MediumModel Class - User Guide

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The MediumModel class is a tool for modelling and analysing mixtures of reacting ideal gases over a range of temperatures, pressures and compositions. It can be used to calculate various basic thermodynamic properties of individual gases and gas mixtures.

Reaction system equations can be defined and solved to find equilibrium compositions for a reaction (or set of reactions) at a range of temperatures.

The model uses data compiled by NASA in the following paper:

NASA Glenn Coefficients for Calculating Thermodynamic Properties of Individual Species. *Bonnie J. McBride, Michael J. Zehe, and Sanford Gordon* Glenn Research Center, Cleveland, Ohio http://www.grc.nasa.gov/WWW/CEAWeb/TP-2002-211556.pdf

All published substances(~2000) are implemented, but for typical needs the following substance names are useful **N2,O2,CH4,CO,CO2,H2,H2O**

All properties are reported in SI units with mol the internal unit of "amount of substance". Molar Mass of the mixture is maintained by all methods so conversions to mass are conveniently available.

Class Properties

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

- **T** - Temperature Range (Kelvin) *Default - 801 values, ranging from 273.15K to 1073.15K in steps of 1K*
- **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** - Stoichiometry 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)

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.

- **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:

Property Set Methods

- **setT**-*sets the object temperature range*
- **setP**-*sets the reaction and atmospheric pressures*
- **setNu**-*sets the object's chemical reaction stoichiometry*
- **setZ**-*sets the object's composition by moles*
- **setX**-*sets the object's composition by mass*

Calculation Methods

- **gibbs**- *uses the Gibbs equation, g=h-Ts to calculate the enthalpy change of reaction for the specified stoichiometry so the lowest free energy state can be calculated.*
- **solveEq**- *solves the relevant Gibbs equations to find the lowest free energy state and hence equilibrium proportions over the temperature range so the end results can be plotted.*
- **props**- *used 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**- *calculates relevant value by moles, if the user specifies values by mass*
- **findTFromH**- *calculates temperatures when enthalpies are specified*

`gibbs` and `solveEq` are executed in Example2 and Example3 below. The remaining calculation methods are internal methods that are not 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.

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.

Example 1 - Instantiating a Simple Medium-Model Object

In this example, the model contains only a single species (steam).

```
Example1 = MediumModel({'H2O'});
Example1.setT([100:100:500]+273.15);
Example1
```

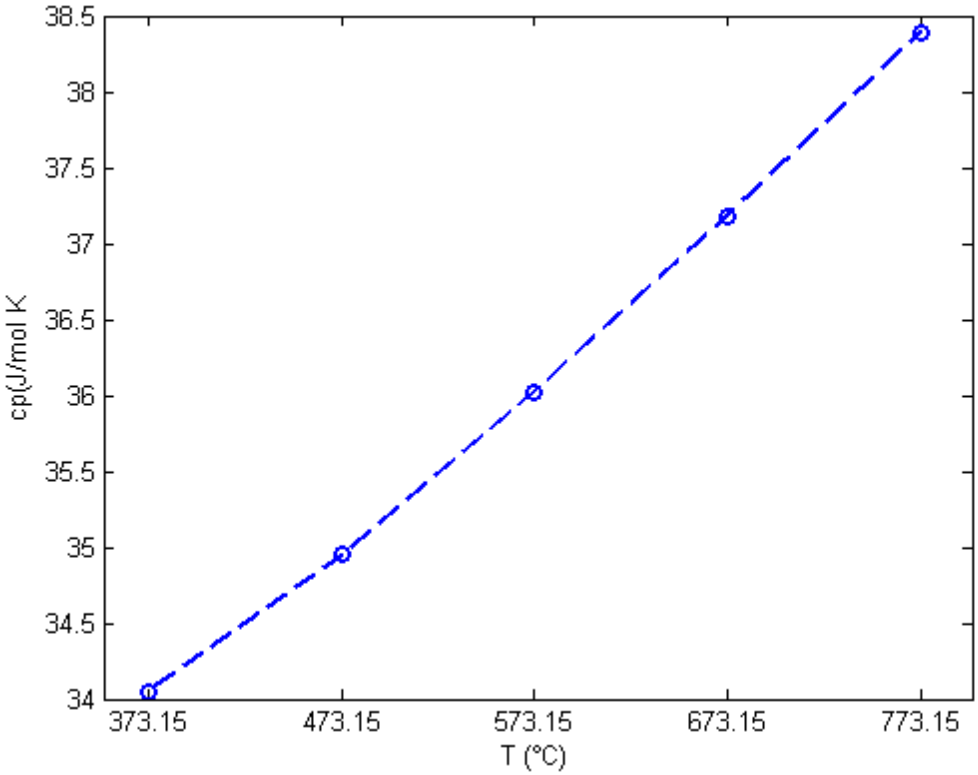
```
Example1 =

  MediumModel handle

  Properties:
              gas: [1x1 struct]
            names: {'H2O'}
             cp_V: [5x1 double]
              h_V: [5x1 double]
              s_V: [5x1 double]
             mu_V: [5x1 double]
               cp: [5x1 double]
                h: [5x1 double]
                s: [5x1 double]
               mu: [5x1 double]
             mm_V: 18.0153
               mm: [5x1 double]
            index: [1x1 struct]
            ln_kc: []
               nu: []
              Zeq: [5x1 double]
              aeq: [5x1 double]
                P: 100000
               P0: 100000
                Z: 1
                X: [1 1 1 1 1]
                T: [5x1 double]
    notCondensed: 1
```

