Thermo-Calc Software

Application of Thermo-Calc towards carbon neutrality

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Carbon neutrality

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- Carbon neutrality is the balance between emitting carbon and absorbing carbon emissions from carbon sinks. Carbon sinks are any systems that absorb more carbon than they emit, such as forests, soils and oceans.

- Corporations may achieve carbon neutrality by reducing their carbon footprint to zero through a combination of efficiency measures in-house and supporting external emission reduction projects.

- Most corporations find inherent business value in a carbon-neutral strategy. Typically, businesses that invest in improving their efficiency operate more cost effectively. Plus, in a society that increasingly values environmental sustainability and climate action, it provides a point of differentiation, as well as assists with employee recruitment and retention.

Application of Thermo-Calc to achieve carbon neutrality

Multiple areas exist where Thermo-Calc can support corporations objectives to reach carbon neutrality or net-zero emission, e.g. by enabling

- ❑ Introduction of new better materials that lead to higher efficiency
- ❑ More efficient processing, resulting in less waste, less energy consumption
- ❑ Increase use of recycled material
- ❑ Use of alternative processes, e.g. hydrogen-based direct reduction

Introduction of new better materials that lead to higher efficiency

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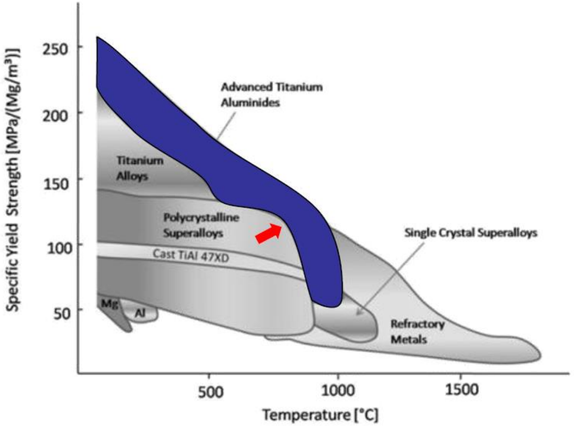
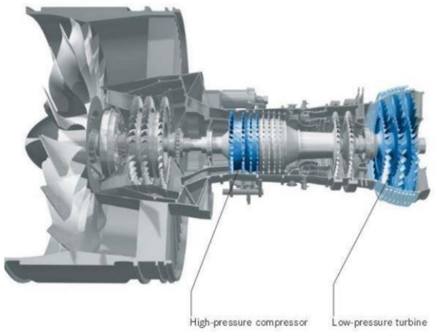
<u>ADVANCE Project:</u> Develop simulation capability that enhance development of novel TiAl-alloys



H. Clemens, S. Mayer; Advanced Engineering Materials 15 (2013) 191-215



Geared turbofan engine ™ (© MTU)

- ❑ Low density 3.7 – 4.2 g/cm3
  - High specific strength
- ❑ Good creep resistance at elevated temperatures
- ❑ Excellent oxidation resistance when coated

<u>Aim:</u> Push the drop-off in specific yield strength to higher temperatures to allow introduction of TiAl’s at earlier stages of the low-pressure turbine => lower weight => less fuel consumption => less CO_2 and NO_x emissions.

ADVANCE

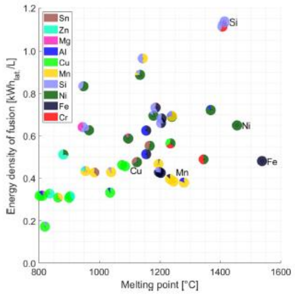
Clean Sky 2

This project has received funding From the European Union’s Horizon 2020 research and innovation Programme under grant agreement No 820647.

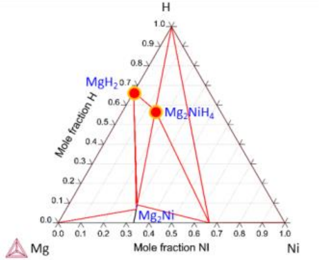
Introduction of new materials for sustainable energy production

Fossil-free and sustainable energy production requires development of new materials, processes & concepts. Several examples exist in literature where Thermo-Calc has been applied to aid such development:

