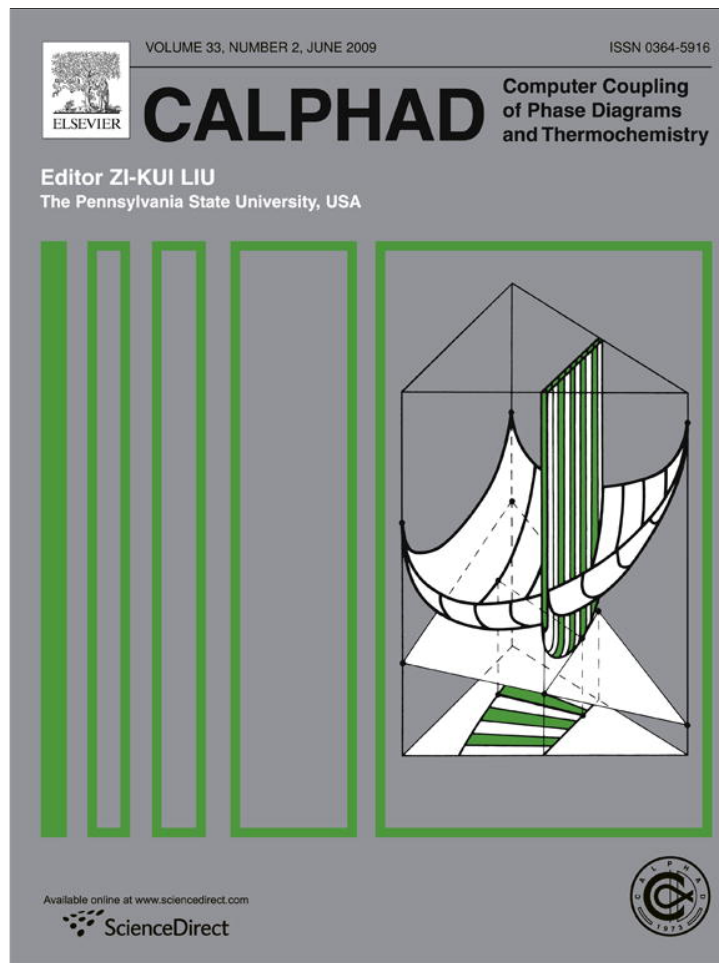


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Property evaluation in The Expert System for Thermodynamics (“TEST”) web application

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ABSTRACT

Ever since its release, TEST has found use as thermodynamic courseware in many universities around the world. TEST offers web-based analysis tools – java applets called daemons – for property evaluation of working substances, energy, entropy, and exergy analysis of generic open and closed systems, IC engines, gas and vapor power cycles, refrigeration, HVAC, combustion, chemical equilibrium, and gas dynamics. Other modules of TEST include animations, problems, examples, and system navigations that are closely integrated with the daemon module to create a comprehensive analysis tool for engineering thermodynamics. In this paper the methodology of thermodynamic state evaluation by TEST is discussed with several examples.

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1. Introduction

In the last two decades, a number of software applications for thermodynamic analysis have been developed. The ASME provides a comprehensive database for thermodynamics analysis [1]. EES [2] is a comprehensive thermal-science programming language that runs in the Microsoft Windows environment. TPX [3] is an Excel plug-in where the core thermodynamic state can be evaluated by entering two independent properties. Thermoptim [4] is a Java application for analyzing thermodynamic cycles and can be run over the web. A graphical menu driven installable program is GasCAD [5]. The Qualitative Reasoning Group at Northwestern University has developed a Windows installable application named CyclePad [6] which allows users to construct and analyze a wide variety of thermodynamic cycles. None of these packages, however, are comprehensive enough to cover the diverse range of topics covered in engineering thermodynamics.

For applications involving mostly gas phase equilibrium computation such as combustion analysis, several commercial and freeware applications are available. GasEQ [7], written by Chris Morley, is a free tool that runs in a Windows environment and can compute equilibrium distributions of

mixtures at fixed temperatures and pressures using Gibbs free energy minimization or fixed temperatures and volumes using Helmholtz free energy minimization. REACT [8], available to Journal of Chemical Education subscribers on the General Chemistry Collection CD-ROM, is an MSDOS program developed in 1995. A similarly named program, REACT! [9], developed in 1992, can be downloaded as a trial version from Yale University. Both of these packages run only in the Windows environment and exhibit somewhat dated user interfaces and installation methods. Developed by the Finnish company Outotec Oyj, the commercial chemical simulation tool HSC Chemistry 6.1 [10] includes an extensive suite of simulation and modeling tools, including modules for performing equilibrium calculations. HSC Chemistry includes two equilibrium solvers: GIBBS, a standard Gibbs free energy minimization solver, and SOLGASMIX [11], developed by Gunnar Eriksson. The numerical method employed in SOLGASMIX has been incorporated into other commercial applications such as FactSage [12] developed at the Center for Research in Computational Thermochemistry [13] at the Université de Montréal in Québec, Canada. FactSage runs only under Microsoft Windows and requires that a security key (dongle) is attached to the USB or printer port of the system on which it is installed, or access to a network license server. FactSage includes an equilibrium module called *Equilib* that employs a standard Gibbs energy minimization algorithm and allows one to perform constrained equilibrium computations with respect to any thermodynamic potential (e.g. $U = U(S, V)$, $A = A(V, T)$, and $H = H(S, P)$ besides $G = G(T, P)$). Perhaps the most well-known

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Nomenclature

c_p	Specific heat capacity at constant pressure, $\text{kJ kg}^{-1} \text{K}^{-1}$
c_v	Specific heat capacity at constant volume, $\text{kJ kg}^{-1} \text{K}^{-1}$
M	Molar mass (or molecular weight), kg kmol^{-1}
p	Pressure, kPa
R	Molar ideal gas constant $\approx 8.314472 \text{ kJ K}^{-1} \text{ kmol}^{-1}$
T	Temperature, K
u	Specific internal energy, kJ kg^{-1}
h	Specific enthalpy, kJ kg^{-1}
j	Specific flow energy, kJ kg^{-1}
s	Specific entropy, $\text{kJ kg}^{-1} \text{K}^{-1}$
v	Specific volume, $\text{m}^3 \text{kg}^{-1}$
V	Velocity, m s^{-1}
\forall	Volume, m^3
x	Mass fraction of a vapor in a saturated mixture
x_A	Mass fraction of species A in a mixture
y	Volume fraction of a vapor in a saturated mixture
y_A	Mole fraction of species A in a mixture
z	Elevation, m

Greek Symbols

Φ	Specific exergy, kJ kg^{-1}
ψ	Specific flow exergy, kJ kg^{-1}
ρ	Density, kg m^{-3}

equilibrium computation software is *Chemical Equilibrium and Applications* (CEA) [14–16] developed by Sanford Gordon, Frank J. Zeleznik, and Bonnie J. McBride at the NASA John H. Glenn Research Center. NASA CEA is open-source and can be downloaded free of charge from the CEA website (NASA Computer Program – Chemical Equilibrium with Applications). Also well-known, especially in the combustion community, is STANJAN [17] developed by Professor William C. Reynolds II of the Mechanical Engineering department at Stanford University.

