THERMO-PROP
THERMOPHYSICAL ANALYSIS PACKAGE FOR MODELLING AND SIMULATION

USER MANUAL OF VERSION 1.4.7

ABSTRACT

This documentation gives background description of Thermo-Prop database for numerical modelling, simulation and calculations. The quality of obtained results, from calculation codes simulating the course of a process, depends on the accuracy of material data used. Only these data, which characterize well the materials and phenomena related to the process, guarantee obtaining of proper conclusions and valuable prediction of the real process behaviour. For example, within the codes of the "generalist" or "professional" types, physical models describe particular stages of the casting development (namely, filling the mould, solidification and the cooling of the metal, the mould heating and the development of stresses). The problem of material data is related to each of these stages.

CONTENTS

1. INTRODUCTION

An important input for physically based simulation models for metal processing, such as production; refining; casting and welding, is the relevant physical properties of the metals and other materials including moulds and slags. Typically enthalpy-related properties (Gibbs energy, enthalpy, entropy, specific heat capacity), heat-transfer coefficient and thermal conductivity or diffusivity are required to model heat flow, and a knowledge of density, viscosity and surface tension is used in fluid flow modelling.

As the models gain in sophistication there is an increasing demand for better physical data. Some work has been performed to establish the sensitivity of the results from simulation models to changes in the values of the input data. The critical properties, which affect the results of the models, are dependent upon behaviour of the process being modelled. For example, a macro heat transfer model is critically dependent on the enthalpy evolved during solidification as well as the heat transfer properties such as the thermal conductivity of the metal.

At the Institute of Engineering Thermophysics (affiliated with the National Academy of Sciences), a Thermo-Prop software, has been developed to calculate important material properties needed in modelling and simulation. The calculations of the Thermo-Prop software have been validated with numerous experiments.

2. SETTING UP

2.1 System requirements

- MS Windows 95/98/NT/ME/2000/XP/2003/Vista/7/8
- A hard disc and CD drive
- VGA display or better
- At least 64 MB of memory
- 5 MB of disk space

2.2 Program installation

- Unzip the downloaded "**thermoprop.zip**" and execute "**thermoprop.exe**"
- Wizards will guide you through installing Thermo-Prop software

3. DESCRIPTION OF THE THERMO-PROP PACKAGE

3.1 Element module

It has long been recognized that the combination of analysis and synthesis of thermodynamic properties is an important source of information on the phase stability of transition metals and alloys. There is an extensive set of experimental thermochemical data available. Thermodynamic data for the condensed phases of pure elements currently used by IET (Institute of Engineering Thermophysics) are the most reliable. IET engages in the compilation of a comprehensive, self consistent and authoritative thermochemical data for inorganic and metallurgical systems. The main purpose of the database lies in its use in calculation of phase equilibria in multicomponent systems which puts a premium on the interconsistency of the data and thereby on their traceability to the data for the elements.

Element module contains thermophysical properties (from the liquid state down to room temperature) for the following elements: Ag, Al, Am, As, Au, B, Ba, Be, Bi, C, Ca, Cd, Ce, Co, Cr, Cs, Cu, Dy, Er, Eu, Fe, Ga, Gd, Ge, Hf, Hg, Ho, In, Ir, K, La, Li, Lu, Mg, Mn, Mo, Na, Nb, Nd, Ni, Np, Os, P, Pa, Pb, Pd, Pr, Pt, Pu, Rb, Re, Rh, Ru, S, Sb, Sc, Se, Si, Sm, Sn, Sr, Ta, Tb, Tc, Te, Th, Ti, Tl, Tm, U, V, W, Y, Yb, Zn, Zr.
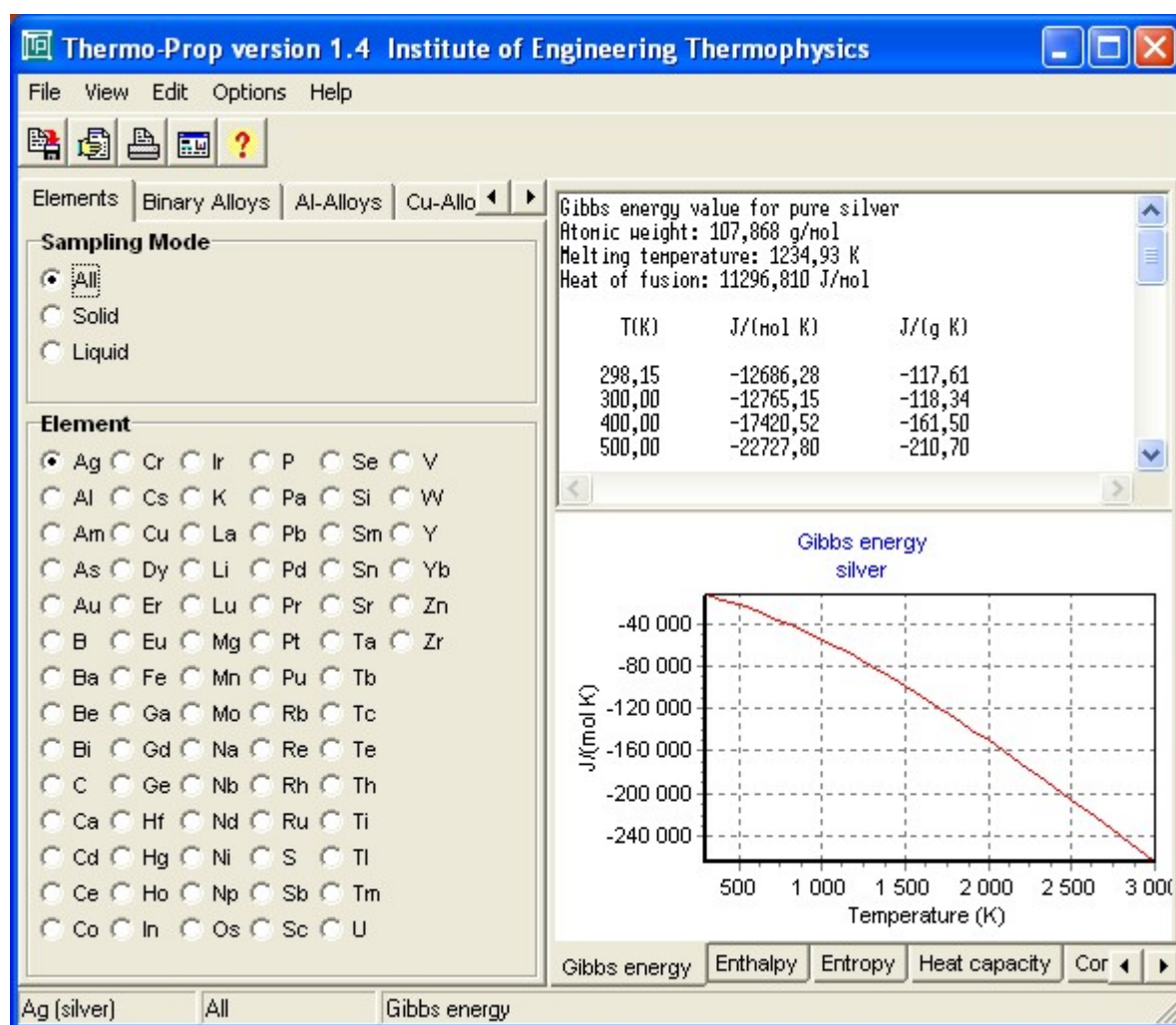
3.1.1 Input data

- **Data of the Thermo-Prop data bank**
  - Program's module contains thermodynamic data
  - Automatic input, not for user

3.1.2 Output data

- **Thermophysical data**
  - Gibbs energy
  - Enthalpy
  - Entropy
  - Specific heat capacity
  - Thermal conductivity
  - Density

- **Abbreviations (Crystal structure types)**
  - CUB - Simple cubic
  - FCC - Face-centred cubic
  - BCC - Body-centred cubic
  - TET - Simple tetragonal
  - BCT - Body-centred tetragonal
  - HEX - Simple hexagonal
  - HCP - Hexagonal close-packed
  - DHCP - Double hexagonal close-packed
  - ORT - Orthorhombic
  - TRI - Triclinic
  - RHO - Simple rhombohedral
  - BETA_RHO - Beta rhombohedral
  - MONO - Monoclinic
  - DIA - Diamond cubic
  - GRAPHITE_HEX - Graphite hexagonal
  - GAMMA - Gamma hexagonal
  - WHITE - White tetrahedral
  - LIQUID - Liquid state

For pure elements, the results are displayed as xx, where xx refers to element's designation (2 characters). In the sampling module, "all" refers to all range; "solid" refers to solid range; and "liquid" refers to liquid range.

