Introduction to the use of MediumModel class on Matlab

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The MediumModel class is used for finding the equilibrium state of a mixture of reacting ideal gases over a range of temperatures, pressures and compositions. It can calculate various properies of individual gases and gas mixtures such and entropy and enthalpy. It can also plot equilibrium composition against temperature and includes methods to calculate and plot Gibbs free energy.

The model uses data compiled by NASA in the paper: NASA Glenn Coefficients for Calculating Thermodynamic Properties of Individual Species.

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http://www.grc.nasa.gov/WWW/CEAWeb/TP-2002-211556.pdf

Instantiating a MediumModel Object

```
Example1 = MediumModel({'H2O'})
```

```
Example1 = 

  MediumModel handle

  Properties:
             gas: [1x1 struct]
           names: {'H2O'}
            cp_V: [801x1 double]
             h_V: [801x1 double]
             s_V: [801x1 double]
            mu_V: [801x1 double]
              cp: [801x1 double]
               h: [801x1 double]
               s: [801x1 double]
              mu: [801x1 double]
            mm_V: 18.0153
              mm: [801x1 double]
           index: [1x1 struct]
           ln_kc: []
              nu: []
```

```
         Zeq: [801x1 double]
         aeq: [801x1 double]
           P: 100000
          P0: 100000
           Z: 1
           X: [1x801 double]
           T: [801x1 double]
notCondensed: 1
```

In this example, the model has only a single species. Later examples include more complex systems.

Class Properties

The model uses the strMaster database, stored in the IdealGases file to find the relevant values using polynomial approximations, as found by NASA, over the required temperature range.

Defined by the user: *(Using standard SI units)*

- **T** - Temperature Range (Kelvin) *Default - 801 values, ranging from 273.15K to 1073.15K*
- **Z** - Initial molar fractions of each species *Default-equal molar proportions*
- **X** - Initial mass fractions of each species. *This is calculated if Z is specified and vice versa*
- **nu** - Stochiometry of defined chemical equations. *Empty by default*
- **P0** -Atmospheric Pressure (Pascals) *Default - 100,000Pa*
- **P** -Pressure of reaction (Pascals) *Default - 100,000Pa*

Calculated based on user inputs: (All of these are matrices of values over the temperature range)

- **cp / cp_V** - Specific heat capacity (J/mol K)
- **h / h_V** - Specific enthalpy (J/mol)
- **s / s_V** - Specific entropy (J/mol.K)
- **mu / mu_V** - Chemical potential (J/mol)
- **mm / mm_V** - Molar mass (g/mol)
- **Zeq** - Molar fractions of each species at equilibrium over the temperature range

The '_V' element of the parameters such as cp_V indicates that it is a vector. It differs from cp by that cp is the specific heat capacity of the mixture as a whole, while cp_V is a matrix showing the specific heat capacity of each individual species. Zeq is calculated after calling the SolveEq method, the others are properties obtained from the IdealGases database polynomial approximations.

Class Methods

Methods are used in the class to set values of properties, perform calculations and plot graphs:

Value setting methods

- **setT**-*sets the object temperature range*
- **setPandP0**-*sets the reaction and atmospheric pressures respectively*
- **setNu**-*sets the object's chemical reation stochiometry*
- **setZ**-*sets the object's composition by moles*
- **setX**-*sets the object's composition by mass*

These methods are called form `object.setT([300 350 400])`. Examples on how to use each one individually are given in Example 2

Calculation methods

- **gibbs**- *uses the Gibbs equation, g=h-Ts to calculate the lowest free energy state for the gas mixture.*
- **solveEq**- *solves the relevant equations to find the equilibrium proportions so the end results can be plotted.*
- **props**- *uses to access the IdealGases database and uses the polynomial approximations to find the values of cp, h and s for the gases.*
- **moleToMassFractions**- *calculates relevant value by mass, if the user specifies values by moles*
- **massToMoleFractions**- *vice-versa*
- **findTFromH**- *calculates temperatures when enthalpies are specified*

`gibbs` and `solveEq` are excecuted in Example2 and Example3 below. The remaining calculation methods are internal methods that aren't directly called by the user. `moleToMassFractions, massToMoleFractions` and `findTFromH` convert from one property to another as described, depending on which properties were initially defined by the user.

Graph plotting Methods

- plot
- gibbsplot

`plot` plots 4 graphs in one window, plotting each gas's cp, h, s and composition against temperature over the temperature range. `gibbsplot` produces two graphs, plotting free energy and equilibrium constant against temperature. `gibbsplot` is used in example2. `plot` is used in example3.