Most of these applications are stand-alone applications and must be installed before use. Also, many are geared towards a specific set of working substances. TEST, on the other hand, is completely web driven and covers the entire range of working substances encountered in engineering thermodynamics applications.

TEST is freely accessible to anyone online from www.thermofluids.net. More than 16,000 students, educators and professionals have registered to use TEST. A visual manual for TEST has been published by Prentice Hall [18]. Some of the daemons have been reviewed and included in various public domain educational web sites such as the MERLOT project [19]. Judging from the comments received from educators, it is fair to say that TEST has the potential to become a very useful tool in thermodynamics education. Work is currently underway to develop a chemical equilibrium module.

An overview of the TEST portal can be found elsewhere [20]. In this work, we will first introduce the methodology TEST uses to classify working substances into different models, with each model based on a set of idealized assumptions. Two types of extended states – the *system* state and the *flow* state – will be developed to capture properties of a uniform system or a uniform flow. In developing the algorithm to evaluate an extended state, the interrelations among different types of properties will be discussed. The graphical user interface for a state and the representation of states on thermodynamic diagrams will be presented next. Finally, TEST codes that can be used to convert the GUI based solution into storable structural codes, and vice versa, will be discussed. Several examples of state evaluation with different material models will be briefly presented.

2. The TEST portal

TEST is a web-based suite of applications for analyzing engineering thermodynamic systems. Accessible from www.thermofluids.net, TEST offers twenty-two customized java applets, called *daemons*, for evaluation of states of different working substances. These working substances include 50 common solids and liquids, 65 phase-change fluids, 60 gases, and several gas mixtures.

TEST has been developed using an object-oriented paradigm in Java so that codes can be reused. All TEST daemons have been thoroughly tested under different versions of IE, Firefox, and Safari running on Windows, MacOS, and Linux platforms. The only browser plug-in required to run the daemons is version 4 (or greater) of the Java Platform, available from www.java.com. An alternative way to run TEST is to install the software locally from a CD distribution. The browser is then used to point towards the locally installed distribution or the index.html file contained on the CD itself. When locally installed, a daemon takes about 2–5 s to load, whereas the load time may vary between 5 and 20 s over the Internet depending on connection speed. The loading time, however, significantly decreases on subsequent access, as browsers cache reusable modules of the daemons. Once loaded, the daemons run just like any other native application installed on the client machine.

2.1. Extended state algorithm

Because engineering systems often involve evaluation of properties in the interior as well as at the inlet and exit ports of open systems, TEST separates states into two types – system states for evaluating properties of a uniform system and flow states for evaluating properties of a uniform flow.

An extended state provides a detailed snapshot of a state beyond the core thermodynamic properties describing a thermodynamic equilibrium. As shown in Fig. 1, an extended state builds upon the thermodynamic state by adding extrinsic and system properties. At the core of any state are material properties – molar mass, gas constant, etc. – which are intrinsic to a working substance and are determined as soon as a substance is selected. Thermodynamic properties – p , T , v , u , h , and s – which are intrinsic to an equilibrium state, also must be common to both system and flow states. Extrinsic properties – properties such as elevation z , velocity V , specific stored energy $e \equiv u + ke + pe$, and specific flow energy $j \equiv h + ke + pe$ – which depend on the observer's speed or location also appear in both types of extended states. Of course, total properties or properties that depend on the extent of a system – mass m and volume \forall for instance – appear only in system states. These are replaced by the rate of transport of mass and volume \dot{m} and $\dot{\forall}$, respectively, in the corresponding flow state.

Each daemon provides an I/O (input/output) panel, where properties that are not included as part of an extended state can be calculated after a state is evaluated. For instance, the total stored energy in a uniform system at state-1, E_1 , can be calculated in the I/O panel from the equation $E_1 = m_1 e_1$. Likewise, the rate of entropy transport by a uniform flow at state-2 can be calculated from $S_2 = \dot{m}_2 e_2$ in the I/O panel after state-2 has been evaluated.

The energy transported by a flow is not only due to the stored energy carried by the flow, but also due to the flow work that is done to sustain the flow:

$$\begin{aligned} \dot{E} + \dot{W}_F &= \dot{m}e + pAV = \dot{m}e + pv \frac{AV}{v} = \dot{m}(e + pv) \\ &= \dot{m}(h + ke + pe) \quad [\text{kW}]. \end{aligned} \quad (1)$$

Because the property group $h + ke + pe$ appears often in open system analysis, TEST introduces a new property symbol

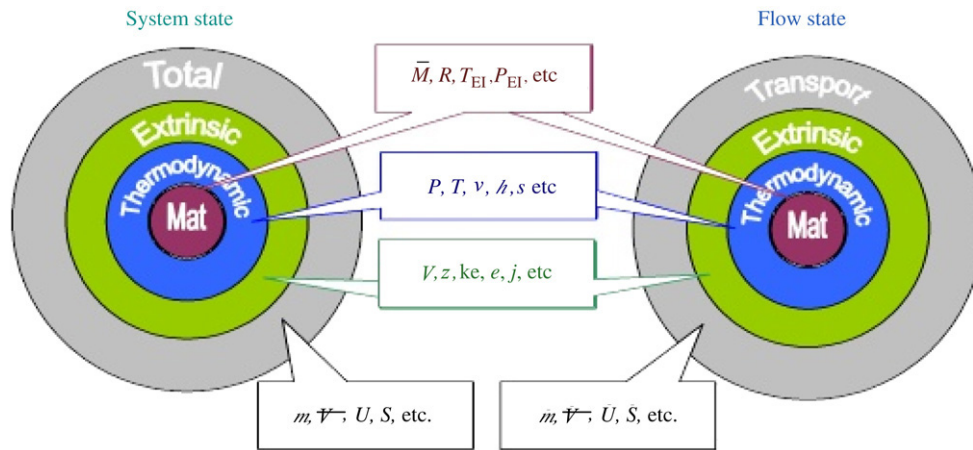


Fig. 1. Two types of extended states evaluated by TEST. They differ only in the outermost layer, where properties depend on system size.

