Thermo-Calc Software

Progress in the Industrial Deployment of Materials Modelling Software

– Experiences from Thermo-Calc Software

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1st material designed using Materials Modelling Software?

Thermo-Calc Software

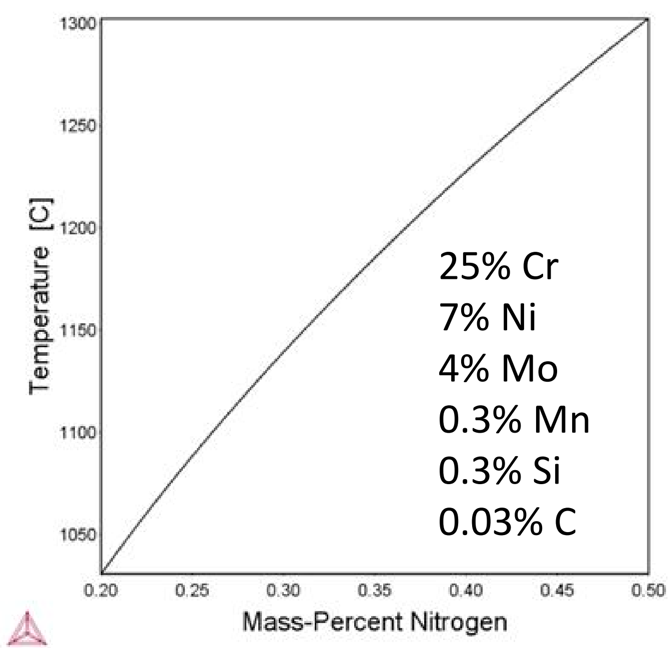
- In 1983, i.e. more than 35-years ago, SANDVIK, a global engineering group, had developed two new steels aided by CALPHAD-based calculations using Thermo-Calc.
- These two steels were SAF 2304 and SAF 2507 that later both became established grades.

Equivalent amounts of FCC (γ) and BCC (α)

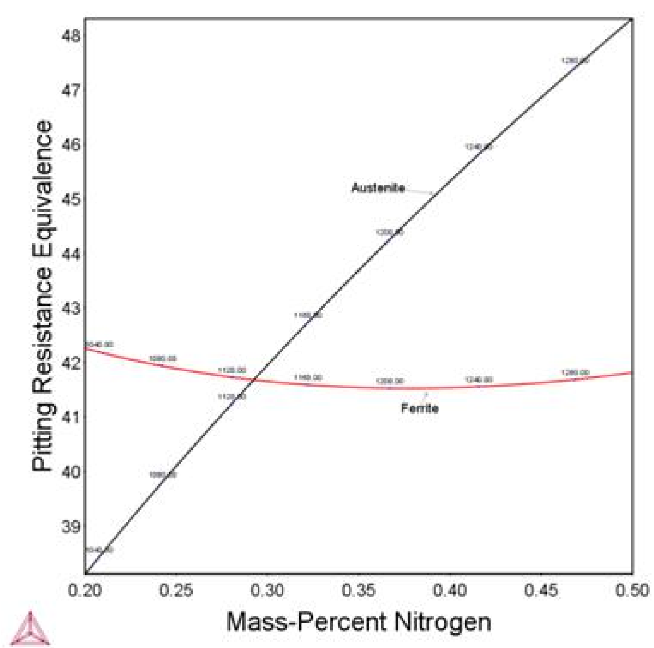
Duplex steel 2507
25% Cr
7% Ni
4% Mo
0.3% Mn
0.3% Si
0.03% C
+ N

Industrial driving force

- The ability to make predictive calculations for a multivariable problem
  - Shorten development time
  - Increase quality of produced and heat-treated steel
- Impossible (or at least very difficult, costly and time consuming) to optimise the chemistry for a duplex alloy with 6-7 elements, to achieve optimal resistance against pitting corrosion, without modelling software



Calculation showing the temperature at which the fraction of ferrite equals 50%, as function of N-content.



Calculated PRE for ferrite (red line) and austenite (black line), as function of N-content.

