis investigation, factors that affect the performance of an automotive turbine engine are being studied. An integral part of the research is to establish the effect of injecting additional water, besides the water vapor normally present in humid air, into the air stream to increase mass flow. Here too, the properties of the air-water mixture may differ appreciably from a perfect-gas model for dry air. A method for accurately calculating the properties of such a mixture is required.

The computer-program subroutine WETAIR was developed to fill these needs. The subroutine interpolates thermodynamic and transport properties of dry air and water from tabular data. It then uses mixing laws to calculate these properties for air-water mixtures. Also, WETAIR determines the thermodynamic state from assigned values of temperature and density, pressure and density, temperature and pressure, pressure and entropy, or pressure and enthalpy.

This paper describes how WETAIR was implemented and the assumptions used to obtain properties of air-water mixtures. A test program is included. It illustrates the use of WETAIR and may be used to obtain property values from WETAIR for comparison with available data.

Symbols

| | |
|----------|---|
| <i>A</i> | sonic velocity |
| <i>C</i> | specific heat |
| <i>c</i> | constant |
| <i>D</i> | density |
| <i>H</i> | specific enthalpy |
| <i>k</i> | thermal conductivity |
| <i>M</i> | molar fraction of one component of a two-component system |
| <i>P</i> | pressure |
| <i>R</i> | gas constant |
| <i>S</i> | specific entropy |
| <i>T</i> | temperature |
| <i>W</i> | mass fraction of one component of a two-component system |
| γ | ratio of specific heats, C_p/C_v |
| η | viscosity |
| ρ | density |

Subscripts:

| | |
|----------|---------------------------------------|
| <i>a</i> | air-component value |
| <i>p</i> | at constant pressure |
| <i>t</i> | at constant temperature |
| <i>v</i> | at constant volume |
| <i>w</i> | water-component value |
| <i>0</i> | function of temperature for ideal gas |

Program Design

In WETAIR, thermodynamic properties of air-water mixtures are obtained by assuming an ideal mixture, that is, one in which the two components occupy the same volume without interacting with one another. Transport properties (viscosity and thermal conductivity) of air and water mixtures are calculated from the constituent values by an empirical equation with one constant. The equation is adjusted to agree with viscosity measurements of air-water mixtures at near-atmospheric pressures.

Properties of Pure Air and Pure Water

The FLUID subroutine (ref. 1) determines the thermodynamic state from assigned values of temperature and density, pressure and density, temperature and pressure, pressure and entropy, or pressure and enthalpy. FLUID considers liquid or two-phase (liquid-gas) conditions as well as the gas phase. It uses a van der Waals model to obtain approximate state values; it then corrects these values for real-gas effects by model-correction factors obtained from tables based on experimental data. Saturation conditions and specific-heat, entropy, and enthalpy data are included in the tables for each gas. Since these tables are external to the FLUID program, FLUID can implement any gas for which a set of tables has been generated.

For the present work, data tables for dry air were prepared from Baehr and Schmier's thermodynamic tables and correlations for air (ref. 2) and from the equations for viscosity and conductivity given in the National Bureau of Standards compilation of gas properties (ref. 3). Data tables for water were prepared by using, as a data base, the computer code WASP (ref. 4), which agrees well with the international skeleton tables for steam and water (ref. 5) and by using the interpolating equation for conductivity recommended for industrial use by Kestin (ref. 6). Preparation of these data tables is described in a later section, Generation of Data Tables.

Properties of Air-Water Mixtures

Pressure. — No information is available on which to base an equation of state for air-water mixtures that takes into account real-gas effects. Instead, we follow Dalton's law, which states that the total pressure of a mixture equals the sum of the partial pressures of its constituents. (The partial pressure is that pressure each gas would exert if it alone occupied the volume of the mixture at the same temperature.) Mixtures of real gases may depart from this behavior at all but low densities. A more precise mixing law would account for the fact that molecules of two species cannot really coexist in the same volume without interaction. At present, however, the data needed to formulate such a model are not available.

The properties of air-water mixtures at a given temperature and density are obtained, according to Dalton's law, from the properties for each component at the specified temperature but for the (partial) component density instead of the (total) mixture density. The pressure of the mixture then is the sum of the pressure of each component.

If we define the gas constant (see Symbols) as

$$R = \lim_{P \rightarrow 0} \frac{P}{\rho T}$$

the equation

$$R = W_a R_a + W_w R_w$$

applies to a mixture that behaves according to Dalton's law, where W_a and W_w are the mass fractions of the two components.