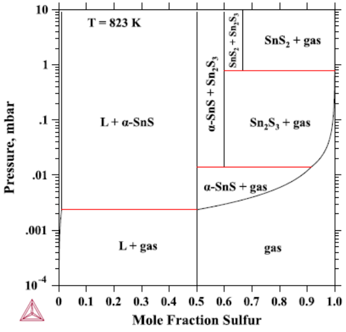
- ❑ Thermal Energy Storage (TES) — *Rawson et al., Journal of Energy Storage (2020) 32;101927*



- ❑ Hydrogen storage/absorption

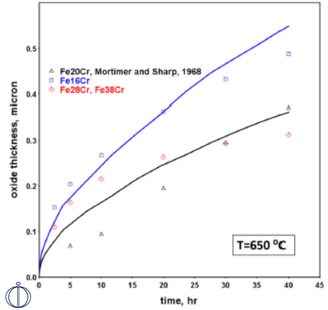


- ❑ Photovoltaics (PV solar panels) — *Lindwall et al., Solar Energy (2016) 125;314-323*



- ❑ Concentrating Solar Power (CSP)

- ❑ Use of Biomass for energy/fuel production — *Bigdeli et al., J. Phase Equilibr. Diffus. (2021) 42;403-418*



Development and use of Thermo Electric Generators (TEGs)

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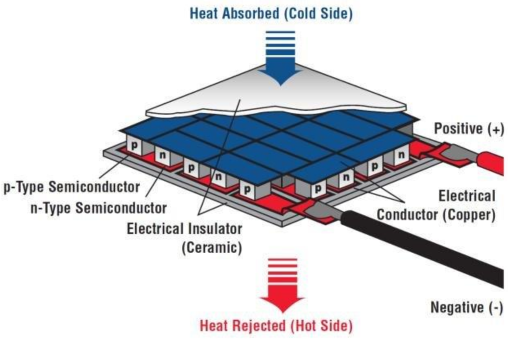
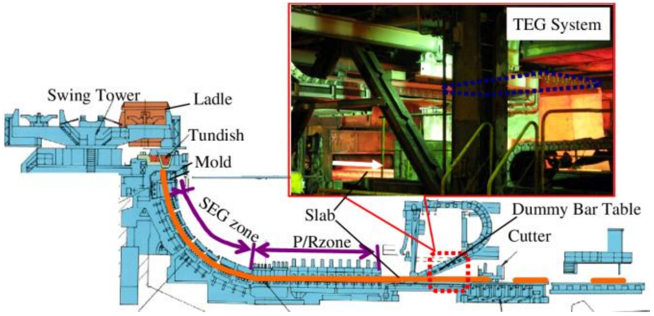
- A thermoelectric generator (TEG), also called a Seebeck generator, is a solid state device that converts heat flux (temperature differences) directly into electrical energy through a phenomenon called the Seebeck effect.

- Thermoelectric generators has potential use in power plants to convert waste heat into additional electrical power, but also for converting waste heat in steel works to electric energy.

- Image to the right show thermoelectric generation utilizing waste radiation heat from the continuous casting facility in the steel mill.





Komatsu technical report: Vol.64 No.171
Published on Mar 29, 2019

Development and use of Thermo Electric Generators (TEGs)