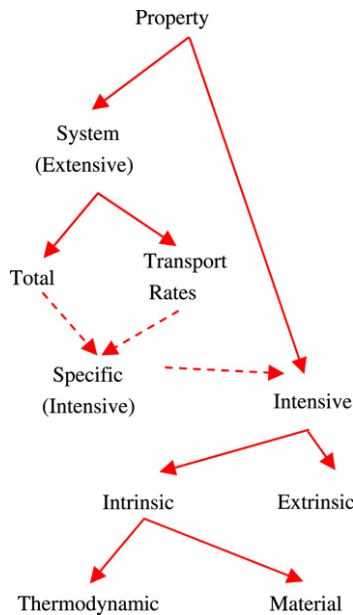


Fig. 2. Property classifications.

$j \equiv h + ke + pe$ to represent the net energy carried by a flow per unit mass. Known as the specific flow energy, (1) can be also written as $\dot{m}(h + ke + pe) = \dot{m}j = \dot{J}$. Specific enthalpy, therefore, can be interpreted as the specific flow energy when the kinetic and potential energies can be neglected in a flow.

Given the large number of properties – some daemons display as many as 23 properties – which can be used as an input by a user, classification of properties (see Fig. 2) plays an important role in the state algorithm. Once a working substance is selected, the material properties are obtained from a look-up table. The following property relations, which are applicable to all working substances, are used to determine thermodynamic properties that may be indirectly supplied. For instance, if mass and volume are supplied, the specific volume can be calculated:

$$m = \rho V; \quad \dot{m} = \rho AV = \rho \dot{V}; \quad \rho = \frac{1}{v}; \quad (2)$$

$$e = u + ke + pe; \quad j = h + ke + pe; \quad h = u + pv.$$

If a sufficient number of thermodynamic properties are known (entered by users or calculated from Eq. (2)), the complete set of thermodynamic properties are then obtained by using an

appropriate model as discussed in the next section. Once the intrinsic properties are found, general property relations of Eq. (2) are used in the reverse direction to populate the missing extrinsic and system properties.

Extrinsic properties calculated by the daemons also include specific stored exergy ϕ and specific flow exergy ψ :

$$\phi = (e - e_0) - T_0(s - s_0) + p_0(v - v_0),$$

$$\psi = (j - j_0) - T_0(s - s_0). \quad (3)$$

Because the exergy of a system depends on its dead state [21], state-0 is designated in TEST as the dead state of a system. To evaluate the dead state, ambient atmospheric temperature and pressure are used for state-0 along with a zero value of velocity and elevation. Once state-0 is computed, all other evaluated states automatically calculate ϕ and ψ .

2.2. Graphical user interface

TEST daemons employ an intuitive graphical user interface to display an array of properties as a complete snapshot of the state. A typical daemon is illustrated in Fig. 3 where a state daemon is used to calculate the flow state of steam flowing at 1000 kPa, 80% quality, and 50 m/s through a cross-section of diameter 10 cm.

All state daemons share a similar graphical interface and appear within a rectangular box containing five horizontal panels. The path name of the daemon such as *State>Flow>PC-Model* shown in Fig. 3, and a version number are shown in the title panel. The row of buttons below the title panel constitutes the global control panel which contains radio-buttons for the choice of units and a few buttons for global calculations (discussed later). Below the global control panel is a panel containing two tabs named the *State Panel* and *I/O Panel* which toggle the state and I/O panel, respectively, displayed between the tab panel and a message panel appearing at the bottom margin of the daemon. Hovering the mouse pointer over any hot spot brings up a helpful tip on the message panel. The state panel is selected in the image displayed in Fig. 3.

The state panel is sub-divided into three panels. The state control panel consists of different control widgets such as a state identification menu, choices for thermodynamic plot, substance selection, buttons for initialization and calculation, and a small textbox to display short messages – in this case the phase composition of the working fluid. Below the state control panel is the property panel where a number of properties are bundled. Below the property panel is an image panel depicting the state.

Property labels are color coded – red for material properties, blue for thermodynamic properties, green for extrinsic properties,

