A MATLAB Toolbox for Thermodynamic Property Evaluation

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I. Introduction

MATLAB has become the technical computing language of choice for the mechanical systems courses in the Department of Mechanical Engineering at Michigan State University. It is used extensively in the undergraduate controls and vibrations courses, as well as several technical electives. With the addition of toolboxes in optimization, signal processing, and controls system, it is truly a powerful tool for analysis in the mechanical systems area. Recently, it has become the structured programming language taught in the freshman engineering computer course at MSU. Unfortunately, the thermal/fluids area has not been able to utilize MATLAB as effectively due to the lack of property evaluation functions. Calculations in thermodynamics, fluid mechanics, and heat transfer rely heavily on the evaluation of thermophysical properties, and without property functions, MATLAB will surely continue to be underutilized in the thermal/fluids area. To address this deficiency, the Thermal Engineering Computer Aided Design (TECAD) group at MSU has developed a thermodynamics property toolbox for MATLAB.

The Thermodynamic Property Toolbox consists of MATLAB functions for the evaluation of thermodynamic properties for several ideal gases, four compressible substances, and three incompressible substances. Both direct functions, such as calculating enthalpy given the temperature and pressure, and inverse functions, such as calculating the temperature given the pressure and enthalpy, are available. As pseudo code functions they may be called directly from the MATLAB workspace or incorporated into other script file programs. A graphical user interface tool has also been developed which allows for interactive property evaluation. Once the type of substance has been determined, the user identifies the two known intensive properties required to fix the state. The GUI then displays the remaining properties. The presentation of the GUI enhances the student's understanding of the methodology of property evaluation and the decision making process that is intricate to the procedure.

This paper continues with some background on the property evaluation for the substance types considered. Next the MATLAB property functions are introduced, followed by a presentation of the MATLAB GUI's. The paper concludes with some observations concerning the development of the MATALB functions and their use.

II. Property Evaluation Background

For an introductory course in thermodynamics, it is often assumed that the world can be divided up into three types of substances

Ideal Gases
Incompressible Substances
Compressible Substances

Each substance has its own mathematical models used to evaluated the properties.

For ideal gases the first of these models is the ideal gas law

$$Pv = RT \tag{1}$$

For the remaining properties we may use

$$\hat{u} - \hat{u}_o = \int c_v dT = \int (c_P - R) dT \tag{2}$$

$$\hat{h} - \hat{h}_o = \int c_P dT \tag{3}$$

$$\hat{s} - \hat{s}_o = \int \frac{c_P}{T} dT - \int \frac{R}{P} dP \tag{4}$$

To carry our these integrals, we must have a functional form of c_P in terms of temperature. The specific heats are evaluated using the polynomial expressions provided by Van Wylen and Sontag [1].

For an incompressible substance, we note that the density must behave as

$$\rho = \text{fn}(T) \text{ only} \tag{5}$$

The remaining properties are governed by

$$\hat{u} - \hat{u}_o = \int c_P dT \tag{6}$$

$$\hat{h} - \hat{h}_o = \int c_P dT + \int v dP \tag{7}$$

$$\hat{s} - \hat{s}_o = \int \frac{c_P}{T} dT \tag{8}$$

For the case of an incompressible substance both the density and specific must be represented by a function of temperature. For the incompressible substances available in the MATLAB toolbox, the data for density and specific heat came from Cengel [2] and was curve fitted using Excel.

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Concerning the compressible substance property evaluation, the steam property functions were obtained by converting the FORTRAN steam functions of RANKINE [3] into MATLAB. The two refrigerants provided in the compressible substance toolbox were evaluated from the formulas and data provided in Reynolds [4].

III. MATLAB Property Functions

Using the property evaluation stated above a series of MATLAB property functions were written as script files for each substance type. Table 1 show the functions available for ideal gases.

The parameter IGAS identifies the specific ideal gas as shown below:

> IGAS = 0: air
> IGAS = 1: N_2
> IGAS = 2: O_2
> IGAS = 3: H_2
> IGAS = 4: CO
> IGAS = 5: OH
> IGAS = 6: NO
> IGAS = 7: H_2O
> IGAS = 8: CO_2

The parameter IMS indicates if the properties are on a per mass basis (IMS = 0) or on a per mole basis (IMS = 1).

