Optimization Framework for Low Pressure Carburization Process

Andreas Markström, Henrik Lasu, Carl-Magnus Lancelot

SHTE Höstmöte, Scandic Skogshöjd, 2023-10-11

Outline