3.2 Binary-alloy module

In the binary-alloy module, interfacial material balance equations and Fick's diffusion laws were combined with a thermodynamic solution model, which links the temperature, the interfacial composition and the phase stabilities to each other. The thermophysical properties of the solution phases are described with a substitutional solution model. Generally, the results depend not only on the alloy composition but also on the cooling rate. The module globally deals with non-equilibrium solidification, i.e., thermodynamic equilibrium is assumed to be achieved at the phase interfaces only. Binary-alloy module embraces thermophysical properties (from the liquid state down to room temperature) for the following components: AlAg, AlCu, AlMg, AlSi, AlZn, CuAg, CuCr, CuFe, CuMg, CuMn, CuNi, CuSi, CuSn, CuTe, CuTi, CuZn, CuZr and FeSn. Depending on the alloy composition and cooling rate, the module also determines the phase fractions and compositions of the liquid during solidification.

In other words, the calculation algorithms are based on thermodynamic theory connected to thermodynamic assessment data, as well as on regression formulas of experimental data, and they take into account the temperature, the cooling rate and the alloy composition.
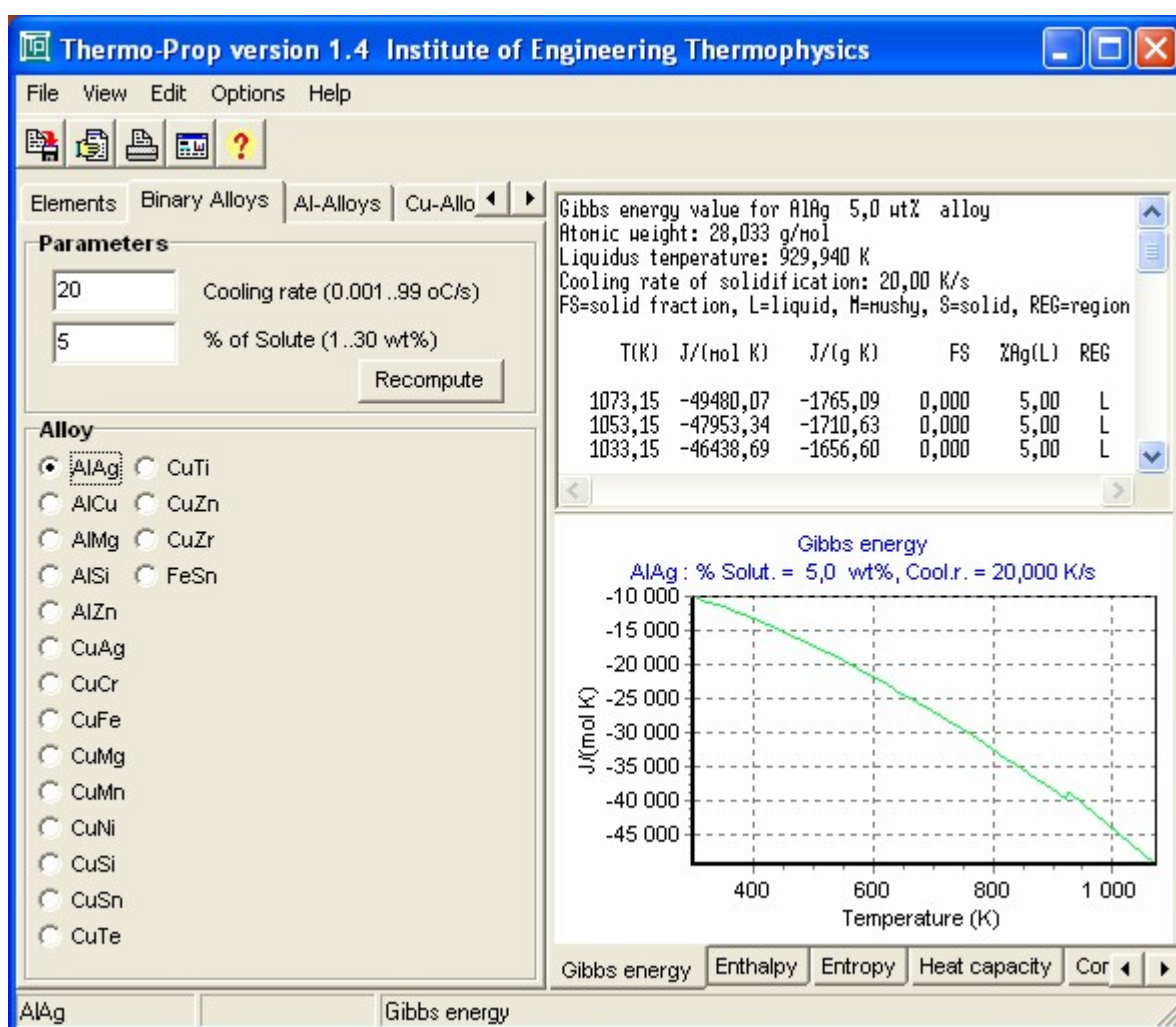
3.2.1 Main instruments

- **Thermodynamic chemical-potential-equality equations**
  - Determination of thermodynamic equilibrium at the phase interfaces
  - Based on substitutional solution and magnetic ordering models
- **Interface mass balance equations**
  - Fick's law of solute diffusion
- **Complete solute mixing in liquid**
- **Diffusion of solutes extremely rapid during solidification**

3.2.2 Input data

- **Solute selection and composition**
  - Nominal composition [wt%] of a selected solute
  - Minimum value: 1.0 wt% of solutes
  - Maximum values given in "composition ranges" section

- **Cooling rate**
  - Cooling rate [°C/s] of solidification
  - Recommended values from 0.001 to 99°C/s]
  - The cooling rate causes different temperature range and location of the mushy zone in the described material properties

- **Data of the Thermo-Prop data bank**
  - Program's module contains thermodynamic data and solute diffusion data
  - Automatic input, not for user

3.2.3 Composition ranges

User should apply the recommended composition ranges given below. Going beyond these ranges does not prevent the calculations but the program restricts itself to these composition ranges.

