



SOFTWARE DELIVERY CONTRACT

1. Technical University Ostrava, Faculty of Metallurgy and Material Engineering

Registered seat: 17. listopadu 2172/15, 708 33 Ostrava - Poruba

Represented by: [REDACTED] Dean of the Faculty of Metallurgy
and Material Engineering

Authorized persons (for technical issues):

[REDACTED]

Business Identification Number: 61989100

Tax Identification Number: CZ61989100

(hereinafter referred to as the "Client")

a

2. GTT Gesellschaft für Technische Thermochemie und -physik mbH

Business seat/location: Kaiserstrasse 103, 52134 Herzogenrath, Germany

Represented by: [REDACTED]

Authorized persons (for technical issues):

[REDACTED]

Business Identification Number: HRB 3197

Tax Identification Number: DE121734435

Bank contact: Commerbank AG, Eschweiler

Account number: [REDACTED]

(hereinafter referred to as the "Contractor")

(hereinafter jointly also referred to as the "Contracting Parties")

Conclude on the below stated day, month and year this contract (hereinafter referred to as the "Contract"):

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I. INITIAL STIPULATIONS

1. The Contractor declares that it is authorized to distribute the software (specified in Article II of the Contract), to provide the corresponding license, service and technical support to the software, and that it is authorized to conclude this Contract and duly fulfill the obligations specified in it.
2. In relation to the result of the tender proceedings related to the public contract called "Software for assessing metallurgical processes", initiated pursuant to Act No. 134/2016 Coll., on Public Procurement (hereinafter referred to as "ZVZ"), as amended, (hereinafter referred to as the "Public Contract"), the Client and the Contractor conclude this Contract for the purpose of implementing the "Infrastructural support of postgraduate study programs FMMI VŠB-TUO" project, reg. no. CZ.02.1.01/0.0/0.0/16_017/0002668 (hereinafter referred to as the "Project").

II. SUBJECT OF THE CONTRACT

1. The Contractor is obliged to supply to the Client software **FactSage 7.2 plus databases FACT Pure Substances, FACT Solution, GTT Oxides (GTox), Steel (FSstel) and Light Metals (FTlite)** (hereinafter referred to as the "Software") and to provide at least a permanent and open ended software license for two independent installations and for one local network with up to 20 simultaneous client accesses, and also (provided the Software will be provided by the means of a physical carrier) to allow the Client to obtain the ownership right to the physical carrier of the Software data. The contractor is obliged to supply the Software including a provision of an unexclusive license, which is granted for the entire time the asset ownership rights to the Software exist. The minimal technical Software parameters are stated in Appendix 1 of this Contract.
2. Together with the delivery of the Software, the Contractor is also obliged to provide the Client with the following services:
 - a) Technical support for a period of 6 years after the Software is delivered,
 - b) Training of the Client employees in relation to operating and working with the Software for at least 2 persons in the extent of 3x8 hours in the Client laboratories or online,
 - c) Software documentation in the printed or electronic form or for downloading online, either in the Czech or English language.
3. The Client undertakes to accept the Software and to pay the Contractor the price in the amount and under the conditions agreed on in this Contract.
4. The Software has to also comply with the requirements stated in the Invitation to Submit Offers for the Public Contract and Contractor Offers, with the stipulation that these documents form an appendix of this Contract, however, they are not physically provided and are stored by the Client.
5. The Contracting Parties declare that the Software is a standard software provided on a commercial basis and the stipulations of Section 61 of Act No, 121/2000 Coll., on Copyright and Rights Related to Copyright and on Amendment to Certain Acts (hereinafter referred to as the "Copyright Act") as amended, thus do not apply to it.

III. PRICE AND PAYMENT CONDITIONS

1. The Contracting Parties agree on the total and final price in the amount of **1,100,239.00 CZK**, excluding VAT, the VAT rate of 0 % (VAT due to the recipient), price including VAT **1,100,239.00 CZK**.
2. The total price cannot be exceeded, with the exception of cases of a legal change of the VAT rate. The total price should include all expenses of the Contractor related to the fulfilment of its obligations arising from this Contract, i.e. it should include the Software delivery, including provision of the corresponding license and documentation, technical support, all transport expenses, all applicable taxes, customs duties, fees related to the corresponding payments – bank transfer of the total price, other payments and all other related expenses.
3. The Client will pay the price for fulfilling the subject of the Contract pursuant to Paragraph 1 of this article upon the Software delivery (provision of the license), including the delivery of the corresponding documentation, based on the appropriate tax document - invoice.