For compressible substance property evaluation there is only one function used, CompSub(ISTM,T,P,v,h,s,u,Q,L,IFLD). To use the function in a MATLAB script file, the general form of the function call is

[T,P,v,h,s,Q,L]=CompSub(ISTM,T,P,v,h,s,Q,L,IFLD)

All variables in the argument-in list (in the parentheses following steam) must have been previously defined in the program. These variables are defined as follows:

ISTM: Integer flag that controls what thermodynamic variables are treated as known and which ones are unknown. It should be assigned a value of 1, 2, 3, 4, or 5 depending on the known and unknown properties.

> ISTM=1 - Calculates h, s, v given T,P, L, and Q. If L is set to -1, the fluid phase will be determined. If the temperature is equal to the saturation temperature at the specified pressure, the fluid phase is assumed to be saturated liquid.
> ISTM = 2 - Calculates P, h, s, and v given T, L, and Q. Used primarily for a two phase mixture when the temperature is known.
> ISTM = 3 - Calculates T, h, s, and v given P, L, and Q. Used primarily for a two phase mixture when the pressure is known.

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Table 1. MATLAB Thermodynamic Property Functions for Ideal Gases

Function	Property Evaluated	Required Inputs
CP(T,IGAS,IMS)	Specific Heat at Constant Pressure	Temperature
CV(T,IGAS,IMS)	Specific Heat at Constant Volume	Temperature
HT(T,IGAS,IMS)	Enthalpy	Temperature
PST(S,T,IGAS,IMS)	Pressure	Entropy and Temperature
PSV(S,V,IGAS,IMS)	Pressure	Entropy and Specific Volume
PTV(T,V,IGAS)	Pressure	Temperature and Specific Volume
STP(T,P,IGAS,IMS)	Entropy	Temperature and Pressure
STV(T,V,IGAS,IMS)	Entropy	Temperature and Specific Volume
TH(H,IGAS,IMS)	Temperature	Enthalpy
TPV(P,V,IGAS)	Temperature	Pressure and Specific Volume
TSP(S,P,IGAS,IMS)	Temperature	Entropy and Pressure
TSV(S,V,IGAS,IMS)	Temperature	Entropy and Specific Volume
TU(U,IGAS,IMS)	Temperature	Internal Energy
UT(T,IGAS,IMS)	Internal Energy	Temperature
VSP(S,P,IGAS,IMS)	Specific Volume	Entropy and Pressure
VST(S,T,IGAS,IMS)	Specific Volume	Entropy and Temperature
VTP(T,P,IGAS)	Specific Volume	Temperature and Pressure

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ISTM = 4 - Calculates T, h, v, L, and Q given P and s. Used primarily for a state following an isentropic process.
ISTM = 5 - Calculates T, s, v, L, and Q given P and h.

T: Temperature in degrees Celsius (°C).

P: Pressure in MPa.

v: Specific volume in m^3/kg.

h: Enthalpy in kJ/kg.

s: Entropy in kJ/(kg·K).

Q: Quality of steam. Q = -1 when quality is not applicable, e.g. for superheated vapor or subcooled liquid.

L: Fluid phase index. Gives the fluid phase of the steam as follows:

L = -1	Unknown
L = 1	Subcooled Liquid
L = 2	Two Phase Mixture
L = 3	Superheated Vapor
L = 4	Saturated Liquid
L = 5	Saturated Vapor

IFLD: Indicates the compressible substance for which the evaluation is being done.

IFLD =1 for steam
IFLD = 2 for Refrigerant-12
IFLD = 3 for Refrigerant-22

There are twelve (12) functions of incompressible substance properties that are available. Also there is one function, **Constants_IC.m**, that is only used internally. The twelve property functions are summarized below.

v_T_IC(T,IFLD): Calculates specific volume for liquid water corresponding to the given temperature (T).

T_v_IC(v,IFLD): Calculates temperature of liquid water corresponding to the specific volume (v).

cP_T_IC(T,IFLD): Calculates specific heat for liquid water corresponding to the given temperature (T).

h_TP_IC(T,P,IFLD): Calculates enthalpy for liquid water corresponding to the given temperature (T) and the given pressure (P).

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T_hP_IC(h,P,IFLD): Calculates temperature of liquid water corresponding to the given enthalpy (h) and the given pressure (P).

P_hT_IC(h,TP,IFLD): Calculates pressure of liquid water corresponding to the given enthalpy (h) and the given temperature (T).

u_T_IC(T,IFLD): Calculates internal energy for liquid water corresponding the given temperature (T).

T_u_IC(u,IFLD): Calculates temperature of liquid water corresponding to the given internal energy (u).

s_T_IC(T,IFLD): Calculates the entropy for liquid water corresponding to the given temperature (T).