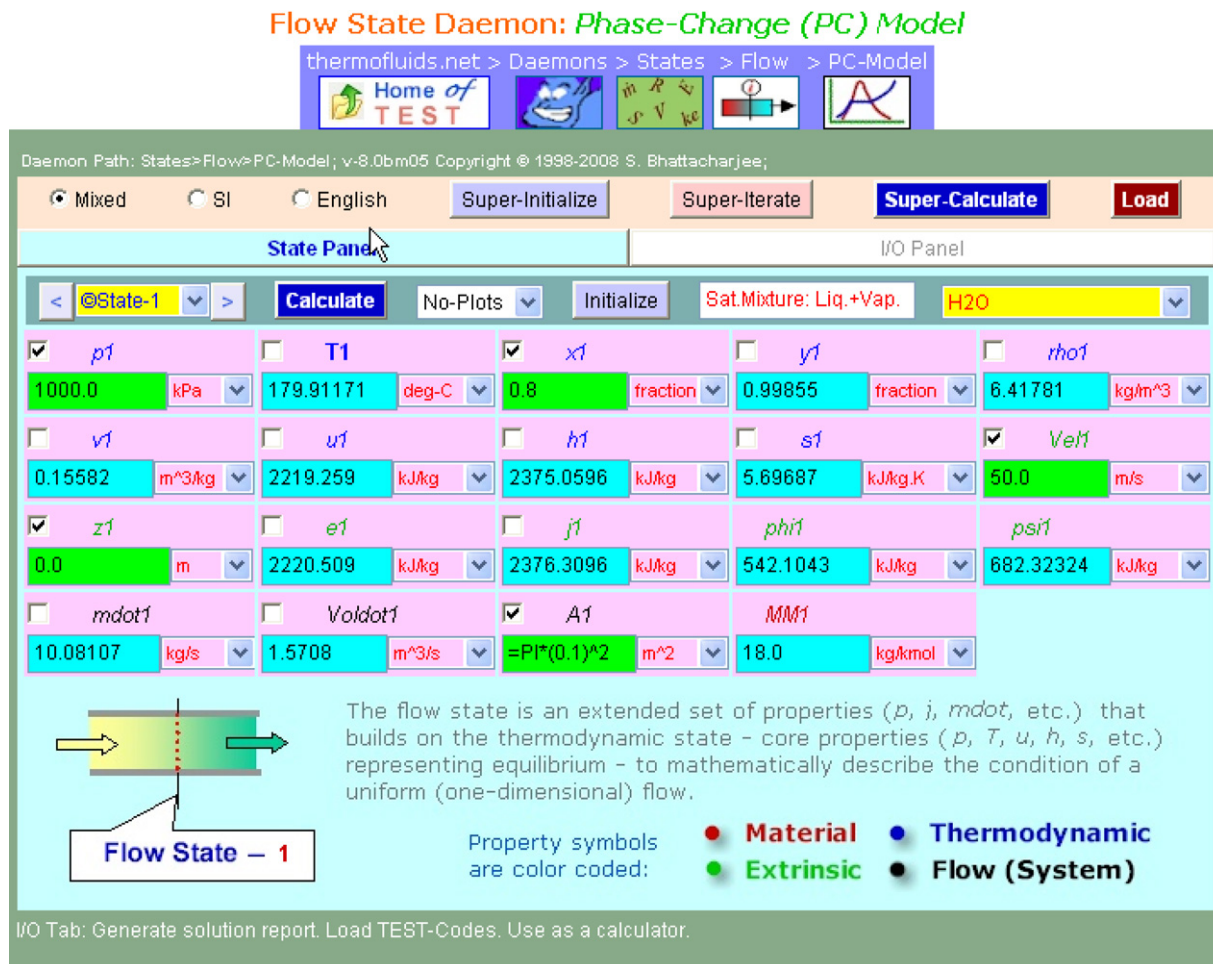


Fig. 3. Image of the PC flow state daemon. The flow state, state-1, is evaluated for a flow of steam at 1000 kPa, 80% quality, flowing with a velocity of 50 m/s through a 10 cm-diameter pipe.

and black for system properties. Each property object consists of a checkbox, a property label, a textfield to display its value, and a choice for selecting a unit. The checkbox toggles the property between the input and display mode. To enter a property, a user starts by clicking its checkbox. A dependency analysis is run in the background to ensure the property cannot be calculated from other properties that have been entered already. If the property is found to be an independent unknown, it goes into the input mode; otherwise, an appropriate error message is displayed and the user is prevented from over-specifying the state. In its input mode, the user enters a property value, selects a unit from the unit menu, and presses the *Enter* button. As shown in Fig. 4 for the temperature object, the background color of the property value changes once the value of 20 °C is read. Each time a new value is entered, the state is updated until the complete state is obtained.

In entering a value for property, simple mathematical expressions can be used. The area A1 in Fig. 3, for instance, has been entered in terms of the diameter of the pipe. Calculated properties from another state can also be used as part of such expressions. For example, suppose state-2 is related to state-1 through a polytropic process $pV^{1.3} = c$ and the volume at state-2 is 0.5 m³. The pressure at state-2 then can be entered through the expression $'= p1 * (Vol1/0.5)^{1.35}'$.

The I/O panel also serves as a calculator that recognizes calculated variables and can be used to evaluate auxiliary quantities. For state-1 displayed in Fig. 3, the transport rate of kinetic energy, stored energy, flow energy, and flow work in kW are calculated in the I/O panel and shown in Fig. 5.

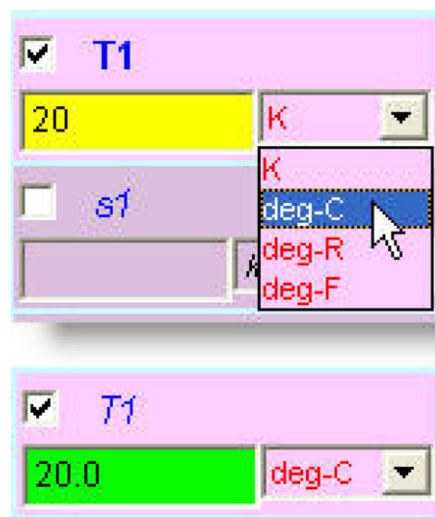


Fig. 4. Example of a property object – setting the temperature T1 of state-1.

2.3. Thermodynamic plots

Plotting calculated states on thermodynamic diagrams is as simple as picking the diagram type from the plot menu which offers $p-v$, $p-h$, $T-v$, $T-s$, $h-s$, $p-T$, $v-T$, $u-T$, $h-T$, and $s-T$ diagrams.

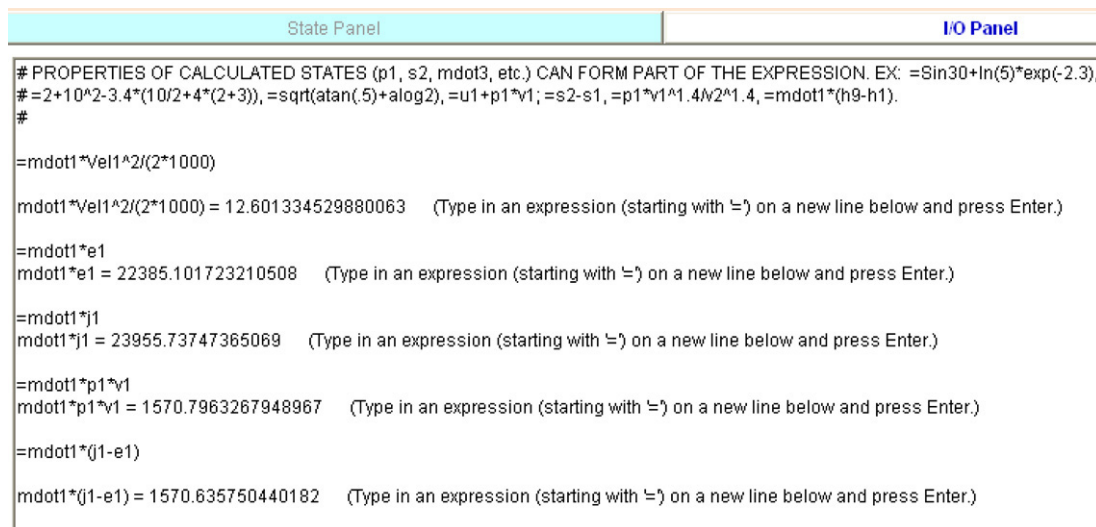


Fig. 5. Use of the I/O panel as a calculator to evaluate auxiliary variables. In this case, the flow work (in kW) is calculated in two different ways for state-1 displayed in Fig. 3.