4. The invoice should be payable within 30 calendar days after the delivery of the appropriate invoice to the Client. The invoice issued by the Contractor has to include the project name, project registration number and identification of this Contract. Furthermore, the invoice has to comply with the conditions prescribed for tax and accounting documents pursuant to Act No 563/1991 Coll., on Accounting, as amended, and Act No. 235/2004 Coll., on Value Added Tax, as amended. Should the invoice not fulfill these conditions or should the price or VAT be charged incorrectly, the Client will not pay it and will return it within 20 days after its delivery for corrections. In this case the payment period of the invoice in question starts running again from the moment the corrected or newly issued invoice is delivered to the Client. The Contractor should deliver the invoice to the Client by the means of certified mail to the address of the Client or electronically to the following email addresses: [\[REDACTED\]@ \[REDACTED\].cz](mailto: [REDACTED]@ [REDACTED].cz) and [\[REDACTED\]@ \[REDACTED\].cz](mailto: [REDACTED]@ [REDACTED].cz)
5. The value added tax should be charge in accordance with the valid stipulations of Act No. 235/2004 Coll., on Value Added Tax, as emended (hereinafter referred to as the "VAT").
6. The Client should pay all payments pursuant to this Contract to the Contractor's account stated in the heading of this Contract.
7. Should the Contractor become an unreliable payee pursuant to Section 106a of the VAT Act as of the day of the taxable payment, the Client should have the right, pursuant to Section 109 of the VAT Act, to make a security payment of the VAT directly to the account of the appropriate financial authorities; in this case the Client is not obliged to pay the VAT amount to the Contractor and the Client will thus pay the Contractor only the given due amount, excluding VAT.
8. The Contractor declares that the bank account stated in this Contract or on the corresponding invoice is its account, which has been published by the tax administrator in a way that allows for remote access in compliance with the stipulations of Section 96 of the VAT Act. The Contractor is obliged to state only such an account on its invoice, which has been published by the tax administrator in compliance with the VAT Act. Should the published account identification change during the duration of this Contract, the Contractor undertakes to inform the Client about such a change in writing and without any unnecessary delay. Pursuant to the stipulations of Section 109, Paragraph 2, Letter c) of the VAT Act, the recipient of a taxable payment is responsible for unpaid taxes arising from such a payment. It means that if the payment in question is made fully or partially by the means of a bank transfer to a different account than the account of the given contractor, which has been published by the tax administrator in a way that allows for remote access, the Client should pay the given price only to an account, which is a published account pursuant to the stipulations of Section 96 of the VAT Act. Should it ever come to light that the Contractor's account, onto which the Contractor requests the payment of the price of the subject of the Contract, is not a published account, the Client is not obliged to make such a payment to the account in question; this situation does not represent a delay of the payment for the price of the subject of the Contract by the Client.
9. Paragraphs 7 and 8 of this Article of the Contract apply only if they are relevant for the given Contractor.

IV.

IMPLEMENTATION TIME AND LOCATION

1. The Contractor is obliged to deliver the Software (including provision of the corresponding license, employee training and delivery of the related documentation) within 21 calendar days after the Contract comes into effect. An exception to the deadline stated in the previous sentence is formed by technical support, which will be provided for a period of 6 years after the Software delivery. The Contractor is obliged to announce the Software delivery date at least 5 days in advance. Otherwise the Client is not obliged to accept the Software; such a situation does not represent a breach of the Client's obligation to accept goods or to provide cooperation.
2. The Software delivery location should be the above stated registered seat of the Client – Technical University Ostrava, Faculty of Metallurgy and Material Engineering, 17. listopadu 2172/15, 708 33 Ostrava - Poruba.

V.