The MediumModel object which is instantiated contains the set of thermodynamic properties for the defined species , as extracted from the NASA thermodynamic properties database. The media is defined for a range of temperatures from 373.115K to 773.15K (100 to 500°C). Below is a plot of the variation in heat capacity over the 5 temperature values.

```
plot(Example1.T,Example1.cp,'--o');xlabel('T (°C)');ylabel('cp(J/mol K');set(gca,'
```



Example 2 - Modelling a Simple Reaction System

This example demonstrates a model of the Haber process reaction, used for making ammonia.

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

The model will be used to find the equilibrium compositions of each gas 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 MediumModel class requires 4 parameters (Initial composition, stoichiometry, temperature and pressure) to be set in order to calculate how any reaction will to progress as follow:

setZ (Composition)

The initial proportions of the species are set by mass or molar fractions.

```
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 (stoichiometry)

The stoichiometry of the chemical reactions must be specified in the model.

```
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. Models with multiple reactions taking place can also be modelled using a nu matrix with additional columns, defining additional reactions. (See Example 3)

setT (Temperature)

The object can be used to find the composition change during the reaction over a range of temperatures by setting temperature property of the model.

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

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

setP (Pressure)

The reaction and atmospheric pressures are set by default to 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 setP(P,P0) to change both values.

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

Solve Equilibrium Conditions

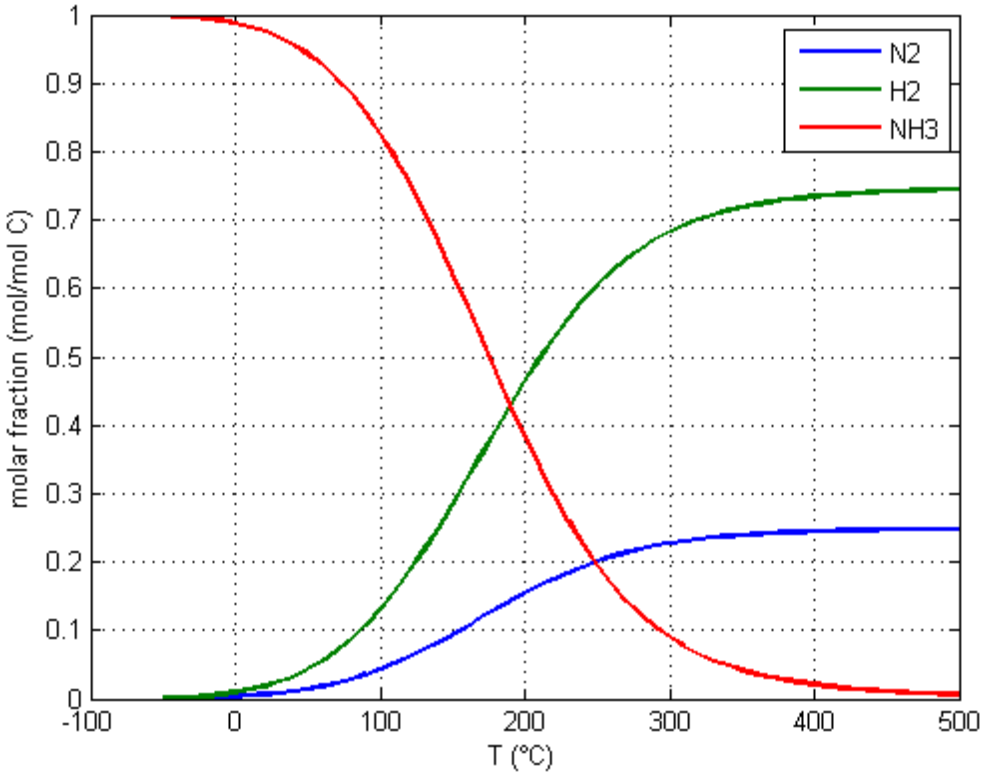
The following commands calculate the equilibrium conditions for the defined system, populating the Zeq (equilibrium composition) property.

```
Example2.gibbs;
Example2.solveEq;
```

