Short user guide for Matlab class thermo

Class thermo

Objects of the thermo class are suited for efficient and accurate calculation of thermodynamic variables and calculations. It requires a model of the molar Helmholtz .free energy as a function of temperature and molar volume. At present such models are available for H_2 H_2O, and CO_2.

The user starts by creating a `thermo` object:

```
>> th = thermo('H2');
>> th = thermo('H2O');
```
or
```
>> th = thermo('CO2');
```

`thermo` reads in parameters for the given species from the relevant parameter file (e.g. H2parameters.m) . Next the thermodynamic state of object must be initialised by specifying the temperature and either molar volume or pressure. Examples:

```
>> th.Tvcalc(300,0.5)

>> th.Tpcalc(300,250e5)
```

`th.Tvcalc` uses the model in `helmholtz.m` to calculate the molar Helmholtz free energy and its partial derivatives with respect to temperature T and molar volume v. It then populates the object with those derivatives as well as a set of thermodynamic properties such as molar enthalpy (`th.h`) and speed of sound (`th.c`). For a full list of properties, type

```
>> th.properties
```

Since the model is explicit in T and v, `th.Tvcalc` is fast and robust.

`th.Tpcalc` uses Newton's method to iterate on v to solve $p(T, v) = p$. Example for H_2:

```
>> th.Tpcalc(300,250e5)
>> fprintf('Speed of sound : %4.0f m/s\n',th.c)
Speed of sound : 1537 m/s
```

`th.Tpcalc` is quite fast and is robust except near the two-phase region. Here one should specify a relevant initial value for the molar volume.

A full list of methods available from the thermodynamic object is shown by typing:

```
>> th.methods
```

Type help thermo.<method> for method help text. Example:

```
>> help thermo.Tpcalc
  Tpcalc(T,p,v0) : Solves of p(T,v) = p by Newton's method
  v0: optional starting point for iteration. Default: Ideal gas value
```

Derivative order

By default, thermo calculates derivatives up to order two. Setting the property max_order to 3 forces the calculation of third order derivatives, at the cost of a longer calculation time. Example:

```
>> th = thermo('H2O');
>> th.Tpcalc(400,1e5);th.f_TTT
ans =
     []
>> th.max_order=3;th.Tpcalc(400,1e5);th.f_TTT
ans =
    0.2000
>> T = linspace(400,500);v = linspace(10,40);
>> tic;for i = 1:100;th.Tvcalc(T(i),v(i));end;toc
Elapsed time is 0.025994 seconds.
>> th.max_order=2;
>> tic;for i = 1:100;th.Tvcalc(T(i),v(i));end;toc
Elapsed time is 0.013975 seconds.
```

Third order derivatives are sometimes needed to calculate jacobians for solving problems involving second order derivatives.

Saturation properties

The parameter files for include model parameters for the saturation pressure as a function of temperature. These models are compatible with the Helmholtz model. Syntax:

```
>> [ps,dpdT,vl,vv] = th.saturation(T);
```

To find other saturated properties, use Tvcalc.
Example: Find the liquid speed of sound for H_2O at 400K:

```
>> T = 400;
>> [ps,dpdT,vl,vv] = th.saturation(T);
>> th.Tvcalc(T,vl)
>> th.c
ans =
   1.5095e+03
```

(Note that this is the speed of sound assuming that no phase change takes place. The two-phase speed of sound is lower.)

For convenience, we also include the file psat.m, which can handle an array of T values, unlike thermo.saturation. Convenient for plotting the saturation curve.

Units

SI units are used throughout; with the exception that kmol is used instead of mol. Intrinsic variables are on a per kmol basis. Properties per kg are found by dividing by th.Mw.

Matlab applications

A small number of application cases are shipped together with the thermodynamic model:

`demo_fill_gas_tank.m`:
Pressure and temperature histories when filling of a H_2 gas tank at a constant rate.

`demo_gas_tank_system.m`:
Pressure and temperature histories when filling gas from one tank into another.

`demo_tank_leak.m`:
Leak from the vapour phase of a liquid H_2 tank. Demonstrates vapour/liquid equilibrium and both sonic (choked) and subsonic flow.

`twophase_region.m`:
Plots the two-phase envelope and selected isotherms in a v-p diagram.