Entropy. — We use Gibbs' theorem to obtain the entropy of an air-water mixture. Gibbs' theorem states that the entropy of an ideal mixture (one in which the constituents do not interact) is the sum of the partial entropies. The partial entropy of a constituent is the entropy it would have if it alone occupied the whole volume at the same temperature. From this theorem and Dalton's law, we obtain for the specific entropy of the mixture

$$S = W_a S_a + W_w S_w$$

Enthalpy and specific heats. — A further consequence of assuming that Dalton's law and Gibbs' theorem apply to an idealized air-water mixture is that the specific enthalpy and specific heats can be obtained from

$$H = W_a H_a + W_w H_w$$

$$C_v = W_a C_{v,a} + W_w C_{v,w}$$

$$C_p = W_a C_{p,a} + W_w C_{p,w}$$

Sonic velocity. — Although sonic velocity is not a thermodynamic property, it is an important parameter in research on gas-turbine engines. The low-frequency sonic velocity of a gas is given by

$$\frac{A^2}{\gamma} = \left(\frac{\partial P}{\partial \rho} \right)_t$$

where γ is the ratio of specific heats C_p/C_v . From the sonic velocity and specific-heat ratio of each component, we can obtain (again using Dalton's law) the sonic velocity for air-water mixtures by

$$\frac{A^2}{\gamma} = W_a \frac{A_a^2}{\gamma_a} + W_w \frac{A_w^2}{\gamma_w}$$

Viscosity and thermal conductivity. — Even at low gas densities, the transport properties of a gaseous mixture do not follow simple cumulative

relationships as do the equilibrium properties such as entropy, enthalpy, and specific heats (ref. 7). The experimental results of Kestin and Whitelaw (ref. 8) on the viscosity of humid air show this quite well. Studnikov (ref. 9) has proposed a one-parameter empirical formula for calculating the viscosity of a water-vapor–air mixture:

$$\eta = (M_a \eta_a + M_w \eta_w) \left(1 + \frac{M_a - M_a^2}{c} \right)$$

where M_a and M_w are the molar fractions of the two components. Studnikov recommends a value of 2.75 for the constant c . Results obtained with this formula compare quite well with the Kestin and Whitelaw measurements.

Simple theory (ref. 7) suggests that the thermal conductivity of air-water mixtures can be obtained from this same equation by replacing η with k . Studnikov's formula is used in WETAIR for both mixture viscosity and mixture conductivity.

Nonhomogeneous mixtures. — If a part of the water component is liquid, specific heat and sonic velocity will be ambiguous quantities. Also, the transport properties cannot be expected to behave according to the equations used for homogeneous mixtures. In WETAIR, specific heats, sonic velocity, and transport properties are calculated by using only gas-phase values for the water component of the mixture.

Solutions for Other Independent Variables

Like the subprogram FLUID, WETAIR was also required to determine the thermodynamic state of air-water mixtures when the given variables may be other than temperature and density. The following four additional cases have been implemented.

Pressure and density (case 2). — In this case, the partial density of each component of the mixture can be calculated exactly, but the partial pressures are unknown.

A starting estimate for the partial pressure of air is made by assuming that

$$P_a = M_a P$$

The temperature (of dry air) is obtained from the estimated partial pressure of air and the known density. This temperature and the known density of the water component are then used to obtain a partial pressure for water. If the difference

$$\Delta P \equiv |P - (P_a + P_w)|$$

is sufficiently small, the results of this procedure are accepted. If not, an improved estimate for the

partial pressure of the air component is calculated from ΔP , and the procedure is repeated.

Temperature and pressure (case 3). — Again, a first estimate is obtained for the partial pressure of the air component. The only difference is that temperature instead of density is the other known variable.

The density (of dry air) is obtained from the estimated partial pressure of air and the known temperature. This density implies a water density, which (with the known temperature) is then used to obtain a partial pressure for water. Iteration is governed as in case 2, in which pressure and density are known.

Pressure and entropy (case 4). — Here too, the starting estimate for the partial pressure of the air component is obtained as in case 2. But a starting estimate for the entropy of the air component is also needed.

The specific entropy of an ideal gas can be expressed as

$$S = S_0(T) - R \ln P$$

where $S_0(T)$ depends only on temperature. In WETAIR, this relationship is used to obtain a starting estimate for the specific entropy of the air component from the given entropy. The pressure and entropy of dry air and of the mixture are obtained for several temperatures and for a density low enough to give ideal-gas behavior. From these values and the preceding equation, a table of S_0 and $S_{0,a}$ is formed. This table is then back-interpolated to obtain a good estimate for the entropy of the air component from the known mixture entropy.