Modelling Reaction Systems

This example is a model of the Haber process reaction, used for making ammonia. The model will be used to find the resulting proportions of each gas at equilibrium during the reaction process over the temperature range -50- to 500°C

```
Example2 = MediumModel({'N2', 'H2', 'NH3'});
```

This creates an object with the specified species included in the model, and must include all products and reactants.

Specify reaction conditions

The class requires 4 parameters to calculate how any reaction is expected to progress: Initial composition, stochiometry, temperature and pressure.

setZ (Composition)

The initial proportions of the species can be set by mass or molar relations. This example uses molar fractions. (Z)

```
Example2.setZ ([0.25, 0.75, 0]);
```

The proportions are defined in the same order as they are given in the class definition, as stored by the 'names' property and must sum to 1.00. (This example has 25% Nitrogen, 75% Hydrogen, 0% Ammonia)

setNu (Stochiometry)

The stochiometry of the chemical reactions must be specified in the model. In the example of the Haber process, the relevant reaction is:

$$N_2 + 3H_2 \leftrightarrow 2NH_3$$

```
Example2.setNu ([-1 -3 2]');
```

Reactants are given negative numbers, as they are used up, and products are given a positive number. This is also done using the same order as they were defined in the class. Note transpose operator, as each reaction is defined in its own column rather than row. Models with multiple reactions taking place can also be modeled using a nu matrix with additional columns, defining additional reactions. (See example 3)

setT (Temperature)

The model is often used to find the composition change over a range of temperatures, so the temperature is set as a range of values.

```
Example2.setT((-50:10:500)+273.15) ;
```

Here, the range is set from -50 to 500°C , in steps of 10°C.

Set Pressure

The reaction and atmospheric pressures are set as a default of 100,000Pa, but can be modified by changing the properties P and P0 of the object. Here, the reaction pressure is changed to 500,000Pa and the pressure of the environment is modified to a more accurate value of 101,325Pa. `setP` can be used in the form setP(P) to just change reaction pressure, or set(P,P0) to change both values.

```
Example2.setP(500000,101325)
```

solve calculations

|The following two commands complete the calculations to model the system, reading for data plotting.

```
Example2.gibbs;
```