DELIVERY OF THE SUBJECT OF THE CONTRACT

1. The Software is considered delivered as of the moment of its acceptance by the Client at the implementation location. The Contractor shall prepare a transfer protocol for transferring and accepting the Software. The protocol has to be signed by both Contracting Parties. The Client is not obliged to accept the Software if it does not comply with the conditions specified in this Contract. When the Software is accepted with defects or some unfinished parts, the acceptance moment for the purpose of this Contract should be the moment when such defects are fixed and unfinished parts completed.
2. The transfer protocol should include the following:
 - a) Software name, including its production number and serial number (provided they exist), Contract name,
 - b) Identification of the Client and the Contractor,
 - c) Date and location,
 - d) Names and signatures of the Client's and Contractor's representatives.
3. The Contracting Parties explicitly agree to exclude the stipulations of Section 2093 of the Civil Code. It means that should the seller supply the buyer with a greater quantity of the goods (Software) than it has been agreed on in this contract, the corresponding purchase contract is not concluded for the surplus quantity even if the buyer does not reject the surplus goods without an unnecessary delay.

VI.

TECHNICAL SUPPORT

1. The Contractor undertakes to provide the Client (or to organize at its own expense its provision) with a complete technical support for a period of 6 years after the Software delivery. The support should include: solving technical issues related to the use of the Software (so-called hot-line), Software upgrades, updates and patches, other updates (security and functional repairs), and solving problems of the Client related to the use of the Software.
2. The Contractor undertakes to ensure the technical support, the so-called. hot-line in electronic as well as phone form. Technical support will be available in the Czech or English language during the working days (Czech Republic) between 9.00 a.m. and 3.00 p.m.: tel.: **0049-2407-59533** and email: **info@gtt-technologies.de**.
3. The Contractor should commence solving any problem within the frame of its technical support within 5 working days after such a problem is reported.
4. As a part of the technical support provision, the Contractor undertakes to provide consultations related to the use of the Software and its interaction with the given hardware, operation environment and other software products. The extent or number of consultations is not limited.

VII.

SANCTION STIPULATIONS

1. Should the Contractor be late with the delivery of the Software pursuant to Paragraph 1, Article IV of this Contract, the Client undertakes to pay the Client a contractual penalty amounting to 0.05% of the total price, excluding VAT, for each started day of such a delay.
2. Should the Contractor not comply with the deadline stated in Article VI of this Contract, the Contractor should be obliged to pay the Client a contractual penalty amounting to 0.02% of the total price, excluding VAT, for each started day of such a delay.
3. The stipulations related to contractual penalties should have no impact on the right of the harmed contracting for compensation for a given damage in the extent that exceeds the contractual penalty pursuant to this Contract.

4. Should the Client be late with a payment of a given invoice, the Contractor should have the right to request a payment of the corresponding interest on late payment.

VIII. OTHER

1. The Contractor undertakes to archive all documents related to the fulfilment of this Contract and to allow the Client to access these archived documents at any time until December 31st, 2028, unless the Czech legal regulations specify a longer period for some of these documents. The Client should have the right to obtain the above stated documents free of charge within ten years after the termination of the technical support pursuant to this Contract.
2. The Contractor undertakes to allow all parties that have the right to oversee the Project, sources of which are used for paying the price pursuant to the Contract, to inspect all documents related to the fulfilment of this Contract. Moreover, the Contractor, as a mandatory person pursuant to Section 2, Letter e) of Act No. 320/2001 Coll., on Financial Control in Public Administration, as amended, is obliged to participate in the financial control process by, for example, allowing the OP VVV control body (Ministry of Education, Youth and Sport) access to also those parts of individual offers, contracts and related documents, which are subject to the protection pursuant to special legal regulations (for example, business secrets or secret facts), provided the requirements specified by the given legal regulations [and particularly Act No. 255/2012 Coll., on Controls (Control Code), as amended] are fulfilled; the Contractor in its contracts with its subcontractors should bind them to allow the OP VVV control body to control the subcontractors in the same extent.

