

User guide for Matlab class thermo

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The Matlab m-files mentioned in this note are all available from GitHub:

<https://github.com/are-mj/thermodynamics>.

Several authors have used methods developed at Ruhr-Universität Bochum (Setzmann & Wagner, 1989) to design high accuracy models for the thermodynamic properties of single-component fluids. These models calculate the molar Helmholtz free energy as a function of temperature T and molar volume v , in a form that allows explicit expressions for all partial derivatives of arbitrary order. These models all have largely the same structure and can be calculated using the same Matlab function (`helmholtz.m`), but with separate parameter sets for the different fluids.

The thermo class and object

The purpose of the Matlab class thermo is to provide a flexible and efficient interface to the `helmholtz` function and to enable efficient methods for solving a range of thermodynamic problems. A Matlab class contains the code for creating one or more Matlab objects. A thermo object is created by calling the class with the name of an available fluid. Example:

```
>> th1 = thermo('O2');  
>> th2 = thermo('H2');
```

A call to `thermo` creates a thermo object, reads the appropriate parameter file and stores the parameters as *properties* of the object. The object also contains *methods* for calculating thermodynamic variables. Note that for a single-component fluid, two independent thermodynamic variables will uniquely determine the *thermodynamic state* and thus all thermodynamic properties.

For a full list of available properties, type:

```
>> thermo.properties
```

For a list of functions available in the thermo object, type:

```
>> thermo.methods
```

Derivative order

The property `max_order` controls the maximum order of partial derivatives of the Helmholtz free energy $f(T, v)$ to be calculated. The default is 2, as nearly all thermodynamic variables may be expressed in terms of these values. However, sometimes we need derivatives of order 3, for example to find analytical Jacobians to use with Newton's method. Setting `max_order` to 3 will force these values to be calculated, at the expense of slightly longer calculation times.

Thermodynamic methods of the thermo object

Tvcalc

The basic method is Tvcalc. A call to the method Tvalc calls the helmholtz function with temperature and molar volume as arguments. The Helmholtz function returns the Helmholtz free energy and its partial derivatives up to order two or three. (Two is the default). It stores these values as object properties together with a number of calculated thermodynamic variables. All variables are in SI units, with the exception that kmol is used instead of mol. For a temperature of 300K and a molar volume of 24 kmol/m³ we write:

```
th1.Tvcalc(300,24)
```

All variables are can be accessed as needed with no extra calculations:

```
>> th1.p          % Pressure (Pa)
ans =
    1.0386e+05
>> th1.c          % Speed of sound (m/s)
ans =
    329.725
```

Tpcalc

In many practical situations the temperature and pressure are known, not molar volume. The method Tpcalc uses repeated calls to Tvcalc to find the molar volume that gives the desired pressure :

```
th2.Tpcalc(300,101325)
```

Let us check:

```
>> th2.p
ans =
    1.0133e+05 % Displays 101325 rounded to five digits
>> th2.v
ans =
    24.6318
```

The Tpcalc method uses Newton's method to find the correct value of the molar volume v . Normally the search converges very fast since the value of the derivative of p with respect to v (at constant T) is always available in the thermo object.

phcalc and pscalc

These two methods find the temperature and molar volume that results in given values for pressure and either molar enthalpy or entropy, respectively. They are less robust than Tpcalc, but will converge fast given good initial values.

saturation

The thermo method saturation returns the liquid-vapour saturation pressure for a given temperature, as well as the corresponding liquid molar volumes of saturated liquid and vapour. Example:

```
>> [ps,vl,vv] = th.saturation(373.1243)
ps =
    1.0133e+05
vl =
     0.0188
vv =
    30.1467
```

(Since the adoption of a new International Temperature Scale in 1990, the boiling point of water is slightly below 100°C.)

Note that the saturation method is not available for all species.

Object vs. separate function calls

Some user may find it conceptually easier to have separate functions for each thermodynamic variable, for instance:

```
h = enthalpy(T,p,'H2')
```

rather than

```
th2 = thermo('H2');
th2.Tpcalc(T,p)
h = th2.h
```

The advantage of the latter approach is that complex calculations need not be repeated if we need more than one property at a given (T, p) pair. Without extra function calls we can get, for example, the heat capacity at constant pressure and the speed of sound:

```
>> fprintf('Heat capacity: %.0f J/K/mol\n',th.cp)
Heat capacity: 28853 J/K/mol
>> fprintf('Speed of sound: %4.0f m/s\n',th.c)
Speed of sound: 1319 m/s
```

Other thermodynamic functions

A number of functions are available as separate Matlab m-files

`choked_flow.m`

State of choked gas flow, given upstream stagnation conditions.
Assumes isentropic process and no condensation.

`compressor.m`

Outlet conditions from gas compressor

`twophase_tank_rhs.m`

Right-hand side for ODE system solving mass and energy balance and phase equilibrium for a two-phase tank being filled or emptied.

`shocktube.m`

`shocktube_ig.m`

See also: `demo_shocktube.m`

Pressures and temperatures in idealised shock tube for real and ideal gas

`shock_from_mach.m`

`shock_from_pressure.m`

`shock_from_velocity.m`

Calculate shock for real gases with various input variables

Demo files

`demo_gas_tank_system.m`

Simple simulation of filling a gas tank from another tank

`twophase_region.m`

Plot phase envelope and isotherms in a p-v plot

`demo_shocktube.m`

Calculate shock tube temperatures and pressures for a range of initial pressures

Parameter files

Parameters for selected species

`parameters_Air.m`

Air treated as a single species. Single-phase only. (Lemmon, Jacobsen, Penoncello, & Friend, 2000)

`parameters_Ar.m`

Argon. Single-phase only. (Tegeler, Span, & Wagner, 1999)

`parameters_CO2.m`

Carbon dioxide. Gas and liquid. (Span & Wagner, 1996)

`parameters_H2O.m`

Water and steam. (Wagner & Pruss, 2002)

`parameters_O2.m`

Oxygen. Single-phase only. (Lemmon, Jacobsen, Penoncello, & Friend, 2000)

`parameters_N2.m`

Nitrogen. Single-phase only. (Lemmon, Jacobsen, Penoncello, & Friend, 2000)

`parameters_H2.m`

`parameters_paraH2.m`

`parameters_orthoH2.m`

Hydrogen. Gas and liquid. (Leachman, Jacobsen, Penoncello, & Lemmon, 2009)

Parahydrogen and orthohydrogen are “spin isomers”. These are relevant for liquid and low temperature gas. The first file is for normal H₂, which is the equilibrium combination at room temperature and higher: 75% orthohydrogen and 25% parahydrogen. See [Wikipedia](#) and (Leachman J. , 2015)

Utility functions

`newton.m`

Solver for nonlinear equation systems using Newton’s method.

References

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