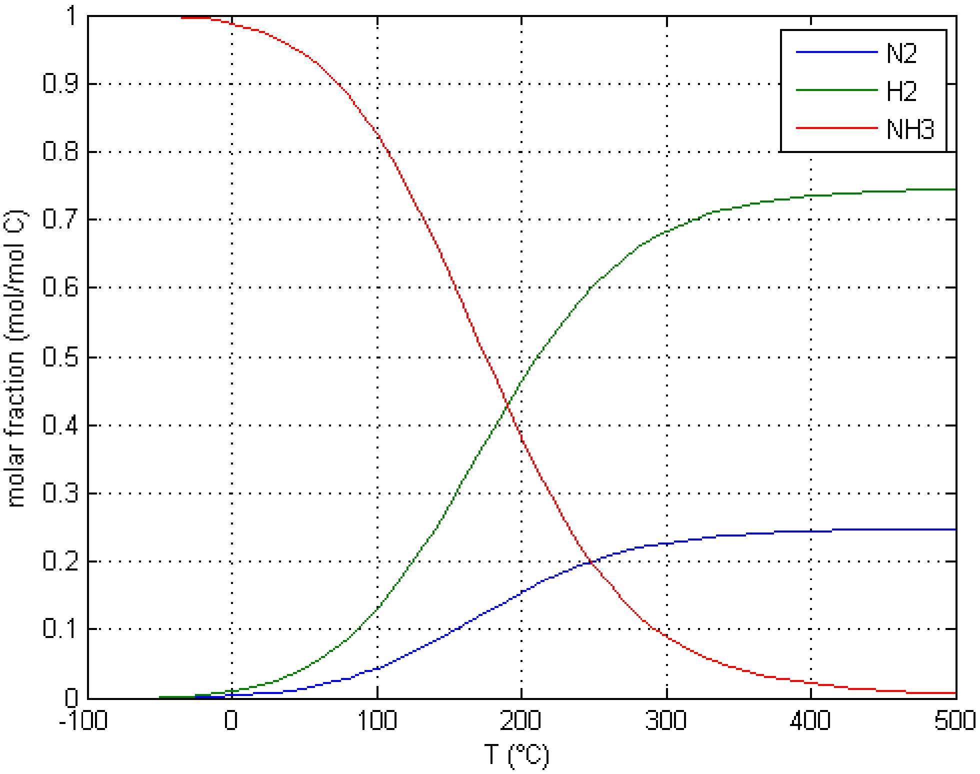
```
Example2.solveEq;
```

Output data and plotting

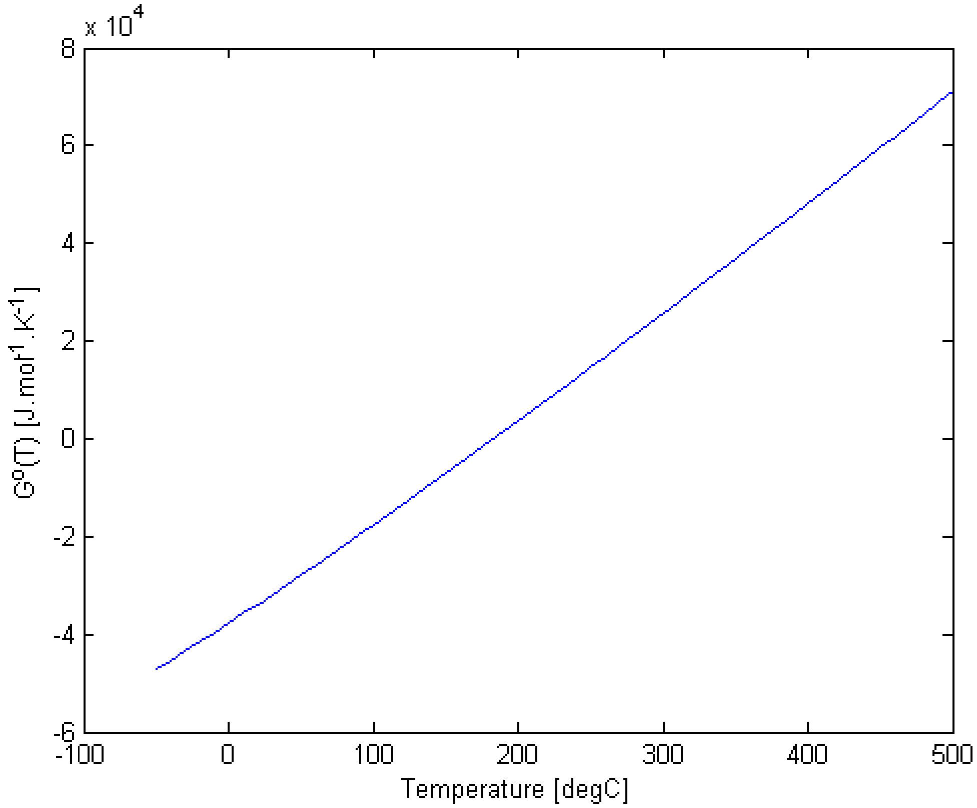
The Matrix **Example2.Zeq** holds the molar compositions of each species in each column of the matrix respectively, increasing in temperature, ready to be plotted against temperature using the code below.

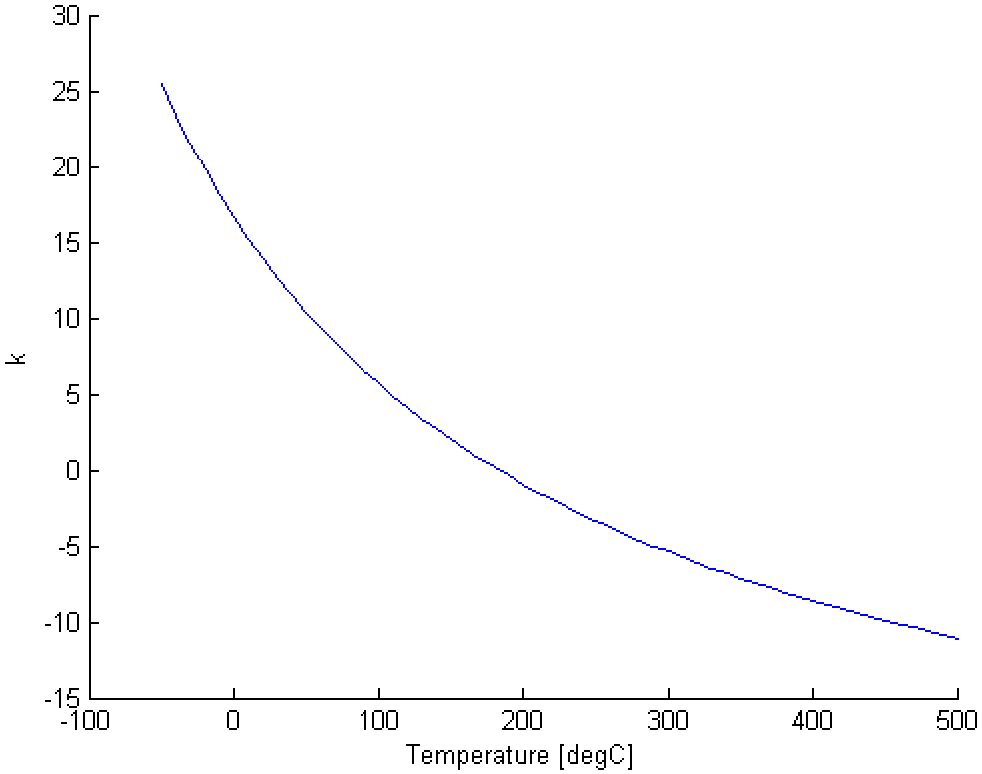
```
figure

plot(Example2.T-273.15,Example2.Zeq);
legend(Example2.names);
grid on;
xlabel('T (°C)')
ylabel('molar fraction (mol/mol C)')
```



```
Example2.gibbsPlot
```