IX. CONTRACT VALIDITY AND EFFECTIVENESS

1. The Contract becomes valid as of the day of its signing by both Contracting Parties. The Contract becomes effective as of the day it is published in the Register of Contracts pursuant to Act No. 340/2015 Coll., on the Register of Contracts.
2. Each Contracting Party has the right to withdraw from this Contract only for reasons specified in this Contract.
3. The Client has the right to withdraw from this Contract in the following cases:
 - a) The Contractor is late with the Software delivery for a period that is longer than 30 days in comparison with the date specified in this Contract;
 - b) Should the Software have defects, which make it unusable, or should it not have the characteristics, which the Client had specified or about which the Contractor had ensured the Client;
 - c) The problem response period within the frame of the technical support is not complied with at least on three problem-solving occasions;
 - d) The Contractor loses its ability to duly comply with the obligations arising from the Contract during the Contract duration.
4. The Contractor has the right to withdraw from this Contract if the Client is late with the payment of the price pursuant to this Contract for a period that is longer than 60 days, despite the fact that the Client was notified about such a delay by the Contractor in writing.
5. Each Contracting Party has the right to withdraw from this Contract in writing if the assets of the other Contracting Party become subject to insolvency proceedings, during which the court declares bankruptcy, if the other Contracting Party submits a proposal for the initiation of insolvency proceedings on its own, or if the other Contracting Party enters liquidation proceedings.

6. The authorized Contracting Party has the right to withdraw from this Contract without any time limitation in relation to the moment when the given breach of this Contract that establishes the right to withdraw from this Contract occurs in cases specified in this Article of this Contract. The effects of the withdrawal from the Contract become effective as of the day the corresponding written notification about the withdrawal is delivered to the other Contracting Party or on a later day stated in the written withdrawal notification.
7. Termination of the effectiveness of this Contract should not have any impact on the stipulations of the Contract that are supposed to remain effective even after the termination of this Contract.
8. Should the contractor provide only a part of the subject of the Contract, the Contracting Parties agree that the Client should have the right to withdraw from the Contract and to decide if it wants to accept the provided part of the subject of the Contract or not. The Contracting Parties hereby exclude the use of Section 2004, Paragraphs 2 and 3 of the Civil Code.

**X.
JOINT STIPULATIONS**

1. The Contracting Parties explicitly declare that they do not wish any rights and obligations to be deduced from the current or future practices established between the Contracting Parties or from generally established customs or customs from the area related to the subject of this Contract beyond the frame of the explicit stipulations of this Contract, unless it is explicitly stated otherwise in this Contract. Apart from the above stated facts, the Contracting Parties declare that they are not aware of any business customs or practices established between them so far.
2. The Contracting Parties agree not to apply the stipulations of Section 557 of the Civil Code, which specify that if a used expression can be interpreted in different ways, it should be interpreted to the disadvantage of the party that used it first.
3. The Contracting Parties agree to exclude interest and expenses pursuant to the stipulations of Section 1806 and Section 1932, Paragraph 2 of the Civil Code.
4. Should either of the Contracting Parties release a quittance or return a bill of debt to the other Contracting Party without the given debt being paid, such an act does not mean that the debt has been forgiven. Should the quittance in question be issued for a claim principal, it does not apply to the given claim accessories.
5. Pursuant to the stipulations of Section 1765 of the Civil Code, the Contractor should bear the risk of a change of circumstances, particularly in relation to increased expenses related to the delivery of the goods pursuant to this Contract.
6. The rights and obligations of the Contractor arising from this Contract or in relation to it must not be assigned to any third party without a prior written approval issued by the Client.
7. Offsetting the claims of the Contractor arising from this Contract is not permitted. The Contracting Parties exclude the application of the stipulations of Section 1987, Paragraph 2 of the Civil Code in relation to the claims arisen to the Client based on this Contract. The Contracting Parties agree that even unsure and/or indefinite claims can be offset, however, only until a possible legal action related to the subject of this Contract is initiated.
8. The authorized persons, stated in the heading of the Contract, are not authorized to act in a way that could directly result in a change of this Contract or its subject. The Contracting Parties have the right to change their respective authorized persons, however, they are also obliged to notify the other Contracting Party about such a change in writing.

**XI.
FINAL STIPULATIONS**

1. The Contracting Parties undertake to comply with the rules of the Research, Development and Education Operation Program.