Output data and plotting

The property **Example2.Zeq** holds the molar compositions of each species in each column of the matrix respectively, against temperature (as defined in **Example2.T**). The output compositions can be plotted against reaction temperature as shown below:

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



Example 3 - Steam Methane Reforming

This example will model the steam methane reforming reaction, which has two reactions taking place simultaneously.

$$CH_4 + H_2O \leftrightarrow 3H_2 + CO$$

$$CO + H_2O \leftrightarrow H_2 + CO_2$$

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

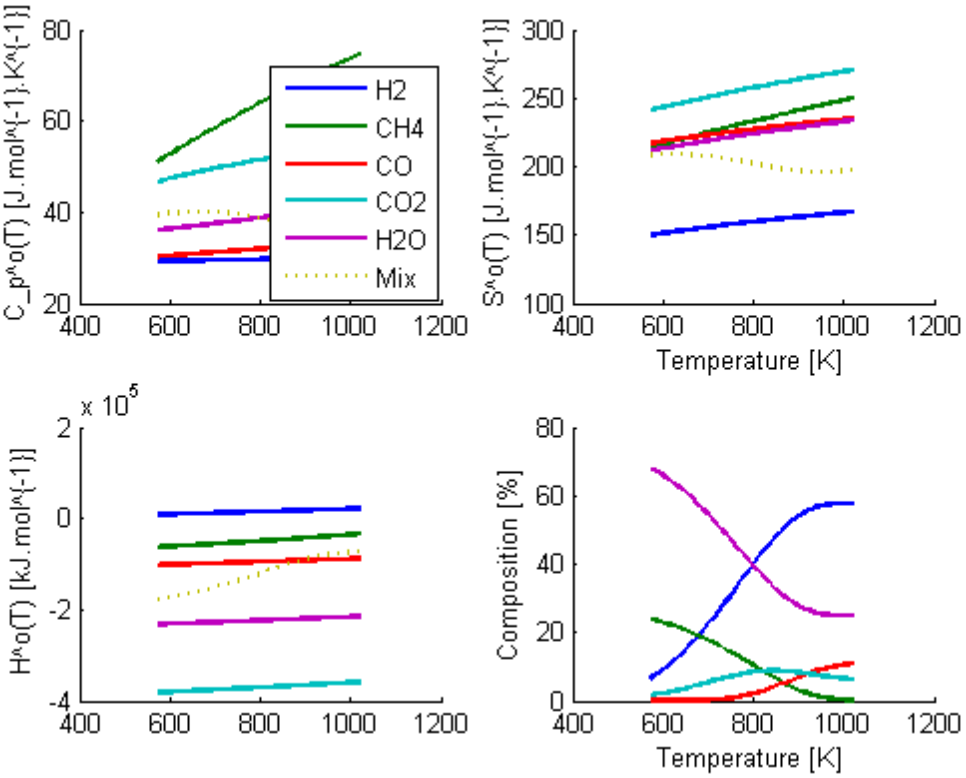
The object is defined with all required species, and the initial molar compositions are set by defining the proportions of each species, then dividing through by the sum to normalise the vector to sum to one as required. In this case, a steam to carbon ratio of 2.8 is defined at the reformer input.

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

The nu matrix now has 2 columns, each with 6 rows, to represent the two reactions taking place. Note: products +ve, reactants -ve. Once again the equilibrium composition of the reaction against a range of temperatures can be found using the `solveEq` method.

The plotting method `plot`, is used to create plots of cp, s, h and equilibrium composition against temperature:

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



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