T_s_IC(s,IFLD): Calculates temperature of liquid water corresponding to the given entropy (s).

Psat_T_IC(T,IFLD): Calculates saturation pressure of water corresponding to the given temperature (T).

Den_T_IC(T,IFLD): Calculates density for liquid water corresponding to the given temperature (T).

IFLD: Indicates the incompressible substance for which the property evaluation is being done.
>   IFLD = 1 is for liquid water
>   IFLD = 2 is for ethylene glycol
>   IFLD = 3: is for engine oil

Note that there is a pattern to the function names. The characters before the first underscore (_) represent the property being calculated, e.g., h for enthalpy, v for specific volume, etc. The characters after the first underscore represent the properties that must be specified, e.g., s for entropy, TP for temperature and pressure. The IC denotes that the substance is an incompressible substance.

As an example of using these functions in a thermodynamics calculation, see Figure 1, where a simple, ideal air compressor calculation is performed.

IV. Demonstration of MATLAB GUI's

To perform interactive property calculations four MATLAB GUI's have been developed. The guide command in MATLAB was used, which allows for a drop and drag approach to the development of the graphical user interface. Figure 2 is the main GUI and requires the user to specify the substance type. Figures 3-5 are specific to the substance type, though they have a

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Figure 1. Example Script File Using the Ideal Gas MATLAB Functions

```
S1 = STP(T1,P1,0,0)
H1 = HT(T1,0,0)
S2 = S1
T2 = TSP(S2,P2,0,0)
H2 = HT(T2,0,0)
WIDEAL = H1 - H2
```

where the inlet temperature and pressure (T1 and P1) and the exit pressure (P2) have been specified by the user.

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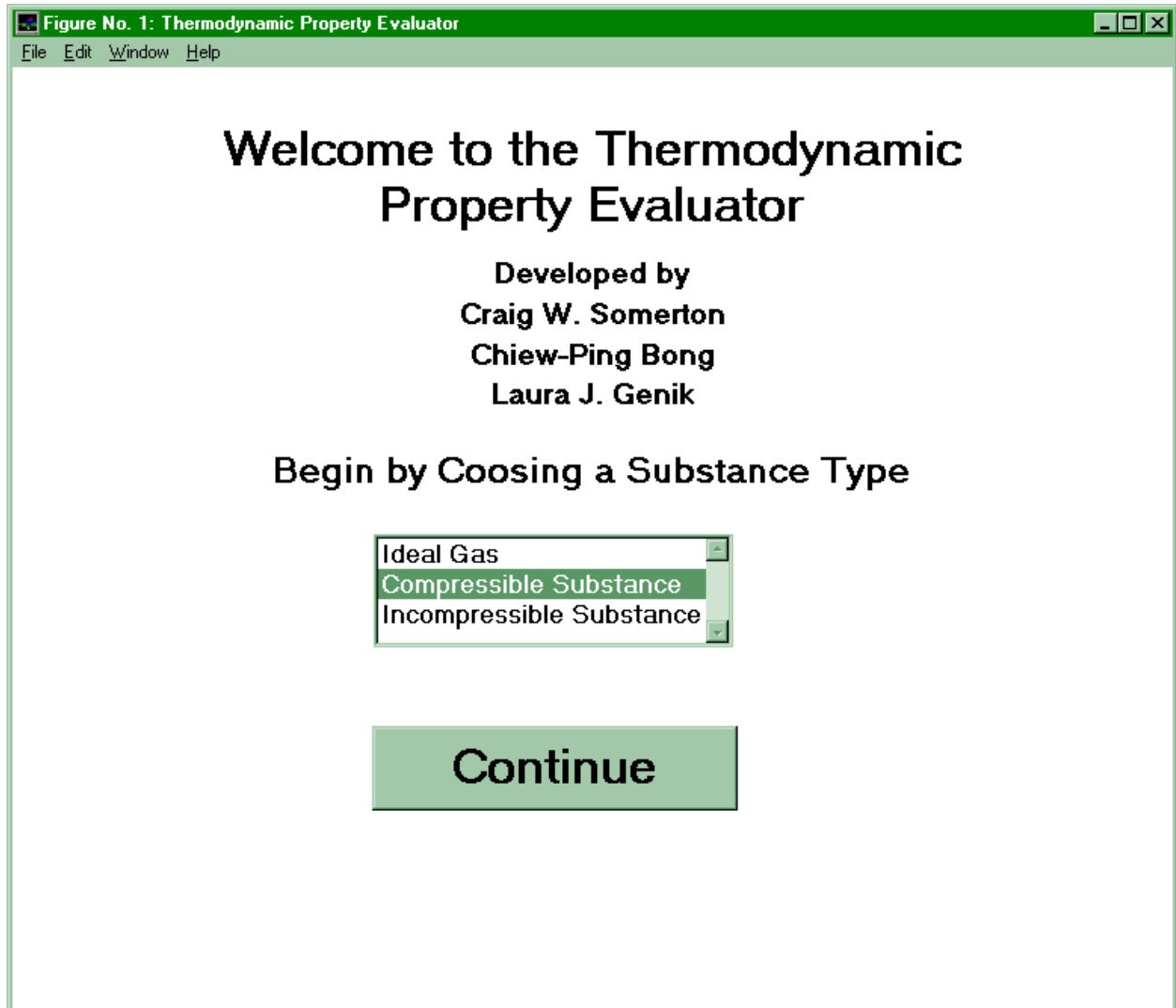Figure 2. Main MATLAB Thermodynamic Property Evaluation GUI