- **Composition ranges [wt%] for aluminium alloys**
  - Ag up to 30
  - Cu up to 20
  - Mg up to 20
  - Si up to 12
  - Zn up to 5

- **Composition ranges [wt%] for copper alloys**
  - Ag up to 5
  - Cr up to 1.4
  - Fe up to 5
  - Mg up to 9
  - Mn up to 10
  - Ni up to 15
  - Si up to 7
  - Sn up to 25
  - Te up to 7
  - Ti up to 16
  - Zn up to 30
  - Zr up to 10

- **Composition ranges [wt%] for ferrous alloys**
 - Sn up to 20

3.2.4 Output data

- **Thermophysical data**
  - Gibbs energy
  - Enthalpy
  - Entropy
  - Specific heat capacity
  - Thermal conductivity
  - Density

- **Miscellaneous data**
  - Solid fraction
  - Nominal liquid composition of solute [wt%]
  - Liquidus temperature (start of solidification)

After the execution of program, the results are displayed as xxxx % Solut. =…, Cool.r. =…, where xxxx refers to alloy designation; % Solut. refers to nominal liquid composition of solute [wt%]; and cool.r. refers to the cooling rate of solidification process.

3.3 Aluminium-alloy module

In this thermodynamic-kinetic module, the main instruments of the convectional solute redistribution models, i.e., the material balance equations and Fick's laws of solute diffusion, were incorporated into the proper set of thermodynamic chemical-potential-equality equations, which relate the phase interface compositions to both the temperature and the phase stabilities. Depending on the alloy composition and cooling rate, the module determines the phase fractions and compositions of the liquid during solidification; and also calculates important thermophysical material data (Gibbs energy, enthalpy, entropy, specific heat capacity, thermal conductivity and density from the liquid state down to room temperature) for aluminium alloys containing Ag, Cr, Cu, Fe, Mg, Mn, Nd, Si, Sn, Ti and Zn.

The module makes use of experimental thermodynamic and phase diagram data as well as solute diffusion data from IET and National Academy of Sciences, which are fed in as measured values.
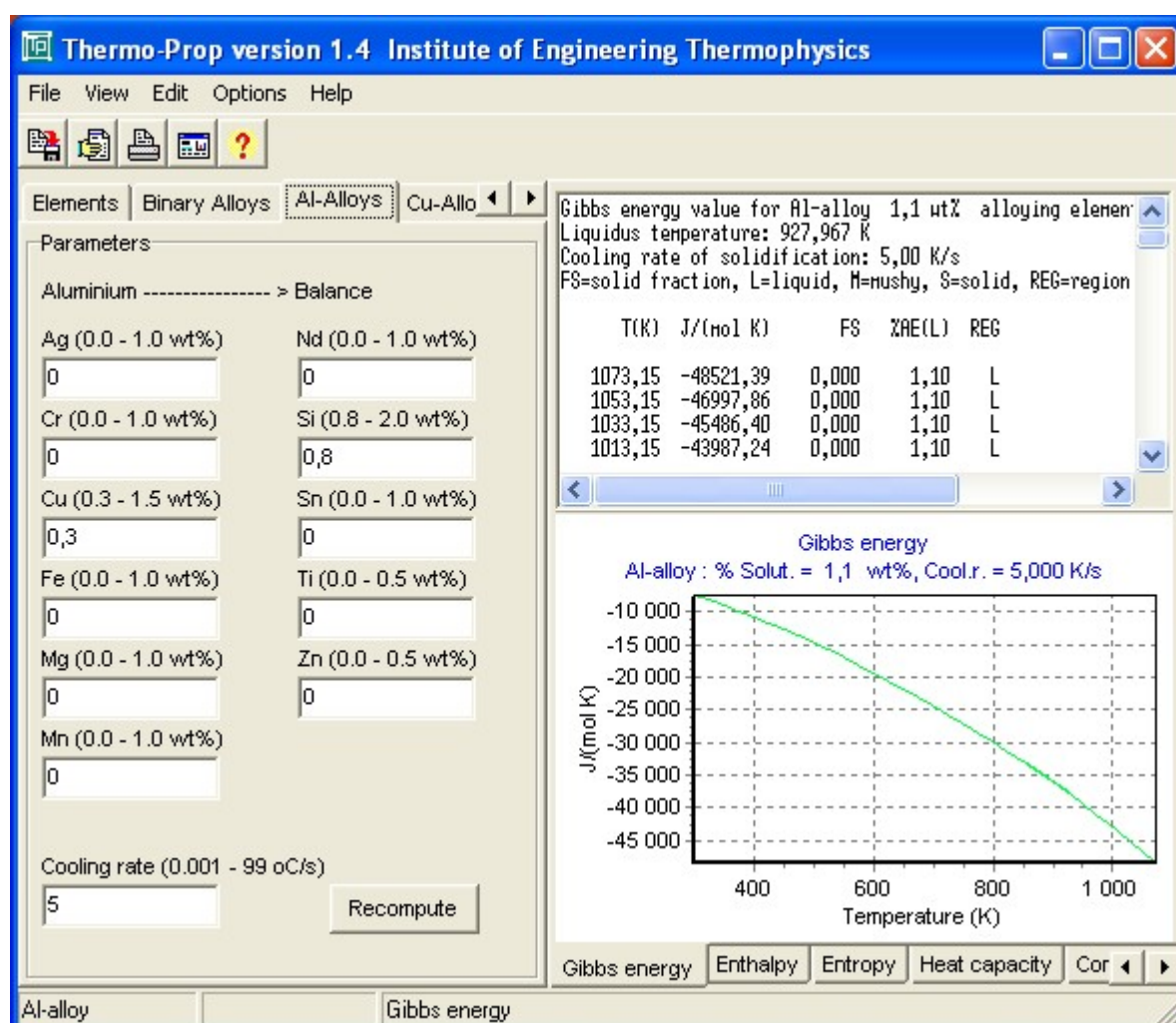
3.3.1 Input data

- **Composition**
  - Nominal composition [wt%] of alloying elements (i.e. solutes)
  - Recommended values given in "composition ranges" section

- **Cooling rate**
  - Cooling rate [°C/s] of solidification
  - Recommended values from 0.001 to 99°C/s]
  - The cooling rate causes different temperature range and location of the mushy zone in the described material properties

- **Data of the Thermo-Prop data bank**
  - Program's module contains thermodynamic data and solute diffusion data
  - Automatic input, not for user

3.3.2 Composition ranges

User should apply the recommended composition ranges given below.

- **Composition ranges [wt%] of alloying elements**
  - Ag: 0.0 - 1.0
  - Cr: 0.0 - 1.0
  - Cu: 0.3 - 1.5
  - Fe: 0.0 - 1.0
  - Mg: 0.0 - 1.0
  - Mn: 0.0 - 1.0
  - Nd: 0.0 - 1.0
  - Si: 0.8 - 2.0
  - Sn: 0.0 - 1.0
  - Ti: 0.0 - 0.5
  - Zn: 0.0 - 1.0

3.3.3 Output data

- **Thermophysical data**
  - Gibbs energy
  - Enthalpy
  - Entropy
  - Specific heat capacity
  - Thermal conductivity
  - Density

- **Miscellaneous data**
  - Solid fraction
  - Nominal liquid composition of solutes [wt%]
  - Liquidus temperature

After the execution of program, the results are displayed as xxxx % Solut. =…, Cool.r. =…, where xxxx refers to alloy type; % Solut. refers to nominal liquid composition of alloying elements [wt%]; and cool.r. refers to the cooling rate of solidification process.

3.4 Copper-alloy module

In this thermodynamic-kinetic module, the main instruments of the convectional solute redistribution models, i.e., the material balance equations and Fick's laws of solute diffusion, were incorporated into the proper set of thermodynamic chemical-potential-equality equations, which relate the phase interface compositions to both the temperature and the phase stabilities. Depending on the alloy composition and cooling rate, the module determines the phase fractions and compositions of the liquid during solidification; and also calculates important thermophysical material data (Gibbs energy, enthalpy, entropy, specific heat capacity, thermal conductivity and density from the liquid state down to room temperature) for copper alloys containing Ag, Al, Cr, Fe, Mg, Mn, Ni, Pb, Si, Sn, Zn, and Zr.