At this point, the density and temperature of dry air are obtained from the estimated partial pressure and entropy. Then, from this temperature and the implied water density, the partial pressure and entropy of the water component are calculated. As in case 2, if the sum of the partial pressures agrees well with the given mixture pressure, the results of the procedure are accepted. If not, new estimates that will improve the pressure balance are calculated for both the partial pressure and entropy of the air component, and the procedure is repeated.

Pressure and enthalpy (case 5). — The method used in this case is similar to that for case 4. For an ideal gas, enthalpy is a function of temperature only.

A special case. — In three of the cases just described (cases 2, 4, and 5), temperature is an unknown and must be solved for iteratively. When the temperature is so low that some of the water component is liquid, this iterative procedure can

fail and an alternative iterative procedure is required.

In this special case, a starting estimate for temperature is the dewpoint temperature at the pressure

$$P_w = M_w P$$

Then the procedure for case 3 is used to obtain a corresponding mixture density, entropy, or enthalpy. If the result agrees well with the given property, it is accepted. If not, a new temperature estimate is calculated and the procedure is repeated. (On the first iteration, a temperature a few degrees below the dewpoint temperature is used. After that, the results of the previous two iterations are used to refine the temperature estimate.)

Data-Table Limitations

For pure-air properties ($W_w = 0.0$), the implemented temperature range is 150 to 1497 K, and the allowed density range is 3.13×10^{-5} to 0.6 g/cm^3 . For pure-water properties ($W_w = 1.0$), the implemented temperature range is 273.2 to 1747 K, and the allowed density range is 0 to 1.01 g/cm^3 . Results are unreliable at pressures above 100 MN/m^2 .

Mixture Limitations

Air-water mixtures are implemented for a water mass-fraction as high as 0.4 (a mole fraction slightly greater than 0.5). The allowed temperature and density ranges for mixtures ($0 < W_w \leq 0.4$) are limited to those values that simultaneously satisfy the previously stated limits for each component.

Calling Conventions for WETAIR

WETAIR was coded in SFTRAN (Structured FORTRAN), a programming language (refs. 10 and 11) recently introduced at the Lewis Research Center. This language was chosen for its self-documenting features. It allows and even encourages the grouping of instructions into small, natural units that can be given unique, descriptive names. In listings, these are displayed in a manner that makes their internal structure immediately apparent to the eye.

Other than the manner in which branching and looping are handled, SFTRAN is very much like FORTRAN. SFTRAN routines can call, or be called by, FORTRAN routines. The SFTRAN language has been implemented as a precompiler that generates FORTRAN source code from SFTRAN source code. The FORTRAN version of WETAIR so generated has been included in the WETAIR package for use

by those not having an SFTRAN precompiler. (This FORTRAN code will not be helpful in understanding WETAIR; the FORTRAN produced by the SFTRAN precompiler is hard to read.)

Units. — Internally, WETAIR assumes SI units, but an initializing entry, WETAIO, provides for other systems of units in the user's calling program. One such system, the so-called engineering system of units, has been implemented.

If a user's program deals in engineering units, it must first call WETAIO with integer argument '2'. (See appendix A for a description of the entry points in WETAIR.) Subsequent calls to WETAIR for property values will then assume these units for both input and returned quantities until another call to WETAIO specifies a change of units.

Calls to WETAIR for property values. — Five combinations of input variables have been implemented: (T, ρ) , (P, ρ) , (T, P) , (P, S) , and (P, H) . A particular one is specified by integer ENTRY. Temperature, pressure, and density are transmitted explicitly as calling arguments. Entropy, enthalpy, specific heats, sonic velocity, and the transport properties are transmitted in the array MIX in common block /WETAIC/. An integer, NP, also in /WETAIC/, is used to specify how many of the properties in MIX are to be calculated.

WETAIR recognizes certain kinds of errors in calling arguments. Fatal errors (due to an error in coding in the calling program) are announced on I/O UNIT 6 and result in a program STOP. Errors due to one or more of the thermodynamic variables being out of range are not fatal; they are flagged by bits in integer ERRS. If for some reason, convergence is not achieved in solving for temperature or density from other input variables, this condition is also flagged by a bit in ERRS.