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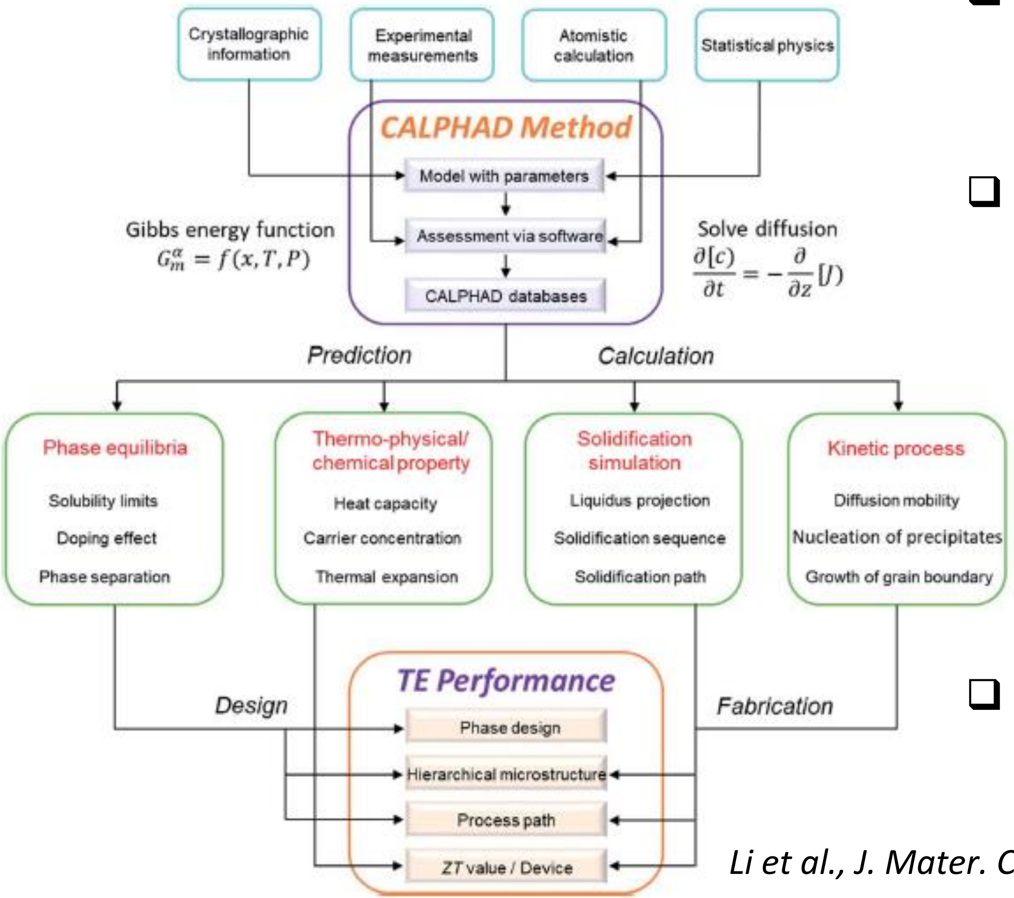


- CALPHAD can determine the solubility limit, phase stability, microstructure modulation, solidification path, etc.
- But also provide much more information, not only for phase diagrams, but also for thermodynamic or kinetic studies, including heat capacity, thermal expansion, diffusion mobility, nucleation of precipitates, …
- Providing a tool that give guidance for both the design and fabrication.

Li et al., J. Mater. Chem. A, (2021), 9;6634-6649

More efficient processing, i.e. less waste, less energy consumption

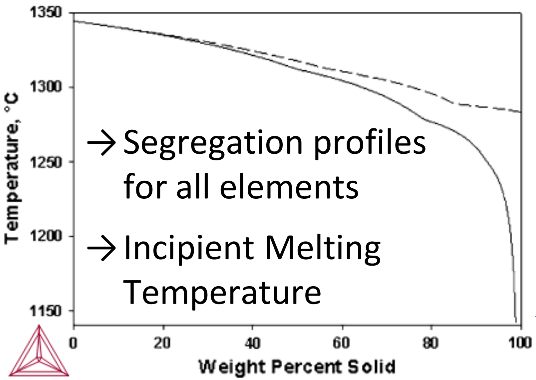
Homogenizing a Nickel-Based Superalloy: Thermodynamic and Kinetic Simulation and Experimental Results

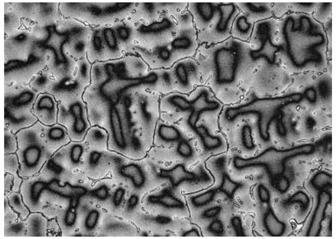
Jablonski and Cowen; Metall. Mater. Trans. B, (2009), 40;182–186

Table I. Target and Measured Chemistry (in Weight Percent) of the Nimonic 105 Alloy Cast for This Study

Nimonic 105	C	Cr	Mo	Co	Al	Ti	Mn	Si	B
Target	0.15	14.85	5	20	4.7	1.1	0.5	0.5	0.05
Measured	0.16	14.61	5.02	20.04	4.43	1.1	0.51	0.51	0.05

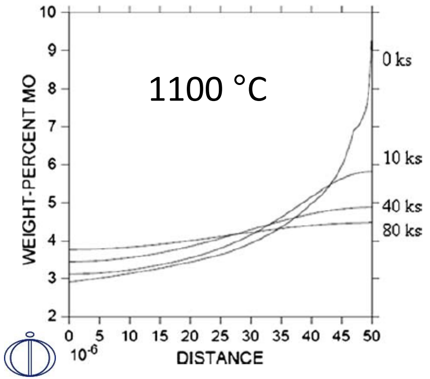
Scheil-simulation of solification:

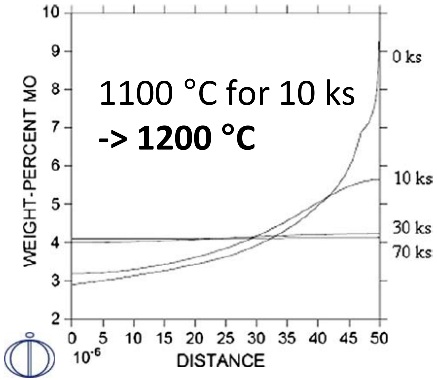




T_{IMP} = 1142 °C

Simulation of homogenization using Diffusion Module (DICTRA):





- After 10 ks we predict that **T_{IMP} = 1275 °C**, as a result of changes in the chemical profile due to homogenization.
- This allows us to significantly increase the temperature and thereby shorten the process, which result in energy savings.

More efficient processing, i.e. less waste, less energy consumption

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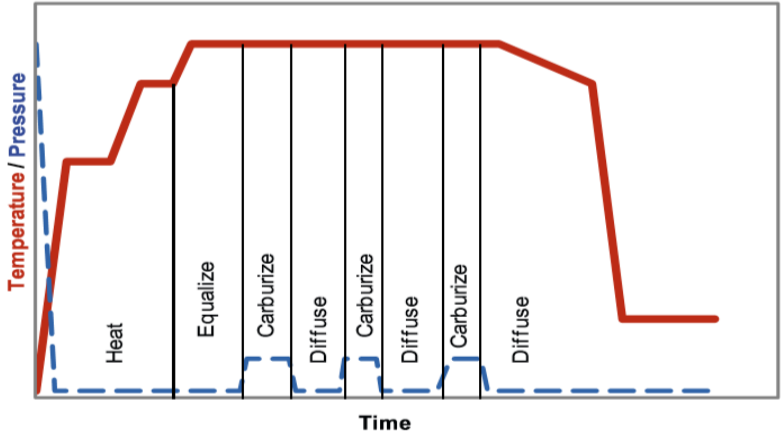
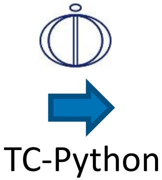
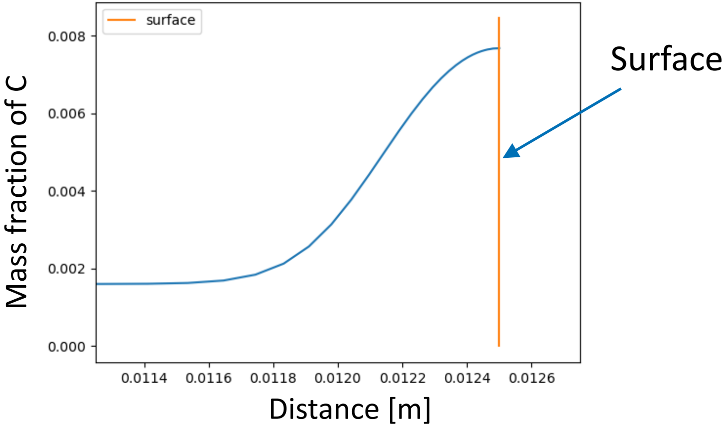
Understanding the relation between process and alloy is key to have:

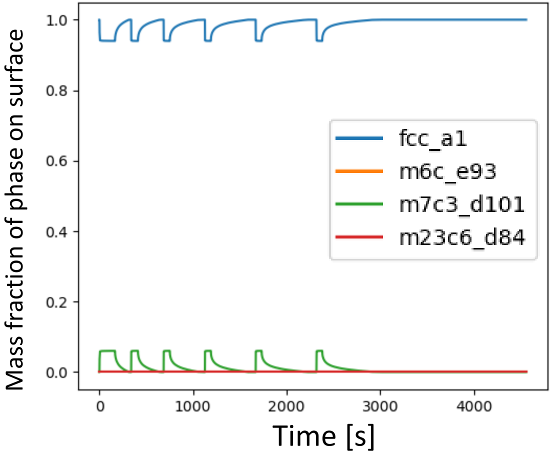
- ❑ Less energy consumption through optimization of process parameters

Low pressure carburization (LPC) of medium & high alloyed steel









- ❑ Aim is to use Diffusion Module (DICTRA) combined with TC-Python to optimize the carburization recipe, eventually in real time.