The module makes use of experimental thermodynamic and phase diagram data as well as solute diffusion data from IET and National Academy of Sciences, which are fed in as measured values.
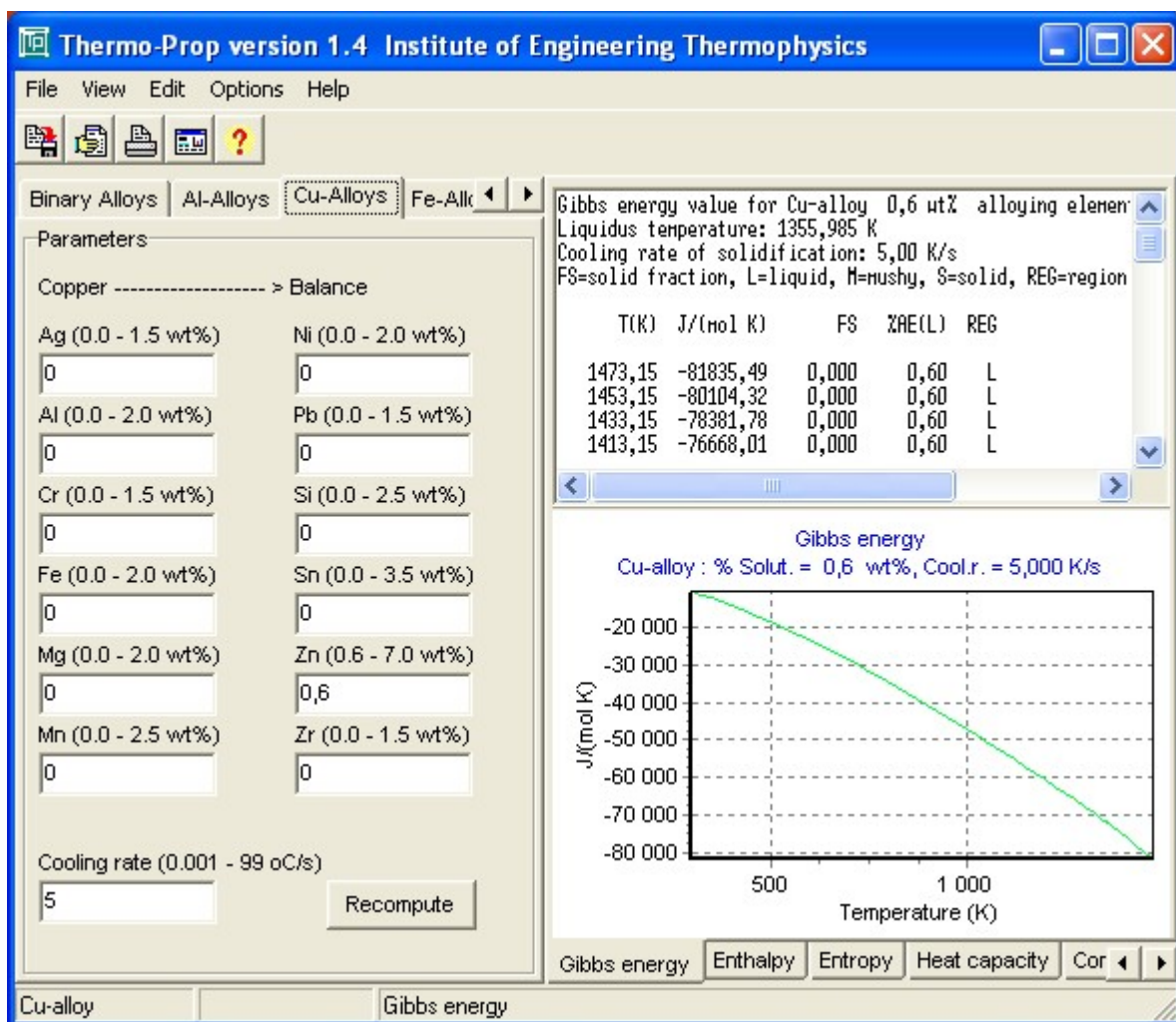
3.4.1 Input data

- **Composition**
  - Nominal composition [wt%] of alloying elements (i.e. solutes)
  - Recommended values given in "composition ranges" section

- **Cooling rate**
  - Cooling rate [°C/s] of solidification
  - Recommended values from 0.001 to 99°C/s]
  - The cooling rate causes different temperature range and location of the mushy zone in the described material properties

- **Data of the Thermo-Prop data bank**
  - Program's module contains thermodynamic data and solute diffusion data
  - Automatic input, not for user

3.4.2 Composition ranges

User should apply the recommended composition ranges given below.

- **Composition ranges [wt%] of alloying elements**
  - Ag: 0.0 - 2.5
  - Al: 0.0 - 2.0
  - Cr: 0.0 - 1.5
  - Fe: 0.0 - 4.0
  - Mg: 0.2 - 2.5
  - Mn: 0.0 - 2.5
  - Ni: 0.0 - 1.5
  - Pb: 0.0 - 2.0
  - Si: 0.2 - 3.5
  - Sn: 0.0 - 2.0
  - Zn: 0.6 - 4.0
  - Zr: 0.0 - 1.5

### 3.4.3 Output data

- **Thermophysical data**
  - Gibbs energy
  - Enthalpy
  - Entropy
  - Specific heat capacity
  - Thermal conductivity
  - Density

- **Miscellaneous data**
  - Solid fraction
  - Nominal liquid composition of solutes [wt%]
  - Liquidus temperature

After the execution of program, the results are displayed as xxxx % Solut. =…, Cool.r. =…, where xxxx refers to alloy type; % Solut. refers to nominal liquid composition of alloying elements [wt%]; and cool.r. refers to the cooling rate of solidification process.

3.5 Ferrous-alloy module

In this thermodynamic-kinetic module, the main instruments of the convectional solute redistribution models, i.e., the material balance equations and Fick's laws of solute diffusion, were incorporated into the proper set of thermodynamic chemical-potential-equality equations, which relate the phase interface compositions to both the temperature and the phase stabilities. Depending on the alloy composition and cooling rate, the module determines the phase fractions and compositions of the liquid during solidification; and also calculates important thermophysical material data (Gibbs energy, enthalpy, entropy, specific heat capacity, thermal conductivity and density from the liquid state down to room temperature) for ferrous alloys containing C, Cr, Cu, Mn, Mo, Nb, Ni, Si, Ti and V.