As an example, consider that at some point in a user's program, a calculation of the properties of an air-water mixture with 5-percent water, by mass, is required. In particular, suppose it is desired to obtain the temperature T , density D , and specific heats at constant volume from pressure P and enthalpy H . For this, the calling program might contain the sequence

```
W=.05
NP=4
ENTRY=5
MIX(3)=H
CALL WETAIR (T,P,D,W,ENTRY,ERRS)
IF (ERRS.NE.0) DO (REPORT ERROR IN WETAIR)
```

(It is assumed that ENTRY and ERRS have been specified as INTEGER type and that the /WETAIC/ common block has been defined exactly as shown in appendix A, with array MIX declared to be REAL

type.) In this example, the highest index in MIX of a desired property is 4 (specific heat at constant volume), and so only four properties need be requested from WETAIR. The remaining properties (five to eight) would not be calculated, for a small saving of computer time.

Other quantities calculated by WETAIR may also be pertinent to the user's program. These quantities are included in the /WETAIC/ common block. See appendix B for another example of the use of WETAIR.

Generation of Data Tables

Reference 1 describes the organization of the data tables used by FLUID. The tables for each gas are external to FLUID; new gases are implemented by building the appropriate tables from an existing properties code, by direct use of tabulated values, or by a combination of these methods. Two sets of tables are used by WETAIR: a set for dry air, and a set for water (and steam). A computer program was written to generate each of these tables.

Data Tables for Dry Air

Baehr and Schwier (ref. 2) have analyzed air-properties data that have appeared in the literature as recently as 1954. In their work, they give coefficients for a reduced equation of state and for the (reduced) ideal-gas specific heat at constant volume. Two pairs of equations and their coefficients are provided: One pair applies to the temperature range -50° to 1250° C, and the other pair applies to the range 60 to 450 K. Coefficients are also provided for equations giving enthalpy, entropy, internal energy, and specific heat at constant pressure. These coefficients were derived from the equation of state and the ideal-gas, specific-heat equation and hence are consistent with them.

The equations of reference 1 were implemented as a subroutine for the present purpose. Below a temperature of 273.15 K, the pair of equations that apply down to 60 K are used. Otherwise, the pair of equations that apply up to 1250° C are used. The subroutine was tested by comparing values calculated by it with values tabulated in reference 2. Good agreement was obtained from 150 to 1500 K at densities to 0.6 g/cm^3 , the ranges implemented in WETAIR. A calculation of the sonic velocity was also implemented in this subroutine; the equation of state is differentiated to obtain the partial derivative of pressure with respect to density and, from this and the ratio of specific heats, the sonic velocity can be calculated.

FLUID cannot accommodate the liquid state of

fluids, such as air, that do not have uniquely defined vapor pressures below the critical point. For this reason, WETAIR was not implemented for temperatures below 150 K. (The temperature below which two phases appear is 132.52 K.) But, even though the range of the dry-air tables does not include the saturation region, an abbreviated saturation table is required by the algorithms used in FLUID when temperature and density are not given quantities. The data used to construct this abbreviated table were taken directly from the table of saturation values given in reference 2.

The viscosity and thermal conductivity of dry air are calculated from the equations

$$\eta_a = \frac{145.8 \times 10^{-7} T^{3/2}}{T + 110.4}$$

$$k_a = \frac{4.1833 \times 0.6325 \times 10^{-5} \sqrt{T}}{1 + \frac{245.4 \times 10^{-12/T}}{T}}$$

from reference 3. These equations are based on experimental data obtained at low densities. Kestin and Whitelaw include some experimental results for the viscosity of dry air in their work (ref. 8). Their results show that viscosity may increase by as much as 10 percent over its low-density value when the density is raised to 0.1 g/cm^3 . But, because of the limited range covered by their data, no attempt was made in the present work to develop an equation for viscosity with density terms.

Data Tables for Water

The computer subprogram WASP (ref. 4) provides thermodynamic and transport properties of water and steam. Its temperature range is from the triple point to 1750 K. Its pressure range is from 0.1 to 100 MN/m^2 for thermodynamic properties but is limited to 80 MN/m^2 for viscosity. WASP was used as a data base for generating the water tables used in WETAIR. Although WASP is not so advertised, it was found capable of supplying thermodynamic properties at pressures from below the triple point to 1000 MN/m^2 when temperature and density were specified. Also WASP gives reasonable viscosity values at pressures to 1000 MN/m^2 . These values were used to construct the tables with both temperature and density as arguments. For those points where temperature and density are both high enough to result in pressures above these limits, extrapolation from lower temperature values at the same density was used to fill out the two-argument tables.