2. Should the Contractor cease to exist without any legal successor, the Client should still have the right to use the Software pursuant to this Contract.
3. Should this Contract require a written form for certain acts, email exchanges or exchanges of other electronic messages will not be considered a written form for these purposes.
4. The Contracting Parties agree that should there be a contradiction between the stipulations of individual appendixes and stipulations of this Contract, the stipulations of this Contract should take precedence.
5. This Contract includes a complete agreement on the subject of the Contract and all requirements, which the Contracting Parties should have and wanted to agree on in this Contract, and which they consider important for the binding character of this Contract. Neither any of the acts of the Contracting Parties executed during the negotiations about this Contract, nor the acts executed after the conclusion of this Contract should be interpreted in contradiction with the explicit stipulations of this Contract and should not establish any obligation of either of the Contracting Parties.
6. The Contractor cannot assign its rights and obligations arising from this Contract to any third party without the approval of the Client.
7. This Contract has been executed in three identical copies. The Client should receive two of the copies and the Contractor one copy.
8. Appendix 1 – Software Technical Parameters – forms an integral part of this Contract.
9. The Contracting Parties identically declare that they are aware of all legal consequences arising from this Contract. The Contracting Parties agree with all its stipulations, with which they have acquainted themselves in detail.

Ostrava, date: _____

Location: Herzogenrath
date: November 14, 2018

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**Technical University Ostrava, Faculty of
Metallurgy and Material Engineering**

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**GTT Gesellschaft für Technische
Thermochemie und -physik mbH**

Technical specification of the SW for assessing metallurgical processes

The subject of the public contract is the provision of a permanent, open ended software license for two independent installations and for one local network with up to 20 simultaneous client accesses, designed for analyses of a thermodynamic equilibrium state of individual systems, in which phase or chemical changes can take place (i.e. for analyses of chemical reactions in a system, related to heat development or absorption). The software has to particularly allow for calculating the composition of steel slag, simultaneously with the development of nonmetal inclusions in the liquid steel, in relation to the selected composition of the slag and creation of the corresponding phase diagrams.

The thermodynamic calculations of an equilibrium phase composition of n-dimensional systems (binary, tertiary, quaternary to multicomponent systems) of the reacting systems have to be based on the thermodynamic balance criteria and they have to seek the minimal values of the Gibbs energy under constant temperature, pressure and chemical composition.

The software has to also allow for calculating the kinetics of individual phase transformations in solid and liquid systems (substances), while focusing on liquid alloys, particularly steels, and slags (oxides, silicates, salts), together with the databases of the necessary thermodynamic and kinetic parameters.

A part of the subject of the contract is also formed by the delivery of the necessary thermodynamic and kinetic parameters of individual materials, particularly steels, slags and nonferrous metals.

SW for assessing the metallurgical processes must meet the following minimal criteria:

| Basic technical parameters | |
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| General requirements for the SW for assessing metallurgical processes | |
| 1) | SW must consist of a series of information, databases, calculation and manipulation modules that access various pure substance and solution databases applicable for industrial, governmental and academic users, especially in materials science and steel metallurgy and non-ferrous metallurgy, |
| 2) | Users must have the access to databases of thermodynamic data for thousands of compounds as well as to evaluated and optimized databases for hundreds of solutions of metals, liquid and solid oxide solutions, molten and solid salt solutions, aqueous solutions, etc. |
| 3) | SW must have the automatic accesses to these databases. The evaluated databases for oxides, slags, etc. have been developed by optimization of literature data using advanced modelling techniques. SW must also enable the access to the databases for alloy solutions and the databases for steels, light metal alloys and other alloy systems. |
| 4) | SW must be able to calculate the conditions for multicomponent, multiphase equilibria, with a wide variety of tabular and graphical output modes, under a large range of constraints. For example, general N-component phase diagram sections can be easily generated with a wide choice of axis variables; metal/slag/gas/solid equilibria can be accurately calculated, tabulated and plotted for industrial systems; multicomponent predominance and EpH diagrams can be readily produced; the course of equilibrium or non-equilibrium solidification can be followed; complex heat balances can be computed; and so on. |
| 5) | SW must be able to: <ul style="list-style-type: none"> ✓ Scan the databases and to display the standard state thermodynamic properties of the compound species and to list the solution phases. ✓ Copy, enter, edit, list and store data in a user's private compound (pure substances) databases. ✓ Enter, edit, list and store non-ideal mixing properties in a user's private solution databases. ✓ Calculate changes in extensive thermodynamic properties (H, G, V, S, Cp, A) for a single species, a mixture of species or for a chemical reaction. The species may be pure elements, stoichiometric compounds or ions (both plasma and aqueous ions). ✓ Calculate and plot isothermal predominance area diagrams for one-, two or three-metal systems using data retrieved from the compound databases. |