The module makes use of experimental thermodynamic and phase diagram data as well as solute diffusion data from IET and National Academy of Sciences, which are fed in as measured values.
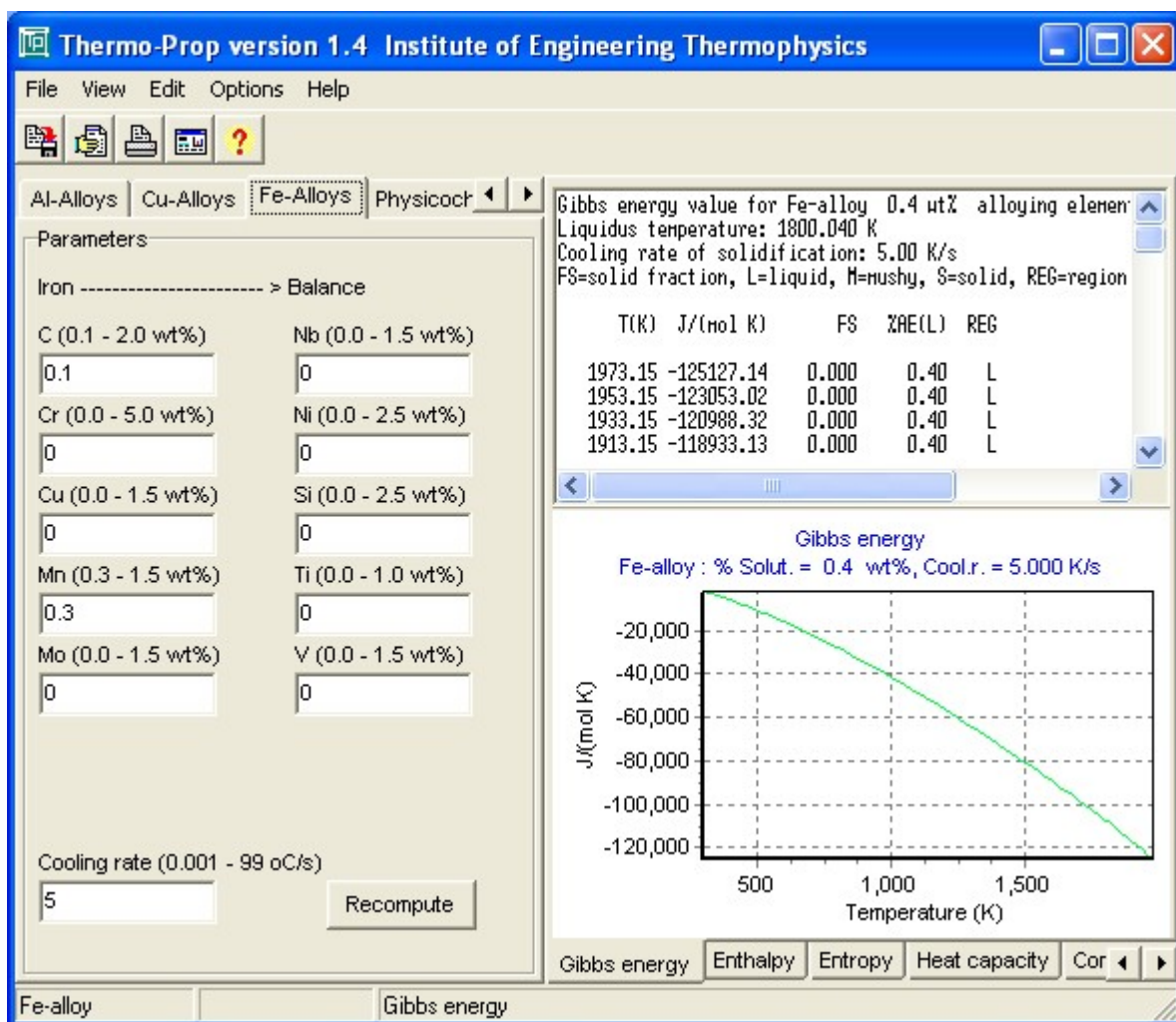
3.5.1 Input data

- **Composition**
  - Nominal composition [wt%] of alloying elements (i.e. solutes)
  - Recommended values given in "composition ranges" section

- **Cooling rate**
  - Cooling rate [°C/s] of solidification
  - Recommended values from 0.001 to 99°C/s]
  - The cooling rate causes different temperature range and location of the mushy zone in the described material properties

- **Data of the Thermo-Prop data bank**
  - Program's module contains thermodynamic data and solute diffusion data
  - Automatic input, not for user

3.5.2 Composition ranges

User should apply the recommended composition ranges given below.

- **Composition ranges [wt%] of alloying elements**
  - C: 0.0 - 1.0
  - Cr: 0.0 - 1.5
  - Cu: 0.2 - 2.5
  - Mn: 0.0 - 1.5
  - Mo: 0.0 - 1.5
  - Nb: 0.0 - 1.5
  - Ni: 0.3 - 2.5
  - Si: 0.5 - 5.0
  - Ti: 0.0 - 1.0
  - V: 0.0 - 1.5

3.5.3 Output data

- **Thermophysical data**
  - Gibbs energy
  - Enthalpy
  - Entropy
  - Specific heat capacity
  - Thermal conductivity
  - Density

- **Miscellaneous data**
  - Solid fraction
 - Nominal liquid composition of solutes [wt%]
  - Liquidus temperature

After the execution of program, the results are displayed as xxxx % Solut. =…, Cool.r. =…, where xxxx refers to alloy type; % Solut. refers to nominal liquid composition of alloying elements [wt%]; and cool.r. refers to the cooling rate of solidification process.

3.6 Heat-transfer module

Heat transfer module is used to determine the heat transfer coefficient at the metal/mould interface from cooling curves of actual casting process. The experimentally determined relationships between temperature and time within the mould and the casting are used in conjunction with finite difference technique to determine the magnitude of heat-transfer characteristics. The method, based on inverse solution, is well conditioned in the sense that it generates bounded solutions and never generates thermal characteristics oscillating with increasing amplitude.

Heat transfer is the driving force in solidification and also has a significant effect on the quality of the cast product. Knowledge of heat transfer phenomena is therefore essential for the improvement of production speed and productivity of the casting process.

The module can also be used to determine the heat transfer coefficient at the interface between two conducting media in other technological processes.
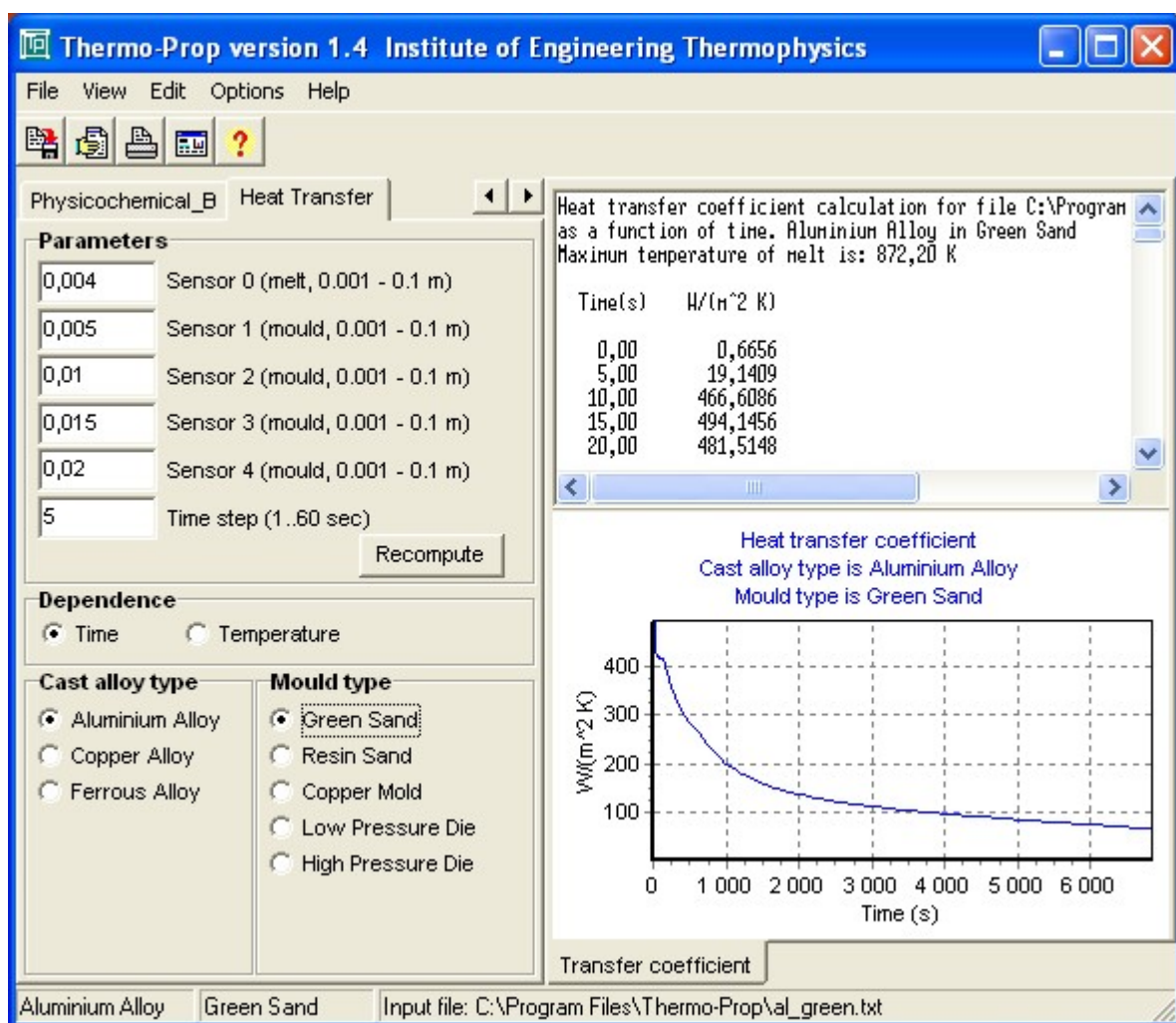
3.6.1 Input data