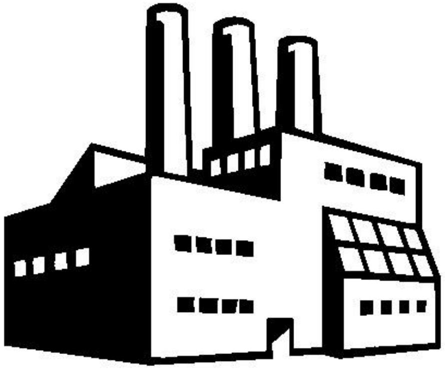
Success factors

- ❑ **Functionality** needed to study the industrial challenge
- ❑ **Access to relevant Data**, that allowed calculations to be performed on alloys of practical importance
- ❑ **Few assumptions**, making calculations predictive
- ❑ **Close collaboration** with academia

Note: When developing these first two steel grades SANDVIK remotely accessed Thermo-Calc (at KTH) via a modem, using an ordinary telephone line.

The Gap


```
Begin["`Private`"];
GaussSolveArraySlice[Real[n_, n_] ain_, Real[n_, m_] bin_, Integer iterations_] → Real[n, m] :=
 Module[{Real[n] dumc, Real[n, n] a, Real[n, m] b, Integer[n] {ipiv, indxr, indxc},
   Integer {i, k, l, irow, icol}, Real {pivinv, amax, tmp}, Integer {beficol, afticol, count}},
  For[count = 1, count ≤ iterations, count = count + 1, (a = ain;
    b = bin;
    For[k = 1, k ≤ n, k = k + 1, ipiv[[k]] = 0];
    For[i = 1, i ≤ n, i = i + 1,
     (*find the matrix element with largest absolute value*)
     amax = 0.0;
     For[k = 1, k ≤ n, k = k + 1,
      If[ipiv[[k]] == 0,
       For[l = 1, l ≤ n, l = l + 1, If[ipiv[[l]] == 0, If[Abs[a[[k, l]]] > amax, amax = Abs[a[[k, l]]];
           irow = k;
           icol = l]]
        ]
      ]
     ];
     ipiv[[icol]] = ipiv[[icol]] + 1;
     If[ipiv[[icol]] > 1, "*** Gauss2 input data error ***" >> "";
      Break];
     (*if irow ≠ icol, then interchange rows irow and icol in both a and b*)
     If[irow ≠ icol, For[k = 1, k ≤ n, k = k + 1, tmp = a[[irow, k]];
       a[[irow, k]] = a[[icol, k]];
       a[[icol, k]] = tmp];
      For[k = 1, k ≤ m, k = k + 1, tmp = b[[irow, k]];
       b[[irow, k]] = b[[icol, k]];
       b[[icol, k]] = tmp]];
     indxr[[i]] = irow;
     indxc[[i]] = icol;
     If[a[[icol, icol]] == 0, Print["*** Gauss2 input data error 2 ***"];
      Break];
     (*prepare to divide by the pivot and subsequent row transformations*)
     pivinv = 1.0 / a[[icol, icol]];
     a[[icol, icol]] = 1.0;
     a[[icol, _]] = a[[icol, _]] * pivinv;
     b[[icol, _]] = b[[icol, _]] * pivinv;
     dumc = a[[_, icol]];
     For[k = 1, k ≤ n, k = k + 1, a[[k, icol]] = 0];
     a[[icol, icol]] = pivinv;
     For[k = 1, k ≤ n, k = k + 1, If[k ≠ icol, a[[k, _]] = a[[k, _]] - dumc[[k]] * a[[icol, _]];
       b[[k, _]] = b[[k, _]] - dumc[[k]] * b[[icol, _]]]]
    ];
    For[l = n, l ≥ 1, l = l - 1, For[k = 1, k ≤ n, k = k + 1, tmp = a[[k, indxr[[l]]]];
      a[[k, indxr[[l]]]] = a[[k, indxc[[l]]]];
      a[[k, indxc[[l]]]] = tmp]])
  ];
  b];
End[];
EndPackage[];
```



Theoretical — Applied

Research — Production

Bridging the Gap or growing the industrial user base (I)

Thermo-Calc Software

- Education, Training & Success stories
  - Support and stimulate use in academia
  - Offer open and on-site training courses
  - Webinars & training (how to) videos
  - Published papers
  - Presentations at technical conferences
- User experience
  - Ease of use (Intuitive GUIs, Wizards, Application modules)
  - On-line documentation, Examples, Tutorials etc.
  - Robustness
  - Reliability
  - Speed
  - Support