Thermal conductivities of water were calculated from Kestin's recommended interpolating equation for industrial use (ref. 6). This equation expresses conductivity directly in terms of temperature and density through relatively simple programming.

A limitation of the van der Waals model of real gases (used in FLUID) is that it predicts a maximum density that cannot be exceeded — a density that is three times the critical density. But for water, the density of the liquid at the triple point exceeds this theoretical limit. To avoid this incompatibility, a pseudocritical density of 0.34 g/cm³ was used to generate the model correction tables, instead of the observed value of 0.317 g/cm³. This ploy is further discussed in reference 1.

Program Performance

Several programs were written to test the WETAIR package for accuracy and to make sure that correct operation is obtained under all possible combinations of input parameters. A listing of one of these (in SFTRAN) is included in appendix B as an example of the use of WETAIR.

Accuracy of Air Properties

As explained, the dry-air tables used in WETAIR trace back to the equations of Baehr and Schmier (ref. 2). One test of WETAIR is to see how well it can duplicate the tabulated properties given in their work. Another test is to see how well WETAIR duplicates the air properties given in the NBS compilation of gas properties (ref. 3).

Compared with reference 2. — Dry-air properties were calculated at pressures of 0.05, 0.1, 0.3, 1, 3, 10, 30, 100, and 300 MN/m² and temperatures from 155 to 1473 K. These properties were compared directly with the tabulated values of reference 2. (Entropies and enthalpies were calculated from reference values that allowed direct comparison with table entries.)

Typically, differences in specific volume were about one part in 10 000. The entropy and enthalpy values also compared well with those of reference 2. Typically, differences in entropy and enthalpy were equivalent to temperature differences of less than 0.1 kelvin, except at temperatures above 1200 K, where enthalpy differences 10 times as large were observed. The specific-heat values compared well with those of reference 2, where they are given to four significant figures. Some exceptions were noted at low temperatures and high pressures, where differences between calculated and tabulated values were as high as 1 percent.

Compared with reference 3. — WETAIR property values were compared with the values given for air

in reference 3. For this comparison, properties were calculated at pressures of 0.1, 1, 4, 10, 40, and 100 atmospheres (1 atmosphere = 0.101325 MN/m²) and temperatures from 160 to 1450 K. The WETAIR densities are consistently about one part in 2000 lower than those given in reference 3. This difference can be traced to a difference in the gas constants given in reference 2 (0.28772 J/g · K) and reference 3 (0.28704 J/g · K). Also, the WETAIR low-frequency-sound velocities are consistently high by about one part in 2000. Entropy, enthalpy, and specific heat at constant pressure agree nearly as well with the reference 3 values as they do with the reference 2 values. The specific-heat ratios at 0.1-atmosphere pressure agree very well with reference 3 values. At high pressures, however, the agreement is not nearly as good; the largest difference was 1 percent at 100 atmospheres and 220 K.

The viscosity and thermal conductivity equations from reference 3 were used to generate the data tables for dry air. The close agreement between WETAIR viscosity and conductivity values and the tabulated values of reference 3 reflects this relationship.

Accuracy of Water Properties

Water properties were calculated at pressures of 1, 15, 30, 60, 100, 300, 500, 1000, 2000, 5000, and 10 000 psi (1 psi = 0.006894731 MN/m²) and at temperatures from 50° to 1500° F (283.16 to 1088.7 K). The results were compared with the 1967 ASME steam tables (ref. 5).

Gas-phase properties for pure water agree well with the values given in reference 5. Typically, differences in specific volume are about one part in 10 000. At high pressures and low temperatures, some differences are as large as one part in 1000. In no case, however, are differences as large as the tolerance estimates for the specific volumes given in the 1963 international skeleton tables for steam (ref. 5). Entropy and enthalpy values also agree well with the values given in reference 5. Typically, the differences between calculated and tabulated values for these quantities are equivalent to a temperature difference of 0.2 kelvin.

Liquid-phase properties for pure water generally agree less well with those of reference 5 than do the gas-phase properties, probably because the van der Waals model correction factors are strongly density-dependent in the liquid region. Differences in specific volume are one part in 500. Typically, the differences between calculated and tabulated entropy and enthalpy values are equivalent to a temperature difference of 1 kelvin.

Gas-phase values of viscosity from WETAIR agree well with those of reference 5. Liquid-phase

values agree less well; typically, WETAIR liquid-phase viscosities are within a few percent of the accepted values.