- Distance of thermocouples from casting/mould interface [m]; 0.001 – 0.1 m
- Time step of solidification process [s]; 1 …60 seconds
- Input file name; text file; array of input data: maximum 1400 rows
- Type of alloy material
- Type of mould material

3.6.2 Columns of experimental data

- 1st column: Time [s]
- 2nd column: Temperature data at the location of Sensor 1 in mould [^{o}C]
- 3rd column: Temperature data at the location of Sensor 2 in mould [^{o}C]
- 4th column: Temperature data at the location of Sensor 3 in mould [^{o}C]
- 5th column: Temperature data at the location of Sensor 4 in mould [^{o}C]
- 6th column: Temperature data at the location of Sensor 0 in melt [^{o}C]
  Note: Columns are separated by space. Five sensors are needed to gather temperature data.

- **Condition**
  Distance of sensors from casting/mould interface must satisfy condition:
  Sensor0 < Sensor1 < Sensor2 < Sensor3 < Sensor4

### 3.6.3 Output data

- Heat transfer coefficient [W/m^{2}K] as a function of time or temperature

3.7 Physicochemical_E (:Element) module

The module comprises physicochemical properties (surface tension and dynamic viscosity) in the liquid state for all the metallic elements in the periodic table.

In this module, the calculation algorithms are based on thermodynamic theory connected to physicochemical assessment data, as well as on regression formulas of experimental data.
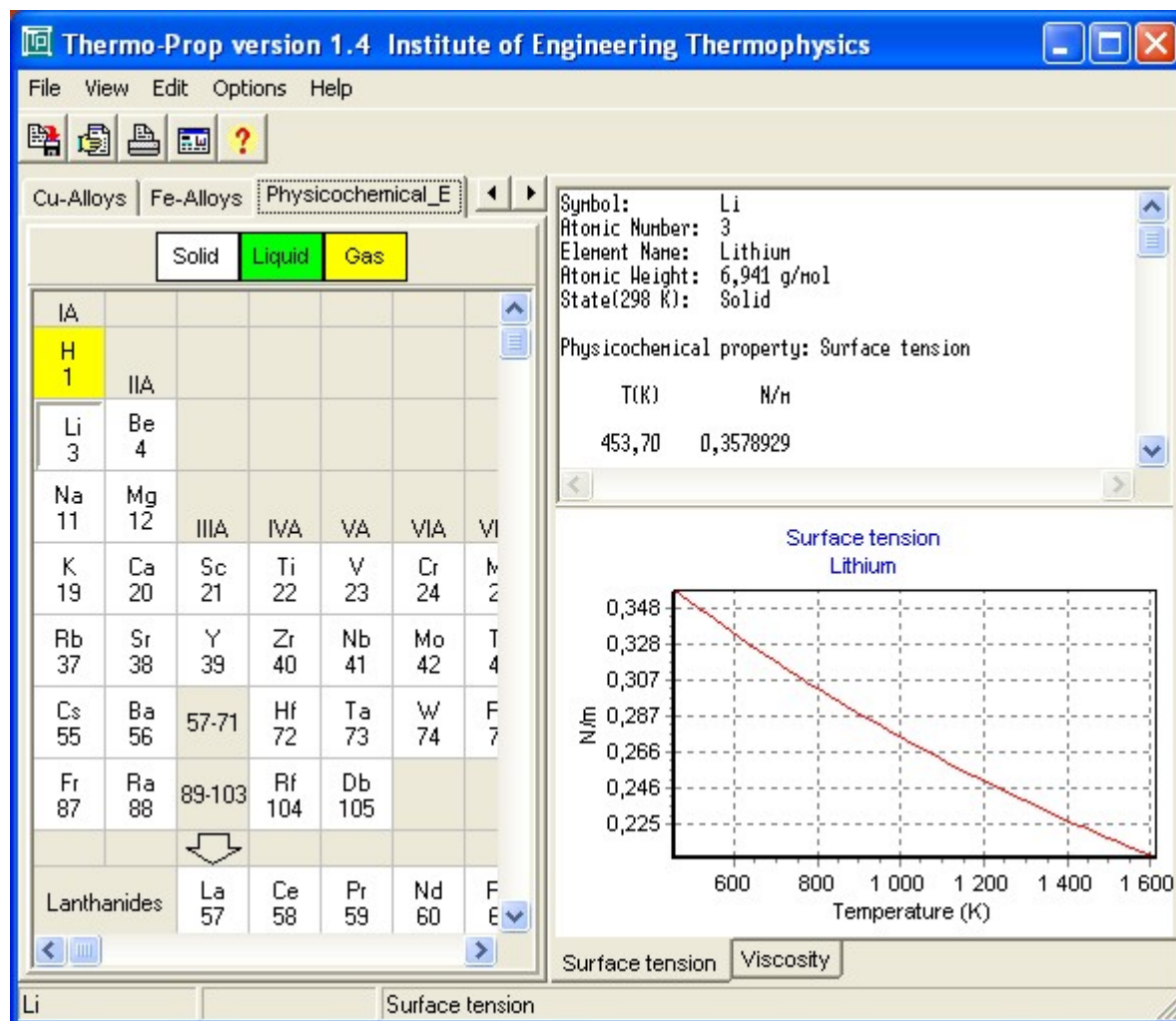
Note: Right-clicking on the periodic table panel initiates popup menu to display list of the elements and their corresponding basic properties.

3.7.1 Input data

- **Data of the Thermo-prop data bank**
  - Program's module contains physicochemical data
 - Automatic input, not for user

3.7.2 Output data

- **Physicochemical data**
  - Surface tension
  - Viscosity

For pure elements, the results are displayed as xx, where xx refers to element's designation (2 characters).

3.8 Physicochemical_B (:Binary-alloy) module

The module embraces physicochemical properties (surface tension and dynamic viscosity) in the liquid state for corresponding binary alloys of all the metallic elements in the periodic table.