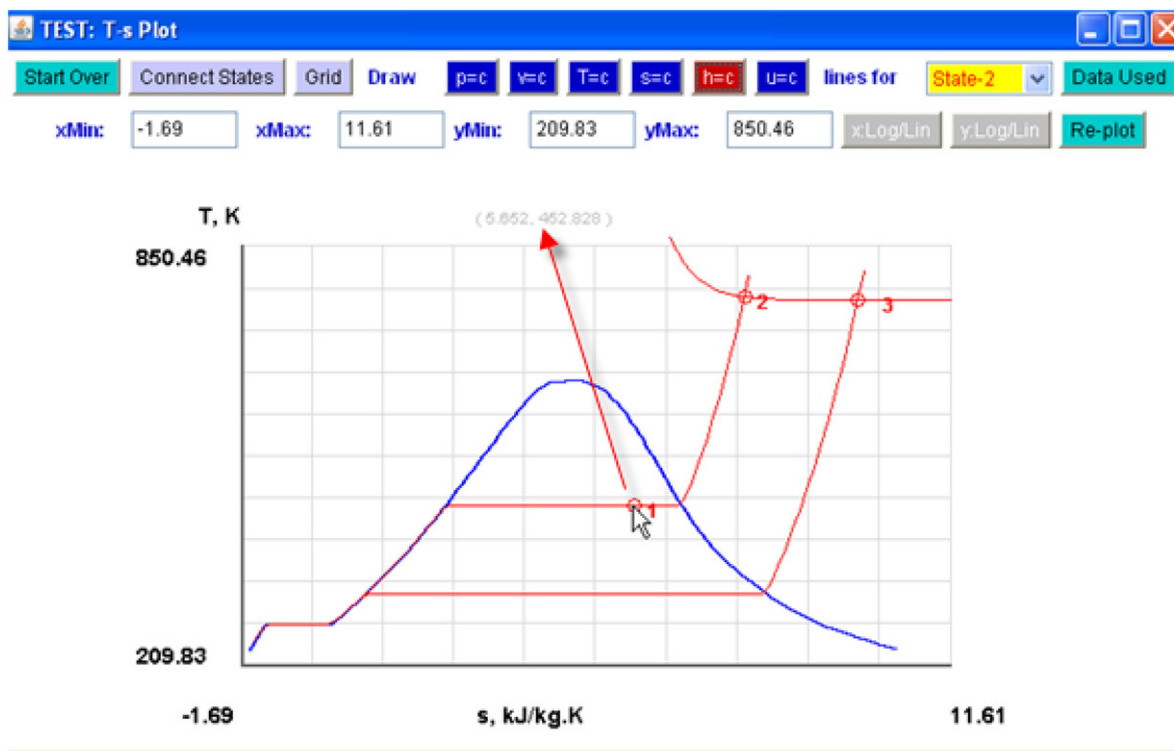


Fig. 6. After three states are calculated, constant pressure lines are drawn. Also, constant enthalpy lines drawn for state-2 indicating $h_2 = h_3$. Parking the pointer at any state point – state-1 in this plot – shows its coordinates.

Fig. 6 shows three calculated states on a $T-s$ plot. The plot window provides many convenient features. Constant property lines can be drawn through any or all states by pressing the constant property buttons. Constant pressure and constant enthalpy lines plotted in this figure reveal that states 1 and 2 have the same pressure, and 2 and 3 have the same enthalpy. Hovering the pointer on top of any point on the plot reveals its Cartesian coordinates. By changing the left-bottom and top-right coordinates, the plot can be zoomed in or out, coordinates can be made logarithmic or linear by using the appropriate buttons, and the raw data used for the plot can be displayed by clicking the *Data Used* button. This raw data can

be copied to a spreadsheet or another plotting routine for further analysis.

2.4. TEST codes and what-if studies

The GUI used by states exposes all the properties of thermodynamic states to the user. Independent properties can be entered in a myriad of possible combinations to calculate a state. Because properties can be entered with relational expressions, a series of states related by certain constraints can be calculated. For example, the states shown in Fig. 6 are related to each other through

```

State Panel
#####
#
# Daemon Path: Test>Daemons>States>Flow>PC-Model; Version: v-8.0bm05
#
#-----Start of TEST-Codes-----
States {
  State-1: H2O;
  Given: { p1= 1000.0 kPa; x1= 0.8 fraction; Vel1= 0.0 m/s; z1= 0.0 m; }

  State-2: H2O;
  Given: { p2= "p1" kPa; T2= 500.0 deg-C; Vel2= 0.0 m/s; z2= 0.0 m; }

  State-3: H2O;
  Given: { p3= 10.0 kPa; h3= "h2" kJ/kg; Vel3= 0.0 m/s; z3= 0.0 m; }
}
#-----End of TEST-Codes-----
    
```

Fig. 7. TEST-codes produced in the I/O panel by the Super-Calculate operation after the states shown in Fig. 6 are computed.

$p_2 = p_1$ and $h_3 = h_2$. All that is required to recalculate the states for a different value of p_1 is to change p_1 and then press the *Super-Calculate* button to update all the computed states.

The Super-Calculate operation also produces a solution macro called TEST-code which is shown in Fig. 7 for the states computed for the plot shown in Fig. 6. The syntax of the macro code is similar to C, C++, and Java and is quite readable. The code describes what is known about each state and can be copied and stored on disk for later use.

To reproduce a visual solution, TEST-codes can be copied back into the I/O panel of the appropriate daemon and then pressing the *Load* button which populates the GUI of the visual solution. The *Problems* module of the TEST portal contains a large library of example TEST-codes.

2.5. Material models and solution algorithms

The numerous working substances used in engineering applications are classified into several material models based on their simplifying sets of assumptions. These models are arranged in a hierarchical manner as shown in Fig. 8 to facilitate their encapsulation in an object-oriented manner. There are two broad categories into which all the models are divided: pure substances and mixtures.

Pure substances are working substances with a constant homogeneous chemical composition and are divided into three categories: (a) solids and liquids, (b) real fluids with possibilities of phase change, and (c) gases. Mixtures of pure substances are divided into two categories: binary and general mixtures.

2.5.1. SL model

The SL (Solid/Liquid) model groups all solids and liquids and is assumed to be incompressible with constant specific heats. An S/L state daemon looks very similar to the PC flow state daemon shown in Fig. 3. As soon as a solid or liquid is selected from the working substance selector, the material properties ρ , v , c_v , and M of the state are populated. Application of thermodynamic relations produces a set of equations relating u and s with T , and h with p and T . Coupled with the general relations of (2), these equations sets are solved iteratively until the most number of unknowns based on user input are calculated.

In addition to common solids and liquids, the SL daemon allows a user to define a custom solid or liquid by assigning the material properties c_v , M , and ρ or v .