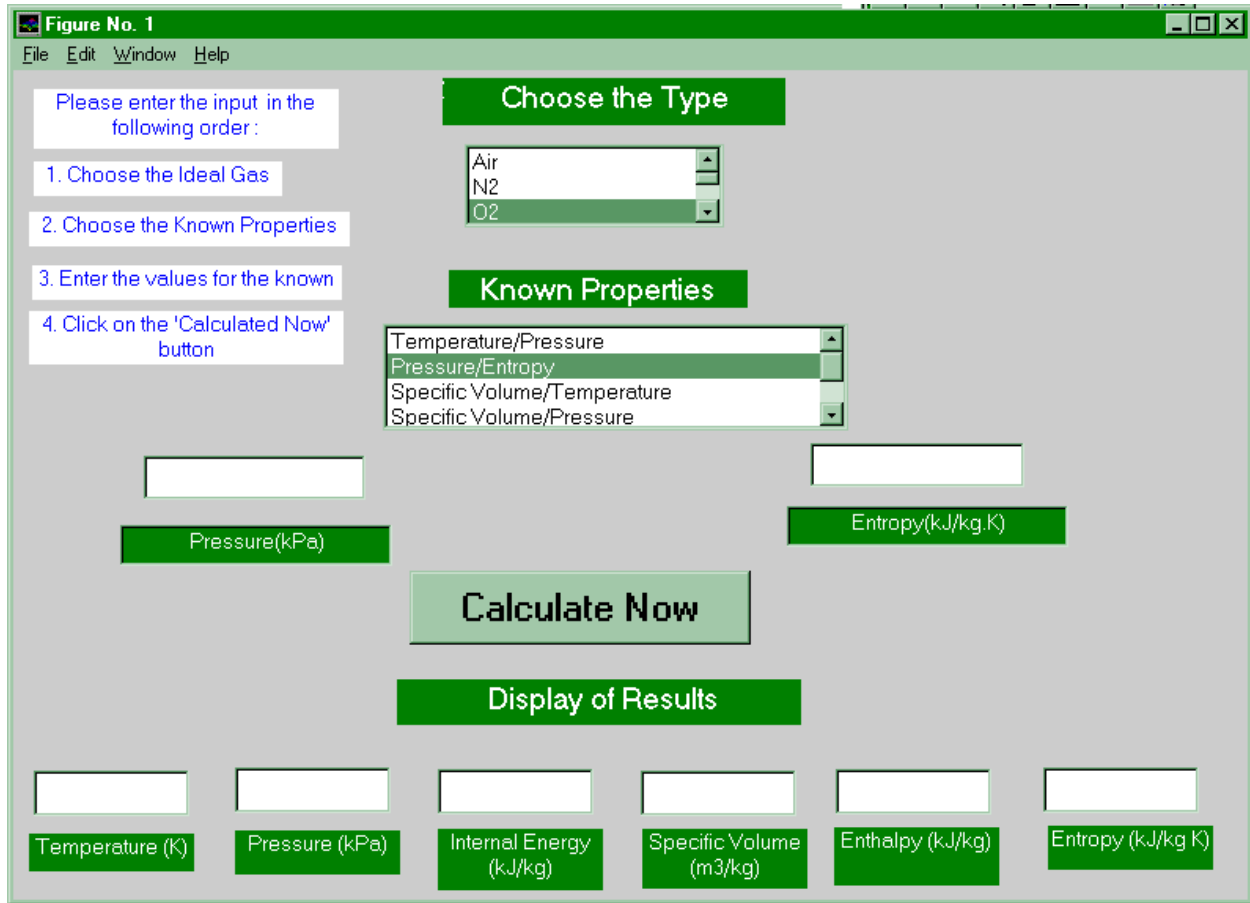Figure 3. MATLAB Thermodynamic Property Evaluation GUI for Ideal Gases

