Thermopy v0.5.1

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This document attempts to give an overview of the databases contained in Thermopy v0.5.1 and literature references for further investigation.
This is not the project's documentation.

1 Overview

Thermopy is a program to calculate thermodynamic variables for thousands of compounds, both inorganic or simple/common organics. Some of these variables are: enthalpy, entropy, specific heat capacity among others. Chemical reactions are also included. For them it is possible to calculate the equilibrium constant, heat of reaction at any temperature and others.

Thermopy has two branches of databases for calculating thermodynamic properties. One branch is a component rich set of databases in polynomial form using NASA polynomials. Gases, solids and liquids (organic and inorganic) are included in this database. The other branch is specific to water/steam calculations using the IAPWS database.

The NASA branch of Thermopy program aims at calculating the following thermodynamic properties: enthalpy, entropy and heat capacity at constant pressure at some temperature. The pressure dependance of these functions is not contemplated by the program. It also calculates derived thermodynamic properties (e.g. Gibbs energy). It does so by using databases of coefficients of known polynomial forms. The databases of coefficients were created with a Fortran program developed by NASA since the late 60's (PAC which stands for Properties and Coefficients).

In the PAC program databases were compiled through calculations based in "spectroscopic constants", "molecular constant data", "group additivity methods", "known

thermodynamic functions" and fitted according to least squares (see [3] for details). To clarify consider the polynomial form of the NASA 7 term polynomials:

$$\frac{C_p^o(T)}{R} = a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4$$

The "a" coefficients were generated by the PAC (Fortran) program external to Thermopy and Thermopy implements this polynomial that so $C_p(500) = 132.83$ in J/mol at 500 K for 2-propanol for example. The range of temperatures depends upon the component but in general it is from 200 K to 6 000 K.

The IAPWS branch works in a similar way. It implements calculations defined by [1] and in this case both temperature and pressure are contemplated by the model. The range for the water properties are from 273.15 K to 2273.15 and 0 MPa to 50 MPa (or up to 100 MPa if the temperature considered is below 1173.15).

2 Previous Thermopy

The author had contact with 2 other versions of Thermopy namely 0.3 by Guillem Borrell i Nogueras and version 0.4 by Adel Qalieh. Both versions were last developed on 31 January 2009 and 27 May 2015 respectively.

The 0.3 version offered saturation equations and $H(T, p)$ data for water (only for region 1 see [1] for details) and made use of Burcat's Database (see [4]) to find enthalpy, entropy, Gibbs energy, etc for various compounds. It also included a units conversion module, physical constants database, simple psicrometry calculations and a combustion module.

The 0.4 version added nothing new to the previous version and is credited here for the sole purpose of the author's possible misjudgment about any contributions.

The author dropped support for the psicrometry and combustion modules present in previous Thermopy versions. The modules were not considered to fit in the purpose of the project and/or were poorly developed.

3 Present databases

The databases present in this version are:

1. NASA 7 polynomials (superseded by NASA 9 polynomials)
2. NASA 9 polynomials
3. Burcat's Database

All these databases share the same framework. The reported values are for species in their ideal state. For gases that is 1 bar (ideal gas). For condensed species that is the pure crystalline or liquid substance at 1 bar. The species are considered as gaseous unless explicitly specified.

Although water is included in the previous databases there is an additional database for more accurate properties of water:

4. IAPWS

Note that in this database solid water is not considered.

3.1 Nasa 9 term polynomials

The maximum error of the quantities reported are in the range of 0.01% [4, p. 5].
See [5] for details.

3.2 Nasa 7 term polynomials

The maximum error of the quantities reported are in the range of 1% [4, p. 5].

This database is present indirectly because Burcat's database uses its fortran program to calculate its polynomials.
See [2] for details.

3.3 Burcat's Database

According to [4] itself: "The database is used by scientists, educators, engineers and students at all levels, dealing primarily with combustion and air pollution, jet engines, rocket propulsion, fireworks, but also by researchers involved in upper atmosphere kinetics, astrophysics, abrasion metallurgy, etc". Calculations were carried using the "McBride and Gordon PAC program. (Gordon and McBride 1967, 1992)".

The database was last updated on 31 December 2014.
See `http://garfield.chem.elte.hu/Burcat/burcat.html` for details.

3.4 IAPWS

The uncertainties are within a specified value for various regions (see fig. 3 and 4 in [1]). The largest uncertainty is ±3% around the triple point for specific heat capacities at constant pressure but most of others are below the ±0.3% interval.
See [1] for details.

4 Transformation of the xml files

The transformation of the xml files contained in Thermopy v0.5.1 were done in a series of different codes each one achieving different levels of complexity. The author considered irrelevant to post the .inp to .xml python codes as they were used once. Credits are given to the module *pubchempy v1.0.3* as it was used to incorporate iupac names, InChIKeys and CAS numbers to the xml file.

In case you are interested in such codes you can email the author.

References

[1] The International Association for the Properties of Water and Steam. Revised Release on the IAPWS Industrial Formulation 1997 for the Thermodynamic Properties of Water and Steam. August 2007.

[2] Bonnie J. McBride, Sanford Gordon and Martin A. Reno. Coefficients for Calculating Thermodynamic and Transport Properties of Individual Species. November 1992.

[3] Bonnie J. McBride and Sanford Gordon. Computer Program for Calculating and Fitting Thermodynamic Functions. November 1992.

[4] Alexander Burcat, Branko Ruscic. Third Millennium Ideal Gas and Condensed Phase Thermochemical Database for Combustion with Updates from Active Thermochemical Tables. September 2005.

[5] Bonnie J. McBride, Michael J. Zehe, and Sanford Gordon. NASA Glenn Coefficients for Calculating Thermodynamic Properties of Individual Species. September 2002.