Thermal conductivity values from WETAIR were calculated at pressures from 0.1 to 100 MN/m² and temperatures from 0° to 800° C. The results were compared directly with values tabulated in reference 6. The WETAIR values generally agree within 1 percent with the tabulated values except when temperature and pressure are both higher than the critical-point values. The greatest difference is 8 percent.

Accuracy of Mixture Properties

Experimental data on air-water mixture properties are generally lacking in the literature, with the single exception of the viscosity measurements of reference 8. Until such data become available, WETAIR represents the state of the art in the calculation of thermodynamic and transport properties of air-water mixtures.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, November 7, 1978,
505-01.

Appendix A Abstract of Entry Points in WETAIR

```
      SUBROUTINE WETAIO (UNITS)
C.....INITIALIZING ENTRY FOR ESTABLISHING UNITS TO BE USED.
C      (THE WETAIR SUBPROGRAM DEFAULT IS UNITS = 1)

C      UNITS = 1: R (GAS CONSTANT) = JOULES / GRAM - DEG. K
C              TEMPERATURE = DEG. K
C              PRESSURE = MEGA-NEWTONS / METER**2
C              DENSITY = GRAMS / CENTIMETER**3
C              SONIC VELOCITY = METERS / SEC.
C              VISCOSITY = GRAMS / CENTIMETER - SEC. (POISE)
C              CONDUCTIVITY = WATTS / CENTIMETER - DEG. K

C      UNITS = 2: R (GAS CONSTANT) = BTU / POUND(M) - DEG.R
C              TEMPERATURE = DEG. R
C              PRESSURE = POUNDS(F) / INCH**2
C              DENSITY = POUNDS(M) / FOOT**3
C              SONIC VELOCITY = FEET / SEC.
C              VISCOSITY = POUNDS(M) / FOOT - SEC.
C              CONDUCTIVITY = BTU / FOOT - SEC. - DEG. R

      INTEGER UNITS

      ENTRY WETAIR (TEMP,PRES,DENS,W,ENTRY,ERRS)
C.....MAIN ENTRY FOR PROPERTY CALCULATIONS.

C.....CALLING ARGUMENTS:
C      TEMP = TEMPERATURE
C      PRES = PRESSURE
C      DENS = DENSITY
C      W = FRACTION (BY MASS) THAT IS WATER
C      ENTRY = INTEGER THAT SPECIFIES WHICH VARIABLES ARE INPUT:
C              = 1 IF TEMPERATURE AND DENSITY ARE GIVEN
C              = 2 IF PRESSURE AND DENSITY ARE GIVEN
C              = 3 IF TEMPERATURE AND PRESSURE ARE GIVEN
C              = 4 IF PRESSURE AND ENTROPY ARE GIVEN
C              = 5 IF PRESSURE AND ENTHALPY ARE GIVEN
C      ERRS = ERROR FLAGS (BITS -- LEAST SIGNIFICANT = 1)
C      BIT 1 = OUT OF RANGE IN SATURATION TABLE FOR AIR
C      BIT 2 = OUT OF RANGE IN G TABLE FOR AIR
C      BIT 3 = TEMPERATURE OUT OF RANGE FOR GG TABLE OF AIR
C      BIT 4 = DENSITY OUT OF RANGE FOR GG TABLE OF AIR
C      BIT 5 = CONVERGENCE NOT ACHIEVED IN AIR CALCULATION
C      BIT 6 = OUT OF RANGE IN SATURATION TABLE FOR WATER
C      BIT 7 = OUT OF RANGE IN G TABLE FOR WATER
C      BIT 8 = TEMPERATURE OUT OF RANGE FOR GG TABLE OF WATER
C      BIT 9 = DENSITY OUT OF RANGE FOR GG TABLE OF WATER
C      BIT 10 = CONVERGENCE NOT ACHIEVED IN WATER CALCULATION
C      BIT 11 = ILLEGAL VALUE OF W (WATER FRACTION)
```

C BIT 12 = CONVERGENCE NOT ACHIEVED IN MIXTURE CALCULATION
C BIT 13 = AIR HAS LIQUIFIED (TEMPERATURE MUCH TOO LOW)
C BIT 14 = GIVEN T, P, D, S, OR H IS BAD