Bridging the Gap or growing the industrial user base (II)

Thermo-Calc Software

- Data Relevance & Quality
  - Extending the validity range and completeness of databases
  - Validation, validation & validation
- Functionality
  - Introducing requested functionality (needed to solve the industrial problem)
- Interoperability
  - Allow for smooth interaction with other simulation tools

Our Customers & their Benefits

Industry

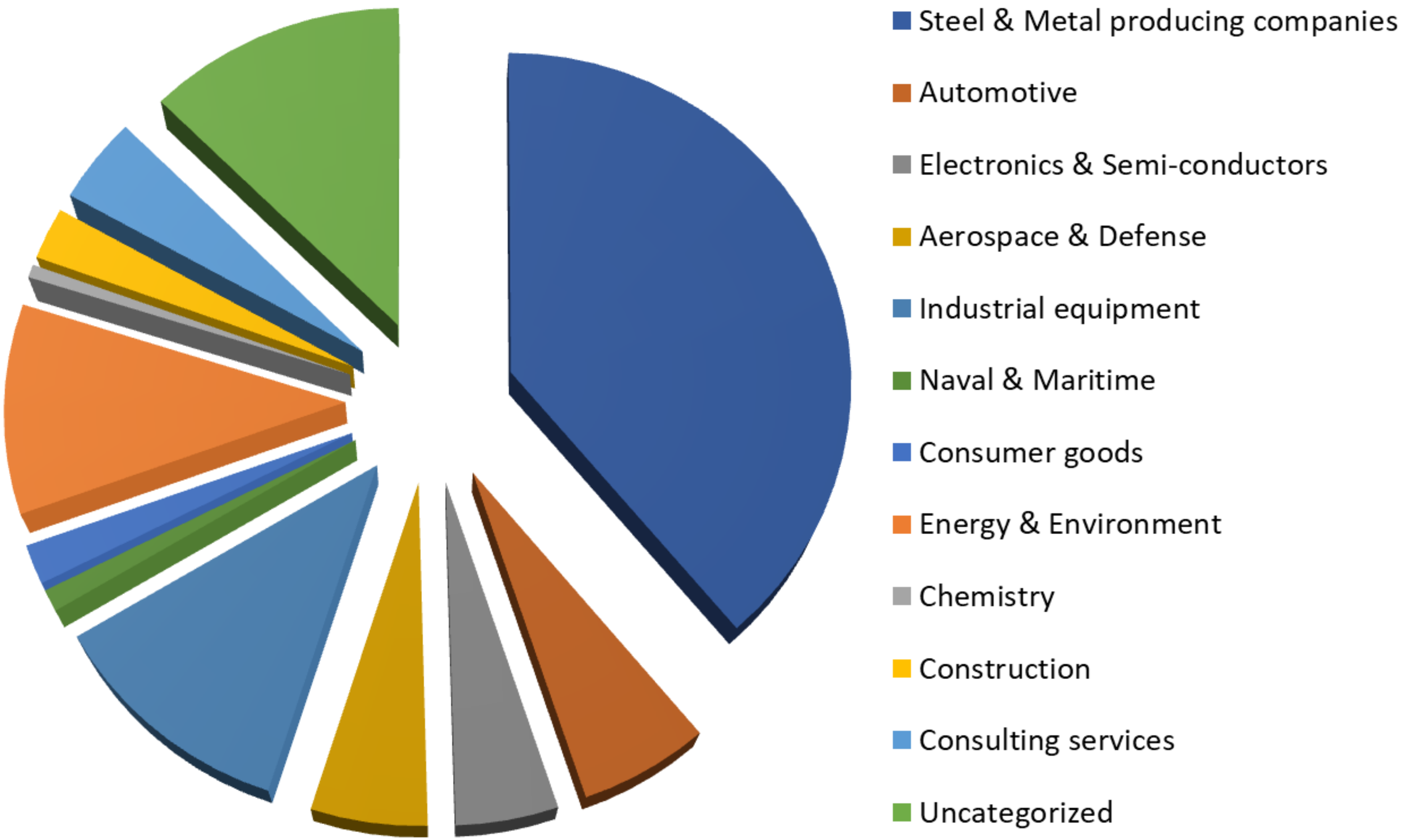
- Steel and metal producing companies
- Manufacturing companies
  - Automotive
  - Electronics
  - Aerospace & defense
  - Industrial equipment
  - Naval, maritime
  - Consumer goods
- Energy & environment
- Consulting services