Increase use of recycled material

- Recycling aluminum require only 5% of the energy necessary to extract it from the bauxite ore, saving 9 tons of CO_2 per 1 ton of recycled aluminum.
- Consequently, there are massive environmental savings to be made from increased recycling of aluminum.
- Used cans are collected, molten together, and used again to create new cans without the addition of any other material.
- For other industries, e.g. the automotive industry, the situation is more complicated.
- The challenge here is to manage or decrease the amount of unwanted impurities in the processed and recycled scrap.
- Several techniques for this exist and Thermo-Calc can give necessary insights.

Increase use of recycled material

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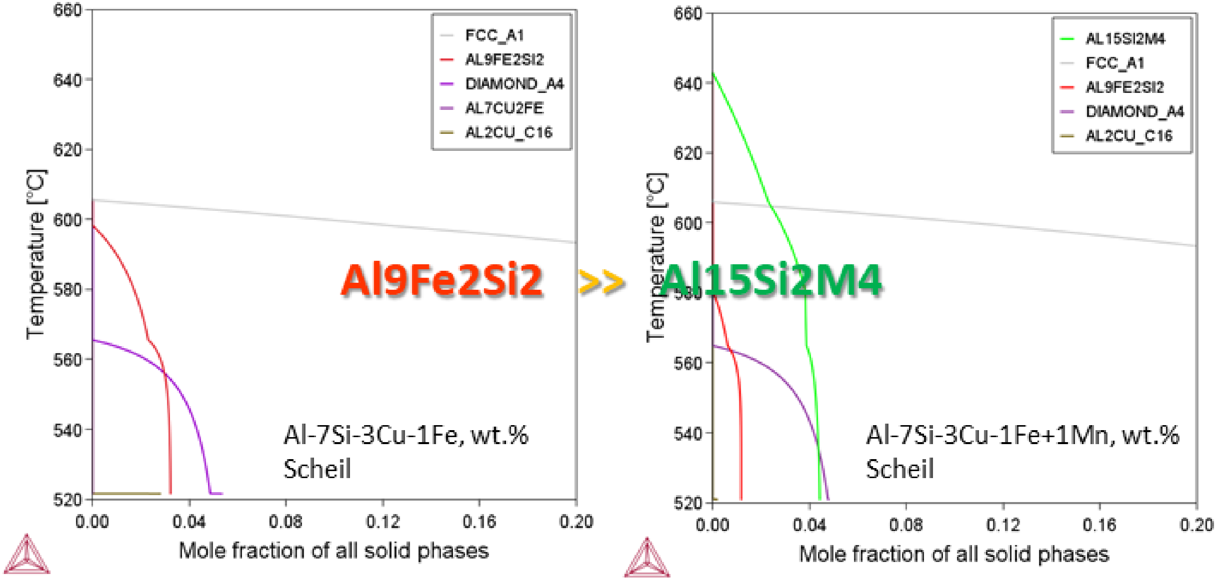
1. One method is to directly convert detrimental phases (especially Fe since it the most common impurity) to less detrimental Al15Si2M4 (which can dissolve Fe) by adding Mn (Cr, Co, V).

   This technique is the simple and the cost might be low, but the Mn addition is limited by the formation of sludge when the amount of Al15Si2M4 becomes high.



- Converting detrimental phases to less-detrimental ones
- e.g. $Al_9Fe_2Si_2$ to $Al_{15}Si_2M_4$ (M = Fe, Mn) by adding Mn.

Increase use of recycled material

2. Form a solid phase (e.g. Al15Si2M4) containing undesired elements and remove it via filtering in the semi-solid state => purified liquid