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| <ul style="list-style-type: none"> ✓ Generate isothermal Eh vs. pH (Pourbaix) diagrams for one-, two or three-metal systems using data retrieved from the compound databases that also include infinitely dilute aqueous data. ✓ Calculate the concentrations of chemical species when specified elements or compounds react or partially react to reach a state of chemical equilibrium. ✓ Calculate, plot and edit unary, binary, ternary and multicomponent phase diagram sections. The resulting phase diagram must be automatically plotted. It must be possible to calculate and plot: classical unary temperature versus pressure, binary temperature versus composition, and ternary isothermal isobaric Gibbs triangle phase diagrams; two-dimensional sections of a multi-component system where the axes are various combinations of T, P, composition, activity, chemical potential, etc.; predominance area diagrams of a multicomponent system (e.g. Fe-Ni-Cr-O) where the phases are real solutions such as mattes, slags and alloys; etc. ✓ Generate a consistent set of Gibbs energy parameters from a given set of experimental data using known Gibbs energy data from well-established phases of a particular chemical system. ✓ Post-process the output from calculations performed in the SW and produces a variety of plots from a single set of equilibrium tables. ✓ Edit mixtures and streams for input to the SW. ✓ Display, edit and manipulate the various figures and phase diagrams produced by SW. It must be particularly well suited for treating figures calculated by the SW. ✓ Calculation of viscosities of single-phase liquid slags and glasses. ✓ Compute optimal conditions for material and process design by coupling SW with the Mesh Adaptive Direct Search (MADS) algorithm for nonlinear optimization. |
| <p>6) SW must have these options:</p> <ul style="list-style-type: none"> ✓ Both 1-dimensional phase mapping (finding phase transitions) and 2-dimensional phase mapping (to create a wide variety of proper phase diagrams) ✓ Multicomponent Scheil-Gulliver Constituent Diagrams for visualizing the solidification of melts under Scheil-Gulliver constraints. ✓ Target calculations with various type of targets and target variables. ✓ macro processing language to automate phase equilibrium and phase diagram calculations. ✓ the calculation of a very wide range of proper publication-ready phase diagrams, and also the easy semi-automatic addition of iso-activity lines and isobars. ✓ Export of the thermochemical data from the databases to application-specific data-files and their using with additional software such as multi-platform, multi-language programmer's library, the thermochemistry add-in for Microsoft Excel, and the software component library for process modelling. |
| <p>7) SW must have these possibilities for results evaluation:</p> <ul style="list-style-type: none"> ✓ Equilibrium results must contain the information on the complete equilibrium state of the chemical system, including information on metastable phases and extensive property balances. ✓ Results from equilibrium calculations can be displayed in tabular and graphical form, as well as saved to text files and Excel spreadsheets. ✓ Post-processor of SW must allow a user to edit the results of a calculation and save customized outputs as templates. ✓ The generation of various types of phase diagrams for systems containing stoichiometric phases as well as solution phases, and any number of system components. |

General requirements for the selected thermo-dynamic databases
The SW must contain minimally these databases which allow the thermodynamic calculation of metallurgical processes during steel and non-ferrous production. For example, it means the calculation of slags systems and inclusion removal during processing of steel and prediction of the chemical composition of inclusions during interaction with slag system, also with drawing of ternary diagrams.

8) **The pure substance database** must contain Gibbs energy data for pure substances, stoichiometric compounds, as well as gaseous and aqueous species. It contains all necessary

