Antti Roine August 10, 2006 09006-ORC-J

31. THERMOCHEMICAL DATA SOURCES

Traditionally, the thermochemical data of species has been measured experimentally using many different kinds of devices and by processing the data obtained by various calculation procedures. In some cases thermochemical data can also be reliably estimated using theoretical methods, but in most cases experimental methods produce the most accurate data.

The data in the HSC Chemistry Main database is not critically evaluated or always internally consistent. However, the accuracy is usually good enough for most thermochemical calculations. HSC provides fast access to data and references found in literature. The following principles have been used in HSC database development work:

1. Where possible, the compiled data has always been taken from the most recent reliable source if the data differs from the older sources.

2. If the same data values in a new source have been published earlier, the old original source is mentioned as a reference.

3. If major discrepancies are found with the data sources, a simple evaluation of the best data has been carried out.

The critical evaluation of the data means that particular data has been collected from many different sources and cross-checked with several different thermochemical dependencies. Errors due to different measurement methods also have be taken into account. All the species must be compared with each others in order to get internally consistent data.

The data in HSC database is not always internally consistent because the data has been collected from more than 900 different sources. However, the data should be more consistent with the external (absolute) scales because the most reliable and recent H, S and Cp data sources have been used. Figure 1 illustrates the meaning of internal and external consistency of house height data.

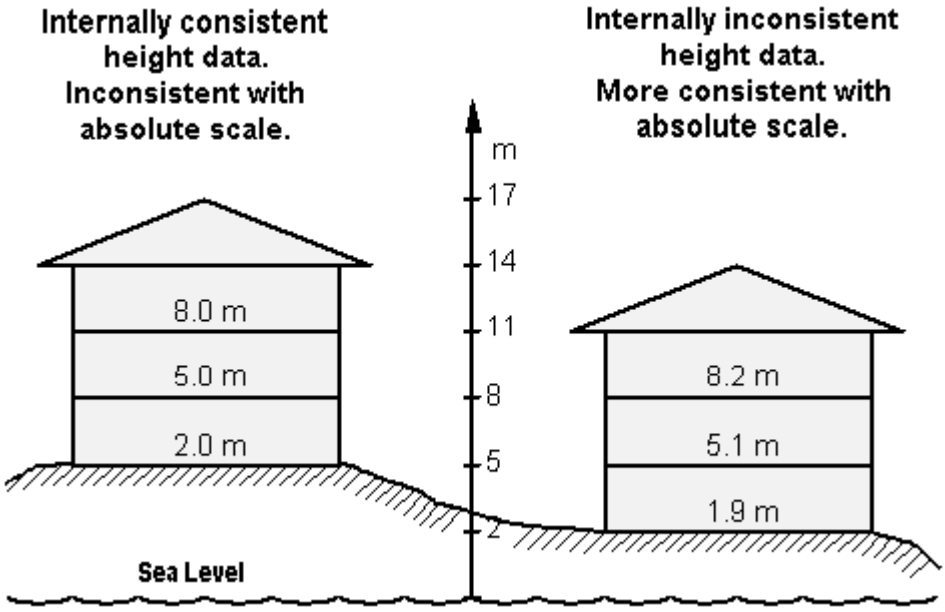

Fig. 1: Internal vs. external (absolute) height scales of the house.

The HSC Main database with some 17000 species is of course incomplete, because the number of different substances is infinite. However, it does offer a fairly good source of thermochemical data for many common substances.

If you do not find some specific compound in the HSC database, you can try to make a computer search from international reference databanks, because thermodynamic data can be found in many articles in scientific journals. For example, you can search from the Chemical Abstracts database, which you can find in DIALOG or STN databanks. Key words can be, for example: compound name, thermodynamics, enthalpy, heat capacity, etc. Of course you need a modem to carry out the search and you have to be a registered user of DIALOG or STN.

The reference lists in **Chapters 32 and 33** give a review of thermochemical data sources. Most of the references have been used to collect data for the HSC Main database. The abbreviations used in the HSC database have been given in the left column in alphabetical order.

If you have some new thermochemical data, which is missing from the HSC 7 database, please send it to Outotec Research Oy. We can then make it available for other HSC users in future HSC versions.

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