Governmental labs

Academia *(material science,....)*

BENEFITS
Reduce costly, time-consuming experiments and testing
Increase the value of experiments through better pre-screening and interpretation of the results
Optimise and define safe processing windows
Base decisions on scientifically supported data and models
Shorten development time and bring products to market faster
Build and safeguard intellectual knowledge
Improve the quality and consistency of products through deeper understanding
Make predictions that are difficult or even impossible with an experimental approach

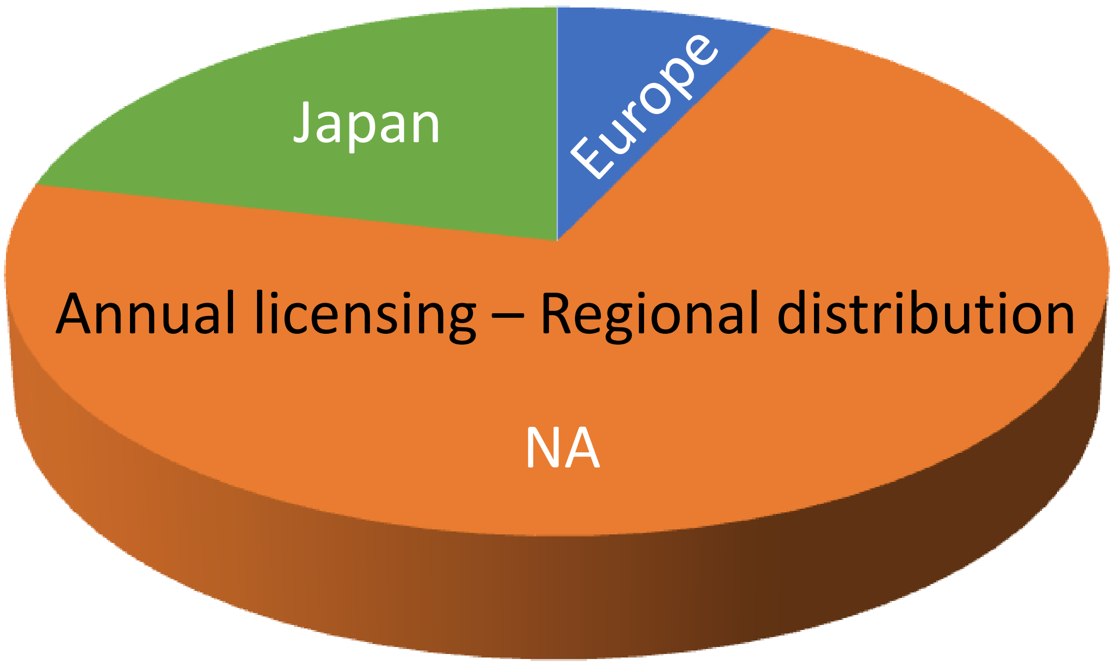
Users by industry segment



Only considering customers in Europe, NA and Japan. Rest of the world (e.g. China, India, Korea, Brazil, Russia) not included.

Perpetual vs Annual licensing (On-Premises)

- Annual leases are very few in our case, i.e. less than 5% of total revenue, albeit starting to increase.
- Annual leases are primarily popular in NA, see below graph.



- We have not seen a strong request from our customer for Cloud computing or SaaS.
- We are seeing issues with the fact a license needs to be tied to a designated Site, and how that is defined.

Organizational aspects & trends

- Our customers have traditionally been R&D units from larger corporations.
- We see fewer and fewer R&D units and more modelling down embedded in business units, i.e. **decentralization of modelling**.
  - We also see growing use of the software for problem solving by the business units, rather than just pure R&D.
- ICME (and also AM) is driving **more cross-team modelling**, which requires connection and interoperability.
  - This also means that non-materials scientists wants to use our tools, which is challenging in terms of what implicit knowledge is needed to run our tools well.
- Customers more and more desire to provide data and models down through their supply chains.

Generating insights on materials and processing operations

Thank You!