The calculation algorithms are based on thermodynamic theory connected to physicochemical assessment data, as well as on regression formulas of experimental data.
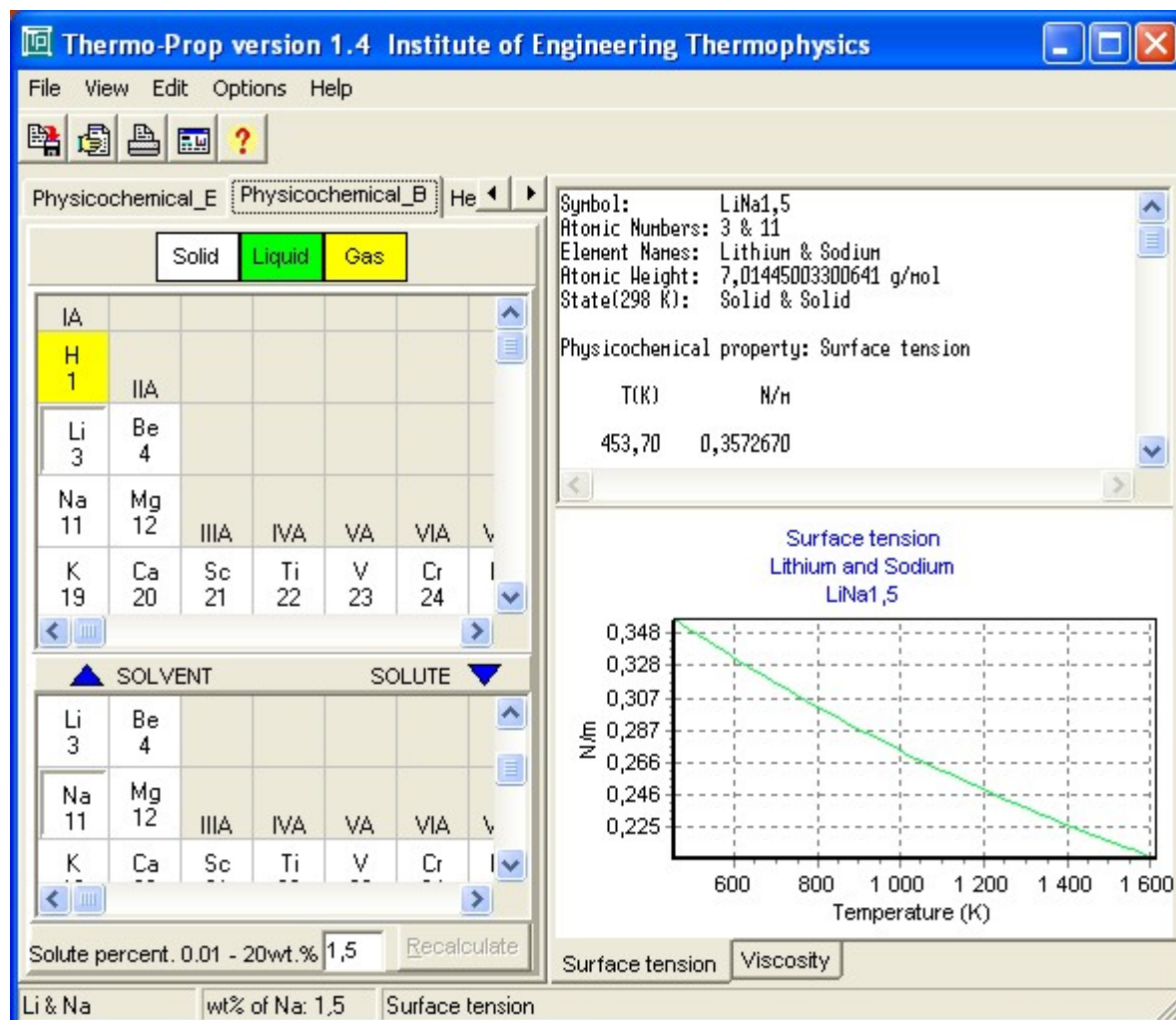
Note: Right-clicking on the periodic table panel initiates popup menu to display list of the elements and their corresponding basic properties.

3.8.1 Input data

• **Composition of selected solute**
User should apply the recommended composition ranges given below. Going beyond these ranges does not prevent the calculations but the program restricts itself to these composition ranges.
  • Nominal composition 0.01 to 20 [wt%] of solutes

• **Data of the Thermo-Prop data bank**
  • Program's module contains physicochemical data and interaction parameter data
  • Interaction parameter describes chemical interaction between the solvent and solute atoms
  • Automatic input, not for user

3.8.2 Output data

- **Physicochemical data**
  - Surface tension
  - Viscosity

After the execution of program, the results are displayed as xxxx%, where xxxx refers to alloy designation; % refers to nominal liquid composition of solute [wt%].

4. DESCRIPTION OF USER INTERFACE

4.1 Main menus

| File	View	Edit	Options	Help
Open	Toolbar	Copy test	Settings	Contents
Save as	Graphics	Copy bitmap	Units conversion	About
Print report	Text	Copy metafile		
Print graph				
Exit				

Shortcut for menu: Press "Alt" and select the appropriate letters for the main menu and submenu.

4.1.1 File menu

- **File - Open:** The File/Open menu opens Dialog, from where input file (for heat transfer calculation) must be loaded.

- **File - Save as:** In Save As menu, there are bitmap, metafile and enhanced metafile, in addition to text. The graphics or text is then save as a file.

- **File - Print report:** Panel to print report in text format.
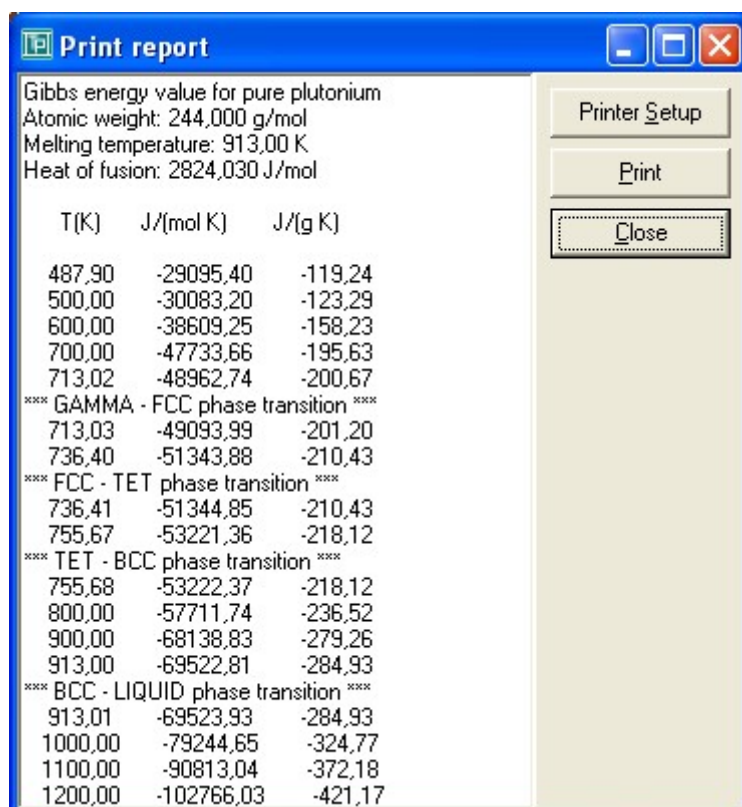
- **File - Print report:** Panel to print report in graph format.
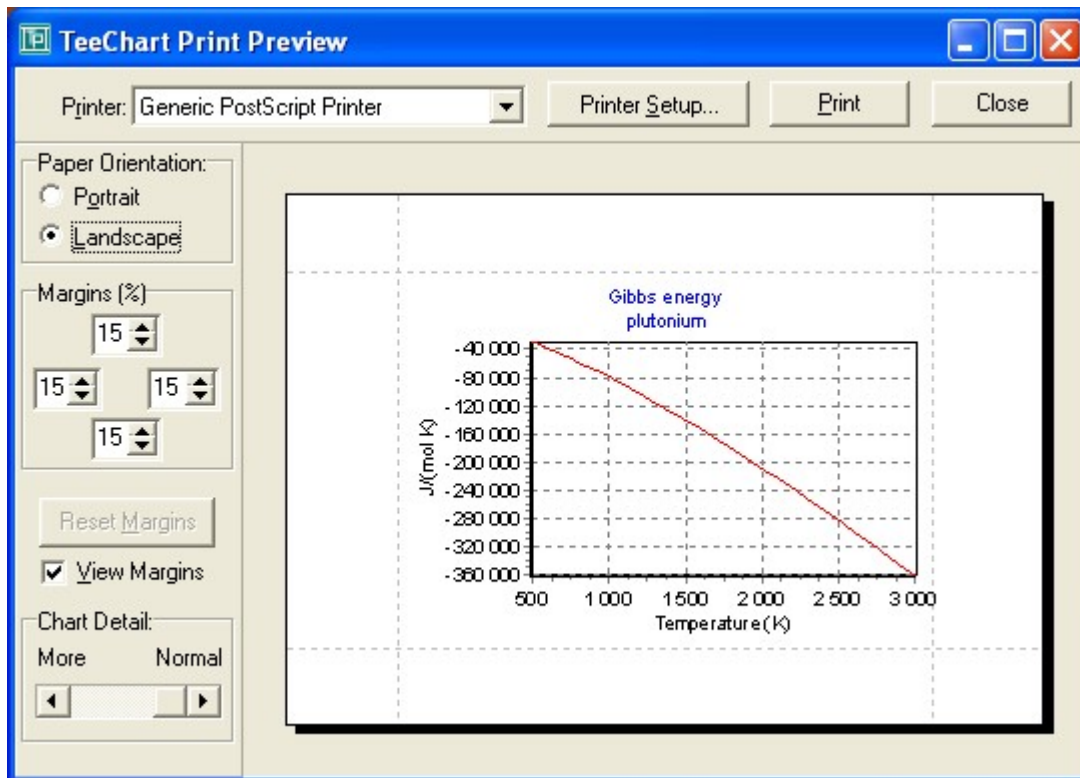
- **File - Exit:** Quit from the program.