COMMON /WETAIC/ MIX,AIR,H2O,NP,R,GAMMA,LIQW,PA,PW,DA,DW,
* WL,WG,DENSL,DENSG,SL,SG,HL,HG

C MIX = PROPERTIES OF WET-AIR MIXTURE:
C MIX(1) = COMPRESSIBILITY, PV/RT
C MIX(2) = ENTROPY, SAME UNITS AS R
C MIX(3) = ENTHALPY, SAME UNITS AS R*T
C MIX(4) = SPECIFIC HEAT, CV, SAME UNITS AS R
C MIX(5) = SPECIFIC HEAT, CP, SAME UNITS AS R
C MIX(6) = SONIC VELOCITY
C MIX(7) = VISCOSITY
C MIX(8) = CONDUCTIVITY
C AIR = PROPERTIES OF DRY-AIR COMPONENT
C (ARRANGED JUST LIKE THE MIX ARRAY)
C H2O = PROPERTIES OF WATER COMPONENT
C (ARRANGED JUST LIKE THE MIX ARRAY)
C NP = NUMBER OF PARAMETERS (LAST ONE) REQUIRED TO BE
C CALCULATED IN MIX, AIR, & H2O ARRAYS
C R = GAS CONSTANT FOR THE MIXTURE
C GAMMA = RATIO OF SPECIFIC HEATS OF MIXTURE
C (ONLY CALCULATED IF NP = 5 OR MORE)
C LIQW = .TRUE. IF WATER IS PART LIQUID, PART GAS
C OTHER CALCULATED PROPERTIES OF POSSIBLE USE:
C PA = PARTIAL PRESSURE OF DRY-AIR COMPONENT
C PW = PARTIAL PRESSURE OF WATER COMPONENT
C DA = (PARTIAL) DENSITY OF DRY-AIR COMPONENT
C DW = (PARTIAL) DENSITY OF WATER COMPONENT
C ADDITIONAL PROPERTIES CALCULATED WHEN LIQW=.TRUE.:
C WL = FRACTION (BY MASS) OF WATER IN LIQUID PHASE
C WG = FRACTION (BY MASS) OF WATER IN GAS PHASE
C DENSL = DENSITY OF WATER IN THE LIQUID PHASE
C DENSG = (PARTIAL) DENSITY OF WATER IN THE GAS PHASE
C SL = (SPECIFIC) ENTROPY OF WATER IN THE LIQUID PHASE
C SG = (SPECIFIC) ENTROPY OF WATER IN THE GAS PHASE
C HL = (SPECIFIC) ENTHALPY OF WATER IN THE LIQUID PHASE
C HG = (SPECIFIC) ENTHALPY OF WATER IN THE GAS PHASE

LOGICAL LIQW
INTEGER ENTRY,ERRS
REAL MIX
DIMENSION MIX(8),AIR(8),H2O(8)

Appendix B

Source-Code Listing (in SFTRAN) of a Test Program for Testing WETAIR Subroutine

C.....TESTS THE WETAIR SUBPROGRAM.

```
INCLUDE (SPECIFICATION STATEMENTS)
INCLUDE (CONSTANTS FOR COMPARING TO NBS-564 AIR VALUES)

NAMELIST /INPUT/ T,P,D,S,H,NP,ENTRY,W,UNITS,NBS,REF,MORE
```

C.....MAIN FLOW:

```
DO WITH
  READ (5,INPUT,DONE=END)
UNTIL (DONE)
  DO (SAVE INPUT VALUES AND ADD SO & HO)
  IF (NBS) DO (CONVERT FROM NBS TO SI UNITS)
  CALL WETAIO (UNITS)
  CALL WETAIR (T,P,D,W,ENTRY,ERRS)
  IF (NBS) DO (CONVERT FROM SI TO NBS UNITS)
  IF (REF) DO (ADJUST SO & HO TO GET INPUT VALUES OF S & H)
  DO (SUBTRACT SO & HO AND RESTORE PROPER INPUT VALUES)
  DO (REPORT RESULTS)
END
STOP
```

C.....DETAILS:

```
PROCEDURE (SAVE INPUT VALUES AND ADD SO & HO)
  TSAVE=T
  PSAVE=P
  DSAVE=D
  SSAVE=S
  HSAVE=H
  S=S+SO
  H=H+HO
END

PROCEDURE (CONVERT FROM NBS TO SI UNITS)
  UNITS=1
  T=T/TCONV
  D=D/DCONV
  P=P/PCONV
  S=S/SCONV
  H=H/HCONV
END
```

```

DEFINITION (CONSTANTS FOR COMPARING TO NBS-564 AIR VALUES)
  DATA TCONV,PCONV,DCONV,SCONV / 1.0, 9.8692, 773.4, 3.4817 /,
*   HCONV,ACONV,CONV7,CONV8 / .01275, 3.017E-3, 5827.5, 4142.5 /
END

```

```

PROCEDURE (CONVERT FROM SI TO NBS UNITS)

```

```

  T=T*TCONV
  D=D*DCONV
  P=P*PCONV
  S=S*SCONV
  H=H*HCONV
  MIX(4)=MIX(4)*SCONV
  MIX(5)=MIX(5)*SCONV
  MIX(6)=MIX(6)*ACONV
  MIX(7)=MIX(7)*CONV7
  MIX(8)=MIX(8)*CONV8

```

```

END

```

```

PROCEDURE (ADJUST SO & HO TO GET INPUT VALUES OF S & H)

```

```

  SO=S-SSAVE
  HO=H-HSAVE
  REF=.FALSE.