Table 1

PC model phase determination for a given temperature and pressure.

Condition	Phase composition	Example ^a
$p_{tp} < p \leq p_{cr}$	$T > T_{sat@p}$ Superheated Vapor (V)	State-1
	$T < T_{sat@p}$ Subcooled Liquid (L)	State-2
	$T = T_{sat@p}$ Saturated mixture (M = L + V)	State-3

^a See Fig. 9. Locating states on a T - s diagram for a given value of p and T .

Table 2

PC model phase determination for a given pressure and one of $\{v, u, h, \text{ or } s\}$.

Condition	Phase composition	Example ^a
$p_{tp} < p \leq p_{cr}$	$b > b_{f@p}$ Superheated Vapor (V)	State-1
	$b < b_{f@p}$ Subcooled Liquid (L)	State-2
	$b_{f@p} \leq b \leq b_{g@p}$ Saturated mixture (M)	State-3

^a See Fig. 9. Locating states on a T - s diagram for a given value of p and T .

2.5.2. PC Model

Real fluids such as water, hydrocarbons, and refrigerants can exist as a compressed liquid, superheated vapor, or a mixture of saturated liquid and saturated vapor. An image of the PC flow state daemon is shown in Fig. 3. In addition to the regular thermodynamic properties, two mixture properties – the quality or the mass fraction x of vapor and the volume fraction y of vapor in a saturated mixture – are introduced by this daemon.

The PC model handles sub-cooled liquids, saturated mixtures, and super-heated vapors of a real fluid. The algorithm used is based on a two-step process of finding the phase composition, followed by property evaluation from saturation and superheated data. To simplify the discussion, we assume the phase compositions to be limited to subcritical liquid, vapor, or saturated mixtures ($p_{tp} < p \leq p_{cr}$).

Case A. Given p and T : From the saturation data, obtain $T_{sat@p}$ and compare it with the given temperature to deduce the phase composition from Table 1.

Note that while the phase composition of state-3 is found, its relative location between the f and g states is an unknown at this point.

Case B. Given p and b (b stands for $v, u, h, \text{ or } s$): From the saturation data, obtain the saturation properties $b_{f@p}$ and $b_{g@p}$ and use Table 2 to determine phase composition.

Case C. Given T and b (b stands for $v, u, h, \text{ or } s$): The procedure is almost identical to the one described in Case B with the property p replaced with T .

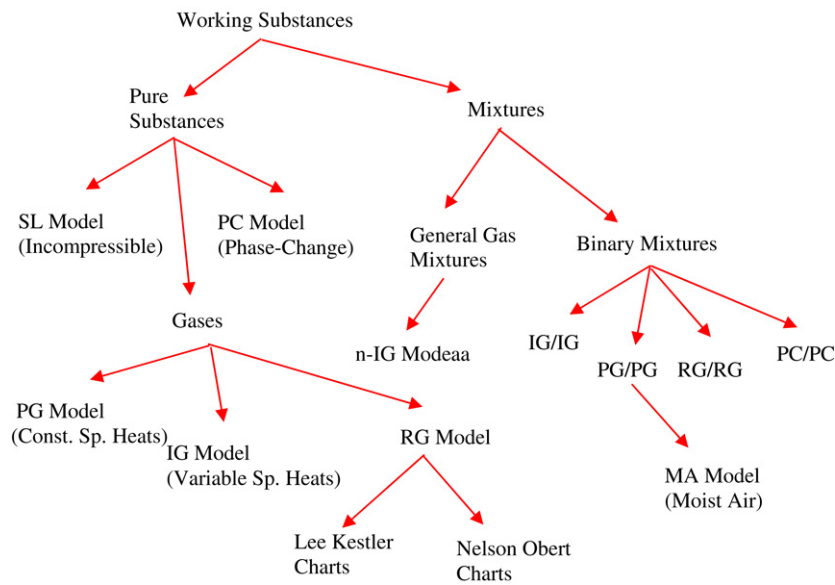


Fig. 8. Modeling working substances.

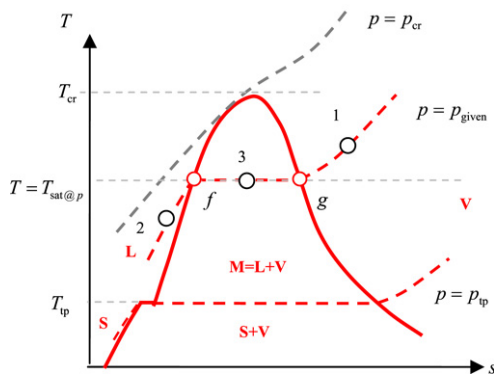


Fig. 9. Locating states on a T-s diagram for a given value of p and T.

Case D. Given x or y: If the quality x or the vapor volume fraction y is given, the phase composition must be a *saturated mixture* ($M = L + V$) because these properties have meaning only in this region.

Case E. Given b_1 and b_2 (b stands for v, u, h, or s): Assume a pressure p and from the assumed p and b_1 , determine b_2 by following case B. Iterate over the entire range of pressures ($p_{tp} < p \leq p_{cr}$) until the calculated b_2 matches with the user supplied b_2 .

Once a phase composition is determined, thermodynamic properties for the vapor region are found from interpolation of the superheated data, which is downloaded along with the applet during loading. For data outside the range of the table, appropriate approximations are made to extrapolate. The message panel displays the assumptions used for such an extrapolation. For saturated mixtures, the vapor mass fraction x, if unknown, is determined by using the following relation that expresses a generic mixture property b in terms of properties of a saturated liquid (f-state) and saturated vapor.

$$b = (1 - x)b_f + xb_g. \quad (4)$$

Once x is calculated, all other specific properties can be calculated by using Eq. (4) since p and $T = T_{sat@p}$ are known. The volume fraction y is determined from

$$y \equiv \frac{V_g}{V} = \frac{xv_g}{v} = \frac{xv_{g@T}}{(1 - x)v_{f@T} + xv_{g@T}}. \quad (5)$$

Since the intersection of the saturated liquid and saturated vapor lines is the critical state, volume fraction can be determined by assigning $x = 0$ (f-line) and $y = 1$ (g-line) in a PC daemon.

Sub-cooled liquid is modeled by the simplifying assumption that v, u, and s are functions of T only so that

$$v = v_{f@T}, \quad u = u_{f@T}, \quad s = s_{f@T}, \quad \text{and} \quad (6)$$

$$h(p, T) = u_{f@T} + pv_{f@T}.$$

Liquid properties, therefore, can be obtained from saturation data. For water, TEST provides compressed liquid data that can be used for higher accuracy. Sublimation data is also available to -40°C .