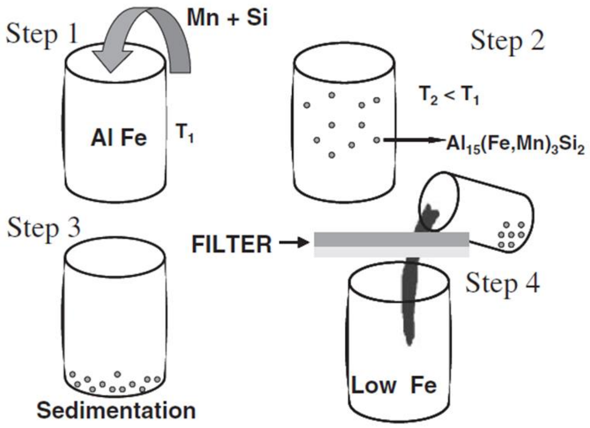
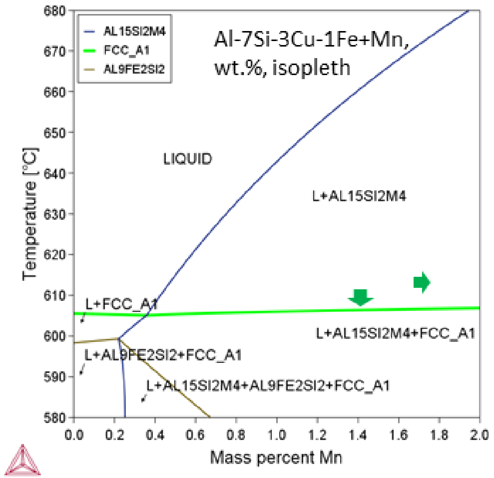
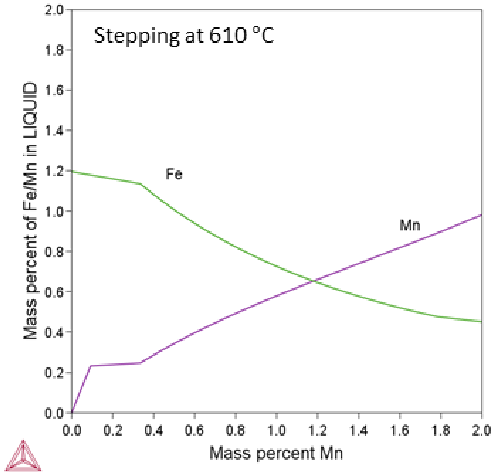


Fig. 1 Schematic diagram of the filtering process.

- Filtration of dross of aluminides, e.g. $Al_{15}Si_2M_4$ (M = Fe, Mn)





  - Lower processing temperature and add Mn to remove more Fe.
  - Not lower than the green line, avoiding (Al), for a high Al yield.

Increase use of recycled material

- Scrap-based electric arc furnace (EAF) steelmaking is limited by a surface cracking problem, which is known as surface hot shortness.
- Originates from excessive amount of copper (Cu) in the steel scrap, which melts and penetrates into the austenite grain boundaries.
- Some elements amplify while others neutralize the negative effect of copper.
- It is known that tin (Sn) increases the negative effect of copper.

Sn added to TCFE12

Copper (Cu) and Tin (Sn) as tramp elements in recycled steel products

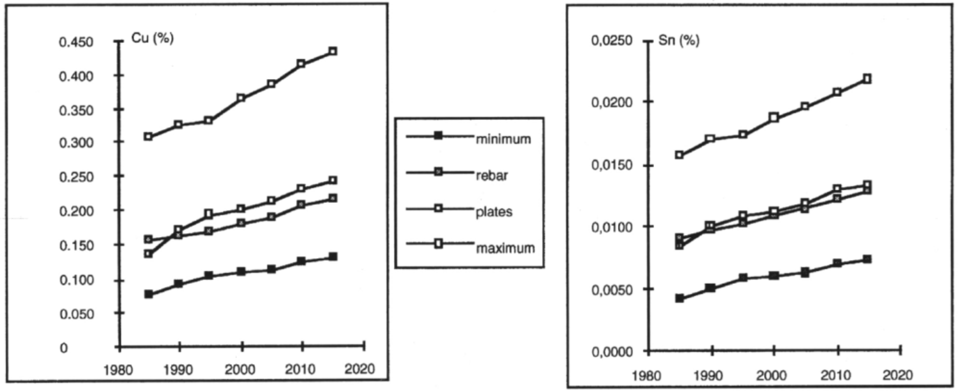
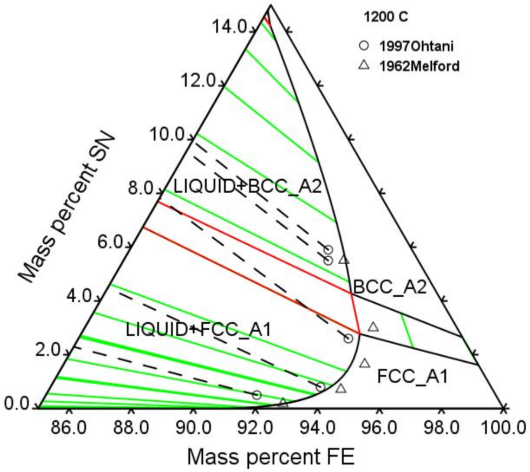


Fig. 2 – Cu and Sn long term evolution in EAF steels as a result of tramp element accumulation in the scrap deposit.

