CD Containing

Thermodynamic Data and Examples of the Use of Excel

For the Fourth Edition of the Text

Introduction to the Thermodynamics of Materials

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CD of Examples and Data provided by

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(http://home.att.net/~thermart/)

Abstract

Computational thermodynamic software is used extensively by scientists and engineers, but there is a notable lack of data and affordable software for educational use. A good way to provide educational software is to utilize an existing calculational platform. In this case, a spreadsheet program is used as a calculational tool. This CD is designed to help the student make detailed thermodynamic calculations relevant to the processing of materials. The CD contains two Microsoft ® Excel* workbooks: ThermoTables.xls and ThermoXmples.xls. The *table* workbook contains thermodynamic data for many of the elements and compounds described in the text. The *examples* workbook shows how common spreadsheet tools can be used to make heat, equilibrium, and mass balance calculations, construct phase diagrams, and examine the feasibility of materials processing techniques.

The CD also contains XmpleExplanation.doc, which describes in detail each example, and outlines the calculational procedure used in the Excel workbook. Each example is keyed into text description, exercises, or problems.

The examples relied heavily on two educationally oriented software programs for thermochemical modeling. Both programs run as Excel spreadsheet files. The first is FREED, a thermodynamic database program containing data files for 2450 species. It contains the entire U. S. Bureau of Mines database, and most of the U. S. Geological Survey database, plus data for scores of other species drawn from various sources. Several modules are available for manipulating and viewing the data. The second program is THERBAL, for making thermodynamic calculations using FREED data. Equilibrium calculations can be made for systems with non-ideal solutions, for a specified set of pressure, temperature, and input amounts of reactants. An optional heat balance can also be calculated.

To take full advantage of this CD, the student should have a good knowledge of Excel and its various features. Excellent references are given in the Appendix.

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Introduction

The personal computer has become a standard tool in engineering education. Programs such as spreadsheets are used by both students and faculty to enhance the educational experience. Although spreadsheet programs were written with the main purpose of serving business and engineering professionals, they were rapidly adopted by the educational market.

Educational software consists of computer programs designed specifically for the educational market, as opposed to shrunken versions of professional programs. Ideally, educational software should be capable of a variety of tasks associated with both undergraduate and graduate education, be generic in application, and run on both the PC and Apple platforms. Other desirable characteristics are a user interface that looks similar to the screens used by other computer programs, and minimal cost.

Prior to its demise in 1996, the U. S. Bureau of Mines prepared a large thermodynamic database that was published in a series of four Bulletins[1–4]. This data had the advantage of being public domain, and hence free for anybody to use. The data were presented as tables of heat content and entropy above 298.15 K, transition temperatures and heats of transition, and other relevant data. The data were developed by the Bureau by fitting experimental data to equations as functions of complex powers of T. These data were now available as the computer database program FREED, constructed to operate as a spreadsheet in an Excel workbook. Several unique mineral species from the U. S. Geological Survey[5]. were added to FREED. Other enhancements include the extension of the upper-temperature limit for many species, the creation of metastable phases for a number of elements (e.g., supercooled and superheated liquid), various fuels (e.g., oil and coal) and species for use as solutes in metals and slags. This CD contains approximately 90 data tables from FREED in the workbook ThermoTables.xls.

It became clear that however valuable the data itself might be, there was a corollary need to develop techniques to use the data to do heat balances and compute the equilibrium composition. To be consistent with FREED, all computations had to operate in Excel. The purpose of Xmples.xls is to illustrate spreadsheet techniques for making thermodynamic calculations on process analysis and design.

ThermoTables.xls Workbook

A collection of about 90 data tables from FREED is on this CD as ThermoTables.xls. The data are based on selection of a standard state for elements and compounds that is the most stable at the specified temperature and 1-atm pressure. The energy unit is Joules, at 50° intervals. Equations for C_p, $H_T–H_{298}$, $\Delta H°f$ and $\Delta G°f$ are listed at the end of the tables.