2.5.3. Gas models

Three different gas models are offered by TEST, as classified in Fig. 3. The gas daemons look very similar to the PC flow state daemon shown in Fig. 3.

The well known ideal gas or IG model is based on the ideal gas equation of state $pv = RT$. As a consequence of this equation, it can be shown that the specific heats of an ideal gas are functions of temperature only. Shomate polynomials [22] are used to correlate c_p with T. The ranges of temperatures over which the polynomial coefficients, obtained from the NIST Chemistry Webbook [23] are valid, are shown on the message panel when a gas species is selected. Beyond that range, c_p is assumed to be a constant.

The IG daemon displays the material properties \bar{M} and R for any selected gas. Application of the ideal gas equation of state, the respective Shomate polynomial, and thermodynamic relations produces a set of equations relating c_p , u, and h with T, and s with p and T. Coupled with the general relations of (2), these sets of equations are solved iteratively until the most number of unknowns based on user entered properties are found.

The PG (perfect gas) model is based on an additional assumption that specific heats are constant in addition to the ideal gas assumption. A perfect gas, therefore, is a simplified ideal gas. The list of material properties for a perfect gas includes \bar{M} , R, c_p , and c_v . Specific heats, therefore, are material properties in the PG model. The solution algorithm follows the same steps as in the case of the IG daemons. A custom perfect gas can be created by the user by assigning a sufficient number of independent material properties. As in the case of any other input property, the daemon checks for independence and sufficiency of the input material properties.

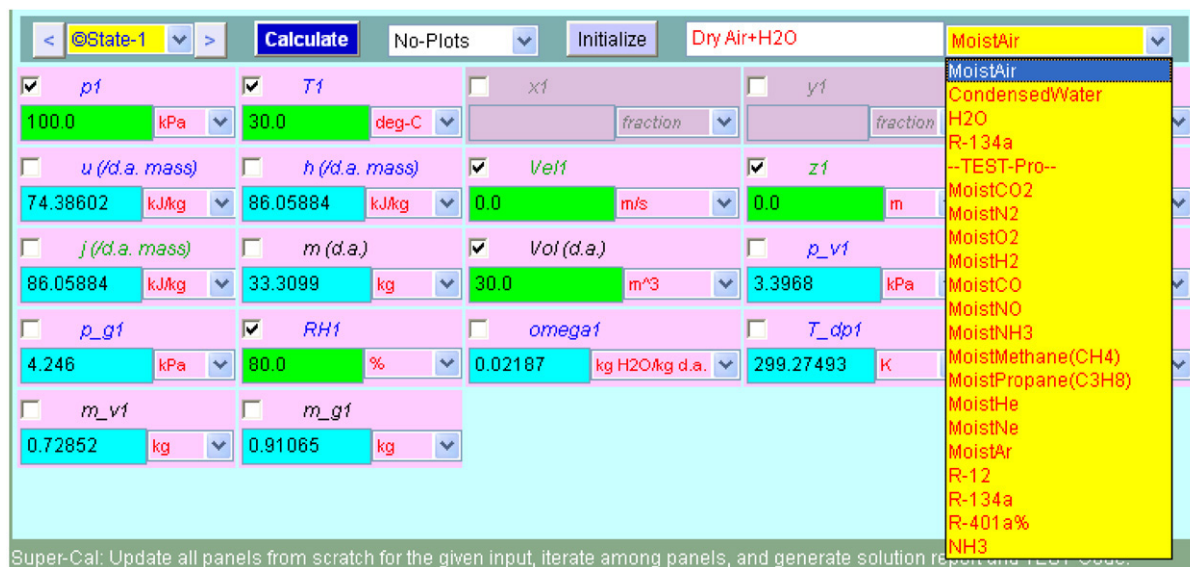


Fig. 10. Image of the moist air system state daemon with a moist air state evaluated at 30 °C, 100 kPa, and 80% relative humidity in a chamber of volume 30 m³. The mass of water vapor calculated is $m_{v1} = 0.728$ kg.

The RG (real gas) model introduces a deviation from the ideal gas behavior at high pressure or low temperature through the compressibility factor and enthalpy and entropy departure factors. The compressibility and the departure charts due to Lee and Kesler [24] as well as those due to Nelson and Obert [25] are both offered by the RG daemons. In the state control panel, the user selects a particular data set before selecting a working fluid. By using data from these charts, the daemon automatically creates the saturation table and superheated table for any selected gas. Once these tables are generated, the PC model algorithm is followed to obtain a solution.

2.5.4. Mixture models

The PG/PG and IG/IG binary mixture models are basically an extension of the corresponding pure gas model with two species selectors A and B. Two new properties x_A and y_A specify the mass and mole fraction of species A in the mixture. One of these properties must be entered to define a mixture. Based on mass or mole fractions, mixture properties are calculated, and temperature tables are created for thermodynamic properties based on the PG or IG model. This table is interpolated for any temperature-dependent property. The rest of the solution follows the IG or PG model algorithm. Note that by entering a value of 1 or 0 for the mass or mole fraction of A, the mixture can be made to consist purely of A or B.

The RG/RG model converts a binary mixture of real gases into an equivalent pure real gas by applying Kay's rule [26] to calculate critical properties for the mixture, based on the mole fraction of the two components. Since the mixture is treated as a pure real gas, the rest of the algorithm follows the procedure of the RG model.

The PC/PC model allows evaluation of a state of premixed blends of refrigerants. The PC state daemons handle such blends indicated by a percent symbol after the fluid name. For example, selecting R-410a% displays its composition as a 50–50 blend of R-32 and R-125 on the message panel. The vapor pressure for a saturated mixture is a function, not only of temperature, but also of the quality x of the mixture. This behavior is captured by using separate data for saturated liquid and saturated vapor and interpolating those data for a mixture. The rest of the algorithm follows that of the standard PC model.

Moist air is a mixture of dry air and water vapor and is an important working fluid in HVAC applications. Because of the

low partial pressure of water vapor and the relatively moderate change in temperature in most applications, water vapor can be treated as a perfect gas. However, the possibility of condensation or evaporation requires saturation data of water. The resulting model is called the MA (moist air) model, which is a modified PG/PG model. The MA state daemons introduce a number of psychrometric properties – p_v , p_a , p_g , ω , ϕ , T_{dp} , T_{wb} – in addition to the mixture properties, which are expressed per unit mass of dry air following the psychrometric convention.