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| <p>substances to properly consider a gas phase, as well as stoichiometric condensed phases which may be formed as inclusions.</p> |
| <p>9) The solution database collection must consist of a number of solutions, which are relevant for thermochemical equilibrium calculations in metallurgical systems. The solution database contains oxide solutions. There are all stoichiometric solid and liquid oxide compounds thermodynamically consistent with the solution database. As an oxide database, the solution database is essential for calculations involving slags.</p> |
| <p>10) The solution database must contain data for pure oxides and oxide solutions of more than 18 elements, as well as for dilute solutions I in the molten (slag) phase.</p> |
| <p>11) Major solution phases in the oxide database → the Liquid/Glass Solutions: OXIDE liquid/glass → oxides of:</p> <ul style="list-style-type: none"> ✓ Al, As, B, Ba, Sr, Ca, Co, Cr(II), Cr(III), Cu(I), Fe(II), Fe(III), K, Mg, Mn(II), Mn(III), Na, Ni, P, Pb, Si, Sn, Ti(III), Ti(IV), Zn, Zr + (S in dilute solution (<10%)). ✓ Oxide liquid/glass containing sulfate → oxides of: Al,As,B,Ca,Fe(III),K, Mg, Mn(II), Na, Ni, Pb, Si, Ti(III), Ti(IV), Zn,Zr + SO₄ in dilute solution (< 10 weight %). ✓ Oxide liquid/glass containing carbonate → oxides of: Al, As, B, Ca, K, Mg, Na, Si, Ti(III), Ti(IV), Zr + CO₃ in solution (< 40 weight %). ✓ Oxide liquid/glass containing water/hydroxide → oxides of: Al, As, B, Ca, Fe(II), Fe(III), K, Mg, Mn(II), Na, Si, Ti(III), Ti(IV), Zn, Zr + OH/H₂O in dilute solution (< 10 weight %). ✓ Oxide liquid/glass containing iodide → oxides of: Al, As, B, Ca, Fe(II), K, Mg, Mn(II), Na, Si, Ti(III), Ti(IV), Zr + I in dilute solution (< 10 weight %). ✓ Oxide liquid/glass containing fluoride and chloride → oxides of: Al, As, B, Ca, Co, Cr(II), Cr(III), Cu(I), Fe(II), Fe(III), K, Mg, Mn(II), Na, Ni, Pb, Si, Sn, Ti(III), Ti(IV), Zn, Zr + (F, Cl in dilute solution (<10%)). |
| <p>12) Solid Solutions: The oxide database must contain a large amount of solid solution phases relevant for metallurgical applications, such as Spinel (cubic); Spinel (tetragonal); Monoxide Solutions; Aluminates of Sodium and Calcium, Phosphates of Calcium and Magnesium; CaF₂, Wollastonite; Ca₂SiO₄ Solutions, Corundum, Calcium Ferro-aluminate solutions, Aluminates of Calcium, Strontium and Barium etc.</p> |
| <p>13) Stoichiometric Solid Oxides: the oxide compound database for evaluation and optimization of properties for more than 350 stoichiometric compounds must be included.</p> |
| <p>14) The solution database must allow the thermodynamic and phase equilibrium calculations involving liquid metal – cryolitic bath – Al₂O₃-based oxides in alumina reduction electrolysis cells, and for molten aluminium treatment with fluoride fluxes. The solution database can be a self-contained database for the Al-Mg-Na-Li-Ca-F-O-C system. No extra phases from other databases are needed for this 8-component system (except Al-Ca and Mg-Ca stoichiometric intermetallic phases Al₄Ca, Al₂Ca, Mg₂Ca, etc..., and the Li-Mg-BCC and Mg-Li-HCP solid solutions). The element "C" refers to the solubility of Al₄C₃ in presence of dissolved metal (with Al₄C₃(s) and Al₄O₄C(s) saturations) and the solubility of CO₂(g) (in the form of carbonates) in the NaF-AlF₃-CaF₂-Al₂O₃ base electrolyte. A density model (taking into account excess volume upon mixing) and a viscosity model could be available for the NaF-AlF₃-CaF₂-Al₂O₃-LiF-MgF₂ electrolyte as a function of temperature and composition.</p> |
| <p>15) The solution database: The SW must contain a number of solutions and corresponding compounds, some of which are very relevant for metallurgical applications. For example:</p> <ul style="list-style-type: none"> ✓ The database for system the S-Cu-Fe-Ni-Co-Cr-Mn system for calculating metal/liquid sulphide/solid sulphide/gas equilibria, for example during hot corrosion or for inclusion formation in steelmaking. ✓ The matte smelting system S-Cu-Fe-Ni-Co-Pb-Zn-As designed for calculation of matte/slag/metal equilibria and is consistent with other parts of databases. ✓ Dilute liquid alloys: Liquid Fe containing Ag, Al, B, Ba, C, Ca, Ce, Co, Cr, Cu, H, , La, Mg, Mn, Mo, N, Nb, Ni, O, P, Pb, , S, Si, Sn, ,Ti, V, W, Zr. ✓ Non-ideal aqueous solution of many solutes with Pitzer parameters. |
| <p>16) The solution database must contain also salt solutions.: The salt compound database must contain all stoichiometric solid and liquid salts and must be thermodynamically consistent with the solution database. Also, a density model can be available for some molten salt systems. The solution databases must contain data for pure salts and salt solutions. The salt database should contain more than 70 solution phases and more than 210 compounds.</p> |