Two worksheets are on the workbook: ELM and CMP. Worksheet ELM contains data on 23 common elements involved in the production and processing of inorganic materials. The data is based on the most stable form of each element at each temperature*, hence $\Delta H°f$ and $\Delta G°f$ are zero at all temperatures. The tables show an extended break in the data at element transitions. Worksheet CMP contains data on 65 common compounds involved in inorganic-materials processing, and on all compounds in the workbook ThermoXmples.xls. Information is given for the composition of compounds in atomic and weight percentages, plus information about the transitions in the reference state elements. The tables show an extended break at the transition temperatures of the compounds, and a minor break at transition temperatures for the constituent elements.

An important part of each table is the listing of the descriptor and, where important, the mineral name. These distinguish between different phases of the same species. Examine the data tables for H_2O(l,g) and H_2O(g) as an example of the care needed in dealing with processes involving water. Your instructor will clarify these distinctions in your lectures.

* An exception is the table for phosphorus, which uses P(white) as the reference state for P.

ThermoXmples.xls Workbook and XmpleExplanation.doc

Excel's tools are good ways to help the student focus on the principles while minimizing tedious arithmetic. The workbook contains 22 examples on the use of spreadsheet software to make various thermodynamic calculations on the processing of materials. Comments have been added to each example, as noted at the top of each worksheet. Excel's formula and goal seek tools are used to set up templates for repetitive calculations. The regression tool is used to develop equations for specific thermodynamic functions. Charts and the trendline tool are used to obtain information not easily calculated. The auditing tool can be used to indicate which cells contain values used in the formula bar. This CD assumes an understanding of Excel and its operation. Resources are available for those seeking further understanding of the use of Excel in technological applications[6,7].

The author of these examples recognizes that there are many different approaches to using a spreadsheet for thermodynamic calculations. No claim is made that the method used here is the best or most efficient. Certainly your instructor can point out ways the examples could have been done in a more elegant manner.

The examples are keyed to sections of the Fourth Edition of the text. Some examples are versions of text problems or exercises, but have been worked out in more detail, or expanded to include conditions not covered in the text. Other examples refer to material discussed in the text that was not used as problems or exercises. In all cases, the object of the workbook was twofold: first, to introduce the student to spreadsheet software, and second, to show how it can be applied to materials processes to gain insight not available by hand calculation.

The document describes each example in detail, and gives background information on the process involved. Equations and equilibrium constant expressions are written for important reactions, and the procedure for making the calculations is described. The relevance of the results is given, and finally, each example contains an assignment to give the student additional practice in using the spreadsheet tools.

Thermodynamic Software

There are 2 thermodynamics programs designed specifically for educational use. The first is FREED, which is a thermodynamic database program in an Excel spreadsheet format. This is the program that produced all of the data in ThermoTables.xls on the CD. In addition to preparing data tables, FREED can also make calculations on the data, construct charts of various thermodynamic variables, and determine parameters for multi-term Cp and $\Delta G°f$ equations from other data tables. More details about FREED and ordering instructions are available from the Thermart web page[8].

The second thermodynamic program is THERBAL, which makes reaction, heat balance, and equilibrium calculations. It uses sub-databases created by FREED. THERBAL was used to make calculations for some of the examples in ThermoXmples.xls. THERBAL is capable of making multiple calculations with varying temperature, pressure, or amounts of input materials. It also contains non-ideal solution models for the regular, sub-regular, Bale-Pelton, and free-form solutions. More details about THERBAL and ordering instructions are available from the Thermart web page[8].

Other software packages are also available for doing calculations similar to those done by FREED and THERBAL. Two of which are: HSC[9], a program from Outokumpu that is often used for educational purposes, and FactSage[10], which has many unique features, notably a set of models for non-ideal solutions such as slags, mattes, and alloys. The FactSage web page also has links to other specialized software programs for process calculations.

References

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