Figure 4. MATLAB Thermodynamic Property Evaluation GUI for Incompressible Substances
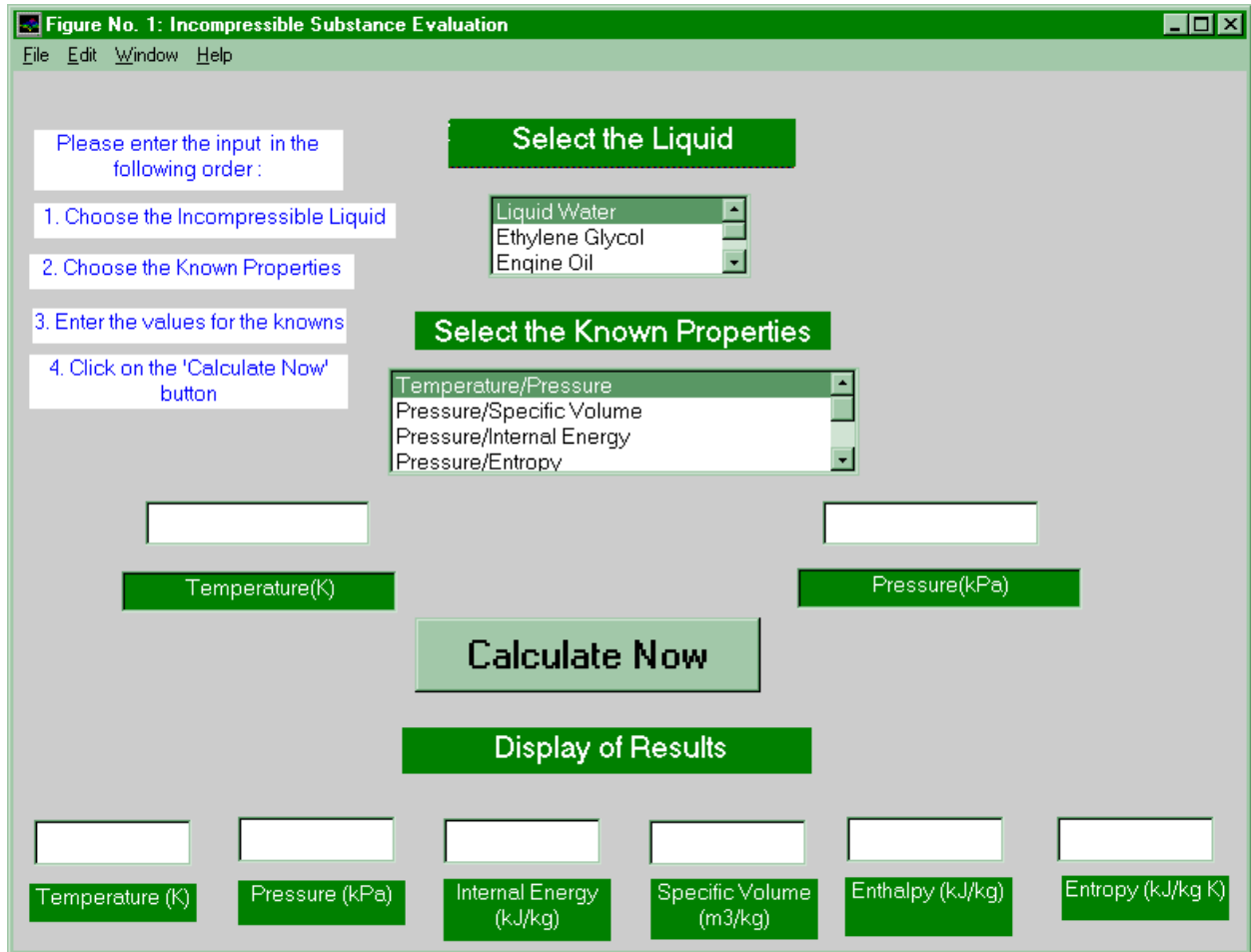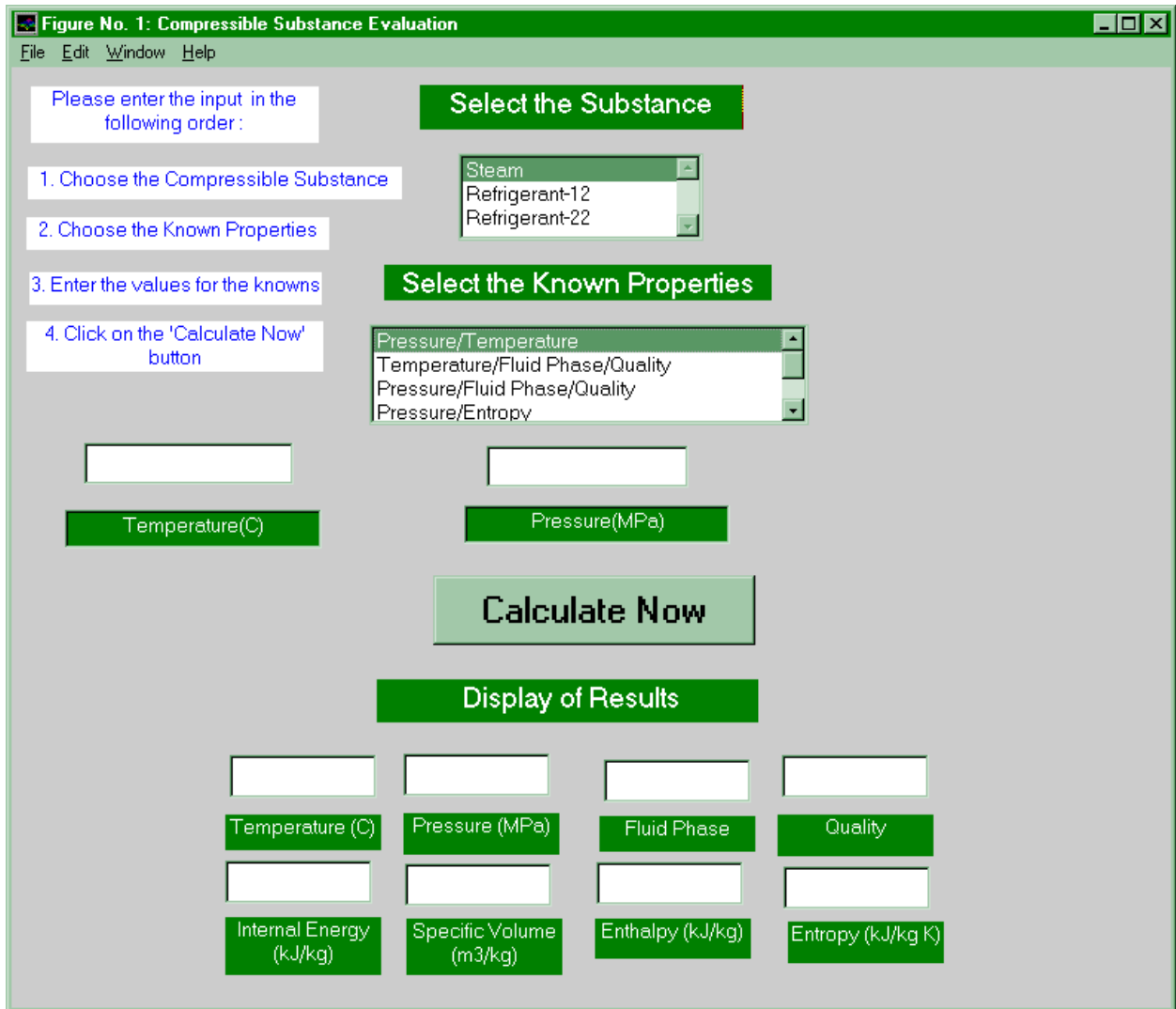
Figure 5. MATLAB Thermodynamic Property Evaluation GUI for Compressible Substances

similar appearance. Using a list box the user indicates the specific substance of interest. Next the known properties are indicated on a list box. The numerical values of the known properties are entered in the appropriate text boxes. The user then clicks on the Calculate Now push button, and the remaining properties are calculated and displayed.

V. Conclusions

Thermodynamic property functions for a number of substances have been developed for use in MATLAB. This includes graphical users interfaces that can be used for interactive property evaluation. All of these functions and GUI's are available for download at the Thermal Engineering Computer Aided Design (TECAD) homepage in the Department of Mechanical Engineering at Michigan State University. The URL address is

$$\text{http://www.egr.msu.edu/~somerton/TECAD.}$$

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