x 10^4
8
6
4
2
0
-2
-4
-6
-100
0
100
200
300
400
500
Temperature [degC]
G^0(T) [J.mol^-1.K^-1]


30
25
20
15
10
5
0
-5
-10
-15
-100
0
100
200
300
400
500
Temperature [degC]
k

Steam Methane Reforming example

This example will use the reforming reaction, which has two reactions taking place side by side whilst including the inert nitrogen.

$$CH_4 + H_2O \leftrightarrow 3H_2 + COCO + H_2O \leftrightarrow H_2 + CO_2$$

```
Example3 = MediumModel({'H2','CH4','CO','CO2','H2O', 'N2'});
Z=[0 1 0 0 2.8 0.2]';
Z=Z./sum(Z);
Example3.setZ(Z);
```

The object is defined with all required species, and the initial molar compositions are set by initially defining the proportions of each species, then dividing through by the sum to normalise the vector to sum to one as required.

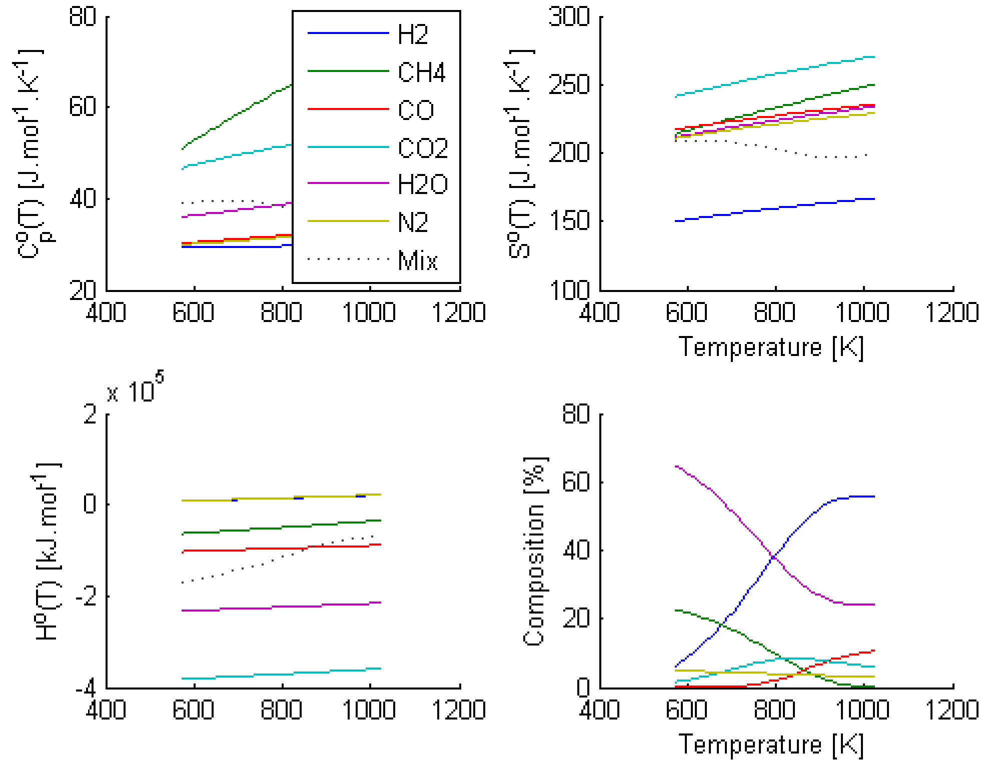
```
Example3.setT([300:10:750]+273.15);
nu=   [ [3 -1 1  0 -1 0]' ...
       [1 0  -1 1 -1 0]']    ;
Example3.setNu(nu);
```

The nu matrix now has 2 columns, each with 6 rows, to represent the two reactions taking place. Remembering products +ve, reactants -ve

The method `plot`, used in Example 3, creates plots of cp, s, h and compostion against temperature, in one window

The Gibbs free energy and equilibrium composition are both calculated, then a plot made which is shown below.

```
Example3.gibbs;
Example3.solveEq;
Example3.plot
```



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