The algorithm for finding a moist air state is straightforward since the mixture of dry air and water vapor can be treated using the Dalton model. Once the partial pressure of water vapor is determined, the rest of the psychrometric properties can be readily evaluated from their definitions. Saturation data for water and ice is downloaded by the MA state daemons. States can be calculated down to -40 °C at any total pressure. The MA model can also be used to determine states of twelve other moist gases including moist carbon dioxide, moist hydrogen, moist oxygen, etc. Psychrometric applications often require evaluation of states of condensed water, saturated steam, and various refrigerants. The MA state daemons, therefore, also include the PC model algorithms.

Fig. 10 displays a screenshot of the MA system state daemon where the working substance selector can be seen to contain a list of moist gases as well as PC fluids such as water and different refrigerants. In Fig. 10, properties x and y are disabled because moist air is selected. When a PC fluid is selected, the psychrometric properties are similarly disabled. The daemon in Fig. 10 calculates the mass of water vapor in a given volume of moist air at a given temperature, pressure, and relative humidity. The psychrometric plot of the calculated state is shown in Fig. 11 where constant wet bulb temperature and constant relative humidity lines through the calculated states are superimposed. By moving the pointer to the intersection of the $T_{wb} = c$ and $\phi = 100\%$ lines, the wet bulb temperature can be obtained from the coordinates displayed on the plot.

Finally, the general mixture model called the n-IG model can be used to evaluate mixture states of any number of ideal gases. A screen shot of the n-IG system state daemon is shown in Fig. 12. The mixture is configured by specifying the amount (in kg, kmol, mass fraction, or mole fraction) of each component. When the first



Fig. 11. As in any thermodynamic plot, constant property lines can be drawn on a psychrometric plot. In this figure, the wet bulb temperature for state-1 computed in Fig. 10 can be deduced by parking the pointer over the intersection of the constant T_{wb} line and the saturation line (shown by the arrow).

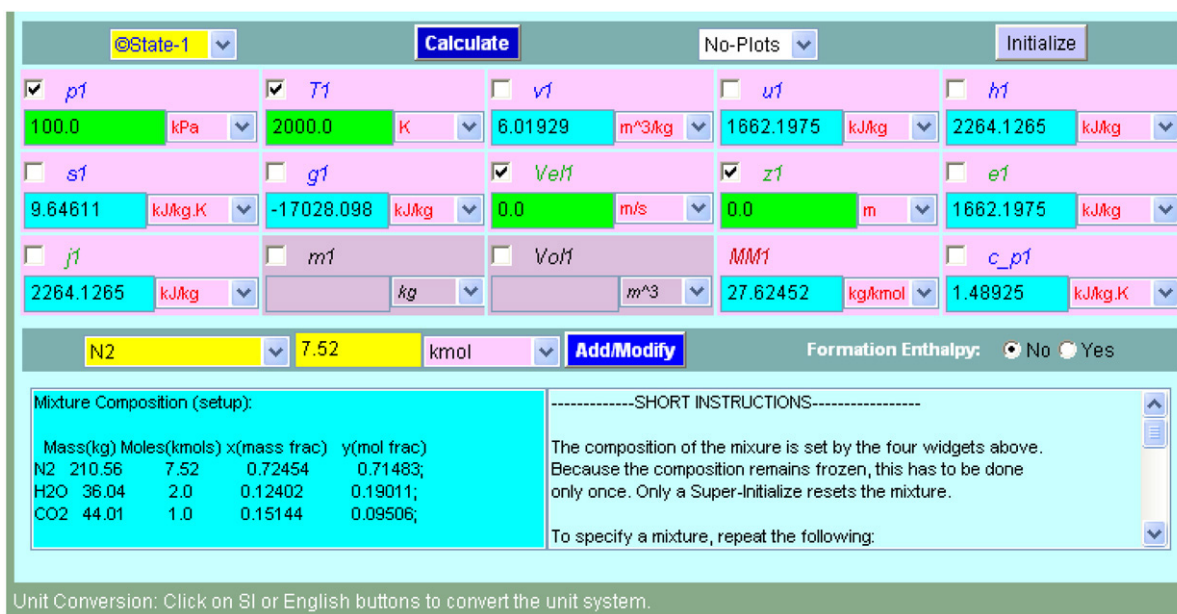


Fig. 12. Image of the n-IG system state daemon evaluating the state of a gas mixture composed of 1 kmol of CO_2 , 2 kmol of H_2O , and 7.52 kmol of N_2 .

component is selected, a mixture gas table is created, based on the material properties and Shomate polynomials of the selected gas. As a new component is added, mixture composition properties are updated and the mixture property table is modified by including a contribution from the newly added species. Once the mixture is fully configured, a state can be evaluated by following the same procedure used in the IG daemons. Note that formation enthalpy can be included or neglected in the state calculation.

3. Examples

A wide range of states involving working substances frequently encountered in engineering applications can be evaluated using the state daemons. In the TEST portal, Chapter 3 of the Problems module contains a number of problems and examples of state evaluation. TEST-codes are posted for each problem so the visual solution can be reproduced. Because of the intuitive user interface,

evaluating a state involves launching the appropriate daemon, entering the known properties in any unit, clicking the *Calculate* button, and then selecting a plot option.

4. Conclusions

Thermodynamic property calculators called *state daemons* for the evaluation of properties of engineering working substances are presented in this paper. These daemons can be browsed online or installed locally from CD to run in a stand-alone mode. The range of substances covered by these daemons include solids, liquids, ideal gases, real fluids with a possibility of phase change, mixture of gases, mixture of real fluids, and moist air. Twelve different models have been developed to capture the behavior of this diverse range of substances. An intuitive graphical user interface has been uniformly implemented for each of these models. To calculate a state, a user simply enters the independent properties in any available unit and then presses the *Calculate* button. A powerful thermodynamic plotter can then display calculated states in any desired thermodynamic diagram and allow the user to draw constant property lines on the plot.

Algebraic expressions can be used to relate one state with another, making it possible to compute a series of states in a cycle. Because the GUI visually exposes every property, so called *what-if* studies can be easily carried out by changing a property and then updating the entire solution. The visual solution can be converted into a few lines of TEST-code which specify the input properties in C language similar syntax. TEST-codes can be saved and reused later to regenerate a visual solution by simply pasting and loading the codes in a daemon's I/O panel.

Efforts are currently underway to deliver these state calculators through Web Services to client side commercial applications such as Microsoft Excel and MATLAB and programming languages such as FORTRAN and Java. State calculators then can be easily integrated into a variety of existing and future applications.

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