S. Sato, et al., The shinseiko project : A new environment friendly steelmaking route based on scrap, Rev. Metall. Cah. D'Informations Tech. 93 (1996) 473–483.



Fe-corner of the Fe-Cu-Sn phase diagram at 1200 °C

Increase use of recycled material

Tin removal by selective evaporation process

The selective evaporation process is a process of separation based on the difference between the vapor pressure of the residual elements and iron in a vacuum state

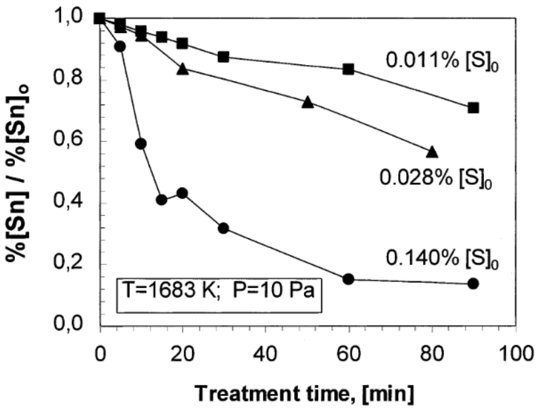
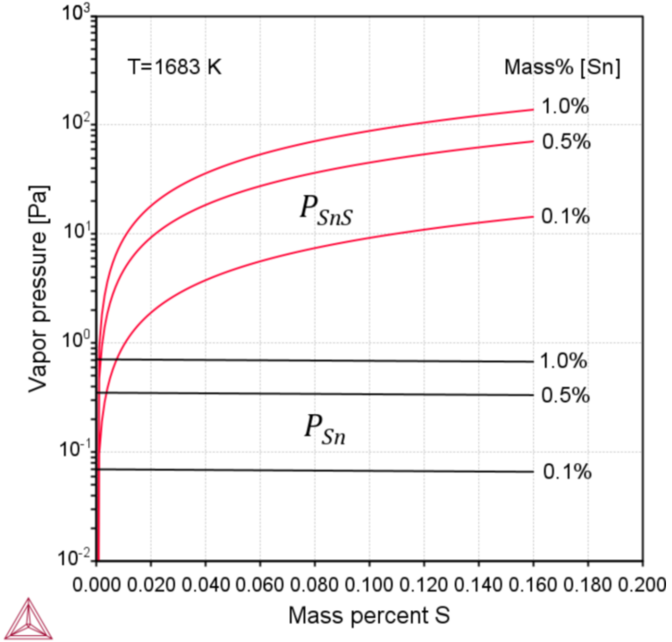


Fig. 1. Influence of the initial sulphur content of Fe–4mass%C–0.7mass%Si melts on the evaporation of tin (test runs VS, VS-2 and VS-3).

L. Savov, S. Tu, D. Janke, ISIJ Int. 40 (2000) 654–663.



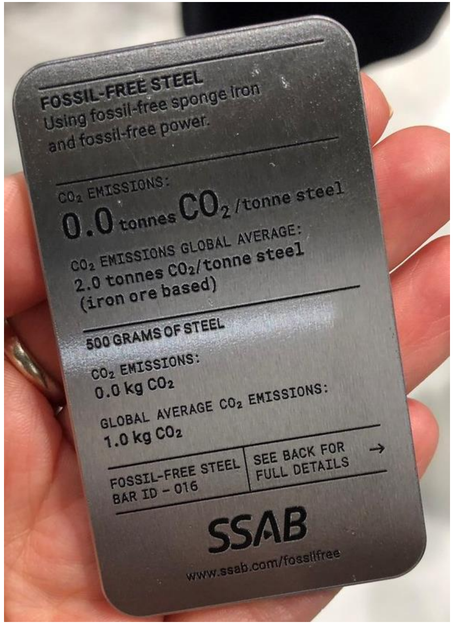
*Calculated vapor pressures of **SnS** and **Sn** in equilibrium with **Fe–4C–0.7Si** wt.% melt containing tin (Sn) and sulphur (S) at a temperature of 1683 K*

Use of alternative processes, e.g. hydrogen-based direct reduction

- ❑ Demand for steel is expected to increase until 2050.
- ❑ Increase of recycling and scrap based steel production will not be enough to meet the future need.
- ❑ Ore based steel production needs to be maintained or even increase.
- ❑ Every ton of steel produced emits on average 1.85 tons of carbon dioxide.
- ❑ 7-9% of all fossil fuel-based CO2 emissions are derived from the steel industry.
- ❑ There are several ongoing initiatives to reduce emissions.