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| 17) | The solution database must contain also infinite dilution properties for aqueous solute species, for pure solid compounds and gases which must be thermodynamically consistent with the part for aqueous solution database. |
| 18) | The thermodynamic database can also allow equilibrium calculations in the Al-(Si-Ca-Mg-Fe-Na)-C-O-N-S system at very high temperatures |
| 19) | The oxide database (for slag systems) must contain the assessment of the Al ₂ O ₃ -Al ₂ S ₃ -CaF ₂ -CaO-CaS-CaSO ₄ -CrO-Cr ₂ O ₃ -CrS-FeO-Fe ₂ O ₃ -FeS-K ₂ O-K ₂ S-K ₂ SO ₄ -Na ₂ O-Na ₂ S-Na ₂ SO ₄ -MgO-MgS-MgSO ₄ -MnO-Mn ₂ O ₃ -MnS-P ₂ O ₅ -SiO ₂ -TiO ₂ -ZnO system. It must contain more than 125 binary, 115 ternary and 5 quaternary fully assessed systems. Other than the liquid slag, the database must contain more than 100 solid solution phases and more than 640 stoichiometric phases. It would be great, if the database can be accompanied by a "Slag Atlas" in PDF form, which shows the relevant calculated phase diagrams and corresponding phase diagrams and experimental information from the scientific literature. |
| 20) | <p>The steel database must include also a "Tramp elements" to allow calculations relating to recycling and removal of unwanted impurities to be performed, for example Al, B, , C, Ca, Ce, Co, Cr, Cu, Fe, Hf, La, Mg, Mn, Mo, N, O, Nb, Ni, P, Pb, S, Sb, Si, Sn, Ta, Te, Ti, V, W, Zn, Zr. The database must contain many completely assessed binary alloy systems, together with ternary and quaternary systems for which assessed parameters must be available for phases of practical relevance. As such, the database must intended to provide a sound basis for calculations covering a wide range of steelmaking processes, e.g.:</p> <ul style="list-style-type: none"> ✓ Reduction of oxygen and sulphur concentration levels through deoxidation and desulphurization of the melt. ✓ Constitution of a wide range of steels, including austenitic, ferritic and duplex stainless steels and including carbide and nitride formation. ✓ Conditions for heat treatment operations to produce a desired constitution. ✓ Conditions for scrap re-melting to maintain as low concentrations as possible of undesirable "tramp elements". ✓ Melt-crucible interactions, etc. <p>The database must to allow calculations primarily for Fe-rich composition ranges, although the assessed data must be also reliable for higher concentrations of alloying components in a number of cases. The database must generally valid for the temperature range of approximately 400°C to 1800°C, although for some steels containing high melting point metals, calculations must reliable to still higher temperatures.</p> <p>The steel database must contain solution phases and compounds.</p> |
| 21) | <p>The light metal database must be designed for thermodynamic and phase equilibrium calculations involving especially Al alloys and Mg alloys</p> <p>The database can be intended to allow calculations over all ranges of composition, in the temperature range of approximately room temperature to 2200°C),</p> <p>The databases must allow to evaluate binary systems, ternary systems and important quaternary systems.</p> |

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| Characteristics of the licences | |
| 22) | A university license for SW and thermochemical databases comes with 2 hardware keys (dongles) for standalone installation. |
| 23) | In addition, university institutes that hold a license are permitted to install a server version of SW on an institute-internal Microsoft Windows-based computer. This SW server can be accessed by up to 20 client installations within the same local network (LAN). |
| 24) | The license as quoted is perpetual, meaning that it does not expire. Maintenance and support for the first 6 years is included. After 6 years, the maintenance and support can be extended. |