4.1.2 View menu

- **View - Toolbar:** Enable/disable toolbar.
- **View - Graphics:** Enable/disable graphic panel.
- **View - Text:** Enable/disable text panel

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4.1.3 Edit menu

- **Edit - Copy text:** Possibility to send text to clipboard.
- **Edit - Copy bitmap:** Possibility to send graphics as bitmap to clipboard.
- **Edit - Copy metafile:** Possibility to send graphics as metafile to clipboard. Format of the metafile is determined by use of enhanced metafile option in Option menu.

4.1.4 Options menu

- **Options - Settings:** Possibility to add/exclude headers, annotations; to determine the format of metafile by use of enhanced metafile option; etc.
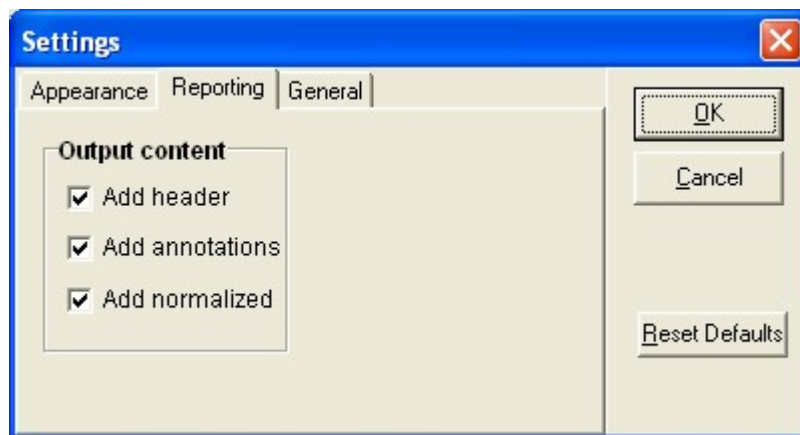
- **Options - Units conversion:** Possibility to select units to use.
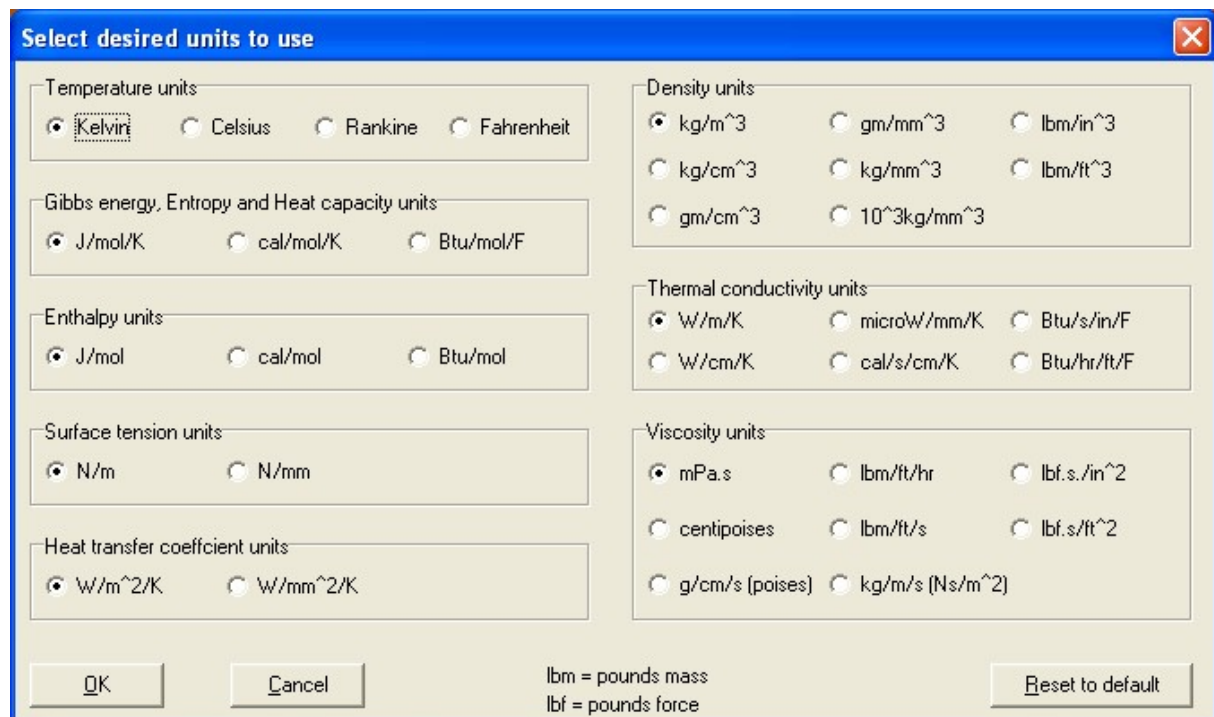
4.1.5 Help menu

- **Help – Thermo-Prop Documentation:** Displays the help contents for the program.
- **Help – About Thermo-Prop:** Shows the about form of the program.

4.2 Numerical input

The representation of number format varies from country to country. As such Thermo-Prop software has been internationalized.

As operands you can use numerical constants in any form (2, 2.0, 2e5, 2e-3) with decimal delimiter "period" or "comma", depending on your computer system configuration. If computer system uses "comma" as delimiter, for example, 2.4 corresponds to 2,4; then 2,4 can also be used as an input.

5. REFERENCE

Up-to-date information about Thermo-Prop software and documentation can be found on the web page **http://www.thermo-prop.com**

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