```

```

END

```

```

PROCEDURE (SUBTRACT SO & HO AND RESTORE PROPER INPUT VALUES)

```

```

  S=S-SO
  H=H-HO
  DO CASE (ENTRY,5)
  CASE 1
    T=TSAVE
    D=DSAVE
  CASE 2
    P=PSAVE
    D=DSAVE
  CASE 3
    T=TSAVE
    P=PSAVE
  CASE 4
    P=PSAVE
    S=SSAVE
  CASE 5
    P=PSAVE
    H=HSAVE

```

```

  END

```

```

END

```

```

PROCEDURE (REPORT RESULTS)

```

```

  IF (ERRS.NE.0) DO (REPORT ERROR BITS)
  WRITE (6,1) W,T,P,D,(MIX(I),I=1,NP)

```

```

      IF (MORE) THEN
        IF (W.LT.1.0) WRITE (6,2) PA,DA,(AIR(I),I=1,NP)
        IF (W.GT.0.0) WRITE (6,3) PW,DW,(H2O(I),I=1,NP)
        V=1.0/D
        WRITE (6,4) V,R,GAMMA
      END
      IF (LIQW) THEN
        SL=SL-S0
        SG=SG-S0
        HL=HL-H0
        HG=HG-H0
        WRITE (6,5) WL,DL,SL,HL,WG,DG,SG,HG
      END
    END
  END

1  FORMAT (' W,T,P,D,MIX(1),.. =',5(1PE12.4)/(20X,5(1PE12.4)))
2  FORMAT ('   PA,DA,AIR(1),.. =',5(1PE12.4)/20X,5(1PE12.4))
3  FORMAT ('   PW,DW,H2O(1),.. =',5(1PE12.4)/20X,5(1PE12.4))
4  FORMAT ('   V,R,GAMMA =',3(1PE12.4))
5  FORMAT ('   TWO PHASES OF WATER'/
*   '   WL,DL,SL,HL =',4(1PE12.4)/
*   '   WG,DG,SG,HG =',4(1PE12.4))

PROCEDURE (REPORT ERROR BITS)
  N=0
  DO FOR I=1,14
    IF (MOD(ERRS,2).NE.0) THEN
      N=N+1
      BITS(N)=I
    END
  ERRS=ERRS/2
  END
  WRITE (6,6) (BITS(I),I=1,N)
END

6  FORMAT (' ERROR FLAGS:',14I3)

DEFINITION (SPECIFICATION STATEMENTS)
  LOGICAL NBS,REF,MORE,DONE,LIQW
  INTEGER ERRS,ENTRY,BITS,UNITS
  REAL MIX
  DIMENSION MIX(8),AIR(8),H2O(8),BITS(14)
  COMMON /WETAIC/ MIX,AIR,H2O,NP,R,GAMMA,LIQW,PA,PW,DA,DW,
*   WL,WG,DL,DG,SL,SG,HL,HG
  EQUIVALENCE (S,MIX(2)), (H,MIX(3))
  DATA UNITS /1/
END

END

```

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| 16. Abstract <p>A computer-program subroutine, WETAIR, has been developed to calculate the thermodynamic and transport properties of air-water mixtures. It determines the thermodynamic state from assigned values of temperature and density, pressure and density, temperature and pressure, pressure and entropy, or pressure and enthalpy. WETAIR calculates the properties of dry air and water (steam) by interpolating to obtain values from property tables. Then it uses simple mixing laws to calculate the properties of air-water mixtures. Properties of mixtures with water contents below 40 percent (by mass) can be calculated at temperatures from 273.2 to 1497 K and pressures to 450 MN/m². Dry-air properties can be calculated at temperatures as low as 150 K. Water properties can be calculated at temperatures to 1747 K and pressures to 100 MN/m². WETAIR is available in both SFTRAN and FORTRAN.</p> | | 13. Type of Report and Period Covered Technical Paper |
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