Use of alternative processes, e.g. hydrogen-based direct reduction

The HYBRIT-initiative in Sweden aim to replace the blast furnace process, which uses carbon and coke to remove the oxygen from iron ore, with a direct reduction process, where fossil-free hydrogen produced from water using electricity from fossil-free energy sources is used.



Worlds first fossil-free steel

Carbon monoxide reduction:

$$3Fe_2O_3(s) + CO(g) \leftrightarrow 2Fe_3O_4(s) + CO_2(g)$$

$$\Delta H^0_{843\,K} = -30.05\ [kJ]$$

$$Fe_3O_4(s) + 4\,CO(g) \leftrightarrow 3Fe(s) + 4CO_2(g)$$

$$\Delta H^0_{843\,K} = -44.478\ [kJ]$$

Hydrogen reduction:

$$3Fe_2O_3(s) + H_2(g) \leftrightarrow 2Fe_3O_4(s) + H_2O(g)$$

$$\Delta H^0_{843\,K} = 6.440\ [kJ]\ (6)$$

$$Fe_3O_4(s) + 4\,H_2(g) \leftrightarrow 3Fe(s) + 4H_2O(g)$$

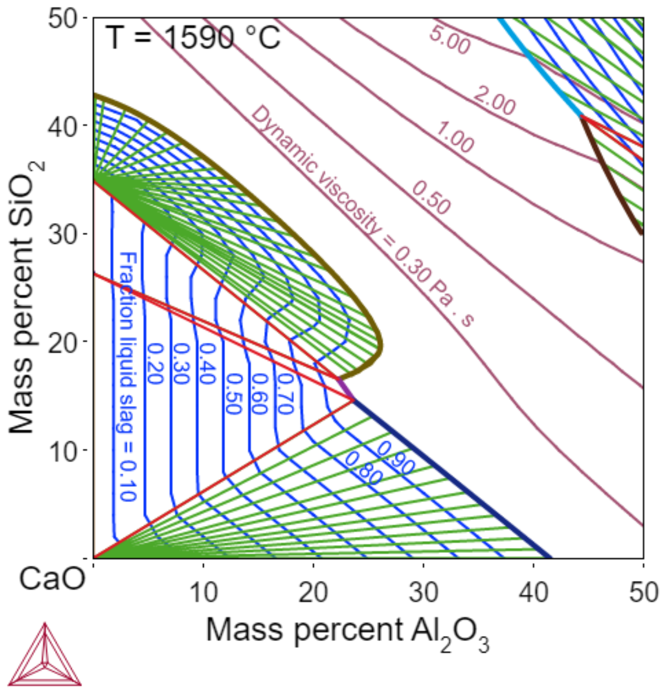
$$\Delta H^0_{843\,K} = 101.482\ [kJ]\ (6)$$

When hydrogen is produced by the process of electrolysis with power from renewable sources and then used as reducing agent the theoretical carbon footprint of steel production is zero.

Use of alternative processes, e.g. hydrogen-based direct reduction

There are many challenges and opportunities:

- ❑ Hydrogen reduced DRI is currently more expensive, compared to ordinary steel.
- ❑ A process route using little or even no fossil-based agents would largely limit Sulphur contamination.
- ❑ A process utilizing hydrogen reduced DRI should, therefore, focus on the removal of phosphorus whilst keeping close control of costs.
- ❑ Thermo-Calc can help design the optimal slag for that purpose.



CaO-Al2O2-SiO2 phase diagram with fraction liquid and slag viscosities superimposed as contour lines.

Summary

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- It is necessary for corporations to reduce their carbon footprint
- This creates many challenges, but also opportunities
- Efficient simulation tools will facilitate this transition
- Multiple examples exist where Thermo-Calc products have successfully helped companies to reduce their emissions, but also to become more cost effective at the same time.

Thermo-Calc Software

Thank You!

When data matters

www.thermocalc.com