

Technical specification of the tender subject in the MATUR project

Subject: Thermocalc software

Requirements: Upgrade of existing software and databases at Designated Site: **11560**

SOFTWARE	Price (EUR)
▪ Thermo-Calc: Academic M&SS for NWL-99 Users, for next 3 years after the first year after purchase being free of charge concerning M&SS;	5 700.00
▪ Diffusion Module (DICTRA): Academic M&SS for NWL-99 Users, for next 3 years after the first year after purchase being free of charge concerning M&SS;	5 700.00
DATABASES	
▪ TCAI: TCS Al-based Alloys Database, Perpetual DNWL, version 9, Upgrade based on valid M&SS;	10 440.00
▪ TCAI: TCS Al-based Alloys Database, Perpetual DSUNLL, version 9, Upgrade based on valid M&SS; Qty 2, free of charge;	0.00
▪ SSOL: SGTE Solutions Database, Perpetual DNWL, version 9, Upgrade based on valid M&SS;	10 020.00
▪ SSOL: SGTE Solutions Database, Perpetual DSUNLL, version 9, Upgrade based on valid M&SS, Qty 2, free of charge;	0.00
▪ SSUB: SGTE Substances Database, Perpetual DNWL, version 7, Upgrade based on valid M&SS;	2 160.00
▪ SSUB: SGTE Substances Database, Perpetual DSUNLL, version 7, Upgrade based on valid M&SS, Qty 2, free of charge;	0.00
NEW DATABASES:	
▪ TCMG: TCS Mg-based Alloys Database, Perpetual DNWL, version 7, Upgrade based on valid M&SS;	11 325.00
▪ TCMG: TCS Mg-based Alloys Database, Perpetual DSUNLL, version 7, Upgrade based on valid M&SS, Qty 2, free of charge;	0.00
▪ TCTI: TCS Ti- and TiAl Alloys Database, Perpetual DNWL, version 6, Upgrade based on valid M&SS;	13 200.00
▪ TCTI: TCS Ti- and TiAl Alloys Database, Perpetual DSUNLL, version 6, Upgrade based on valid M&SS, Qty 2, free of charge;	0.00
Total Net	58 545.00

Requirements – minimum technical demands, that MUST BE MET:

Software Requirements:

1. Phase diagram calculations:

- Ability to generate binary, ternary, and multicomponent phase diagrams.
- Calculation of phase boundaries and critical points.
- Support for Scheil-Gulliver solidification simulations.
- Capability to plot potential diagrams and Pourbaix diagrams.

2. Thermochemical and thermophysical Properties Calculations:

- Calculation of specific heat, enthalpy, and heat capacity.
- Determination of heat of formation and phase transition temperatures.
- Lattice parameters, density and coefficient of thermal expansion calculations.
- Viscosity and surface tension of liquids.
- Interfacial energy and thermal conductivity, thermal resistivity and thermal diffusivity.
- Electrical resistivity, conductivity and other relevant properties.

3. Material Properties:

- Prediction of solubility limits and transformation temperatures.
- Calculation of non-equilibrium solidification properties, kinetic coefficients (atomic mobility, tracer diffusion, intrinsic diffusion, interdiffusion).
- Calculation of driving forces for phase formation.
- Calculation of mechanical properties (yield strength, hardness)
- Activities and chemical potentials of components.
- Generation of property diagrams for various materials.

4. Database and Compatibility:

- Access to comprehensive thermodynamic and kinetic databases.
- Compatibility with third-party databases and software.
- Ability to integrate with other simulation tools and custom code via SDKs

5. Technical Support and Training:

- Comprehensive installation and setup assistance.
- Training sessions for users to maximize software capabilities.
- Ongoing technical support and access to expert advice

6. User Interface and Usability

- Intuitive graphical user interface for easy setup and execution of calculations.
- Detailed user manuals, guides and access to online resources.
- Regular updates and improvements based on user's feedback.

7. DICTRA

The offer must also include the Add-on diffusion Module DICTRA to simulate diffusion-controlled reactions in multicomponent alloy systems.

This module should allow to simulate:

- ❖ Homogenisation of alloys,
- ❖ Micro segregation during solidification.
- ❖ Growth/dissolution of secondary phases, such as carbides, nitrides or intermetallics.
- ❖ Coarsening of precipitate phases.
- ❖ Allotropic phase transformations, such as austenite to ferrite in steel.

❖ Carburization, nitriding and carbonitriding of high-temperature alloys and steels. ❖ Interdiffusion in compounds, such as coating systems, dissimilar joints and others. ❖ Post weld heat treatment (interdiffusion and related phase changes). ❖ Sintering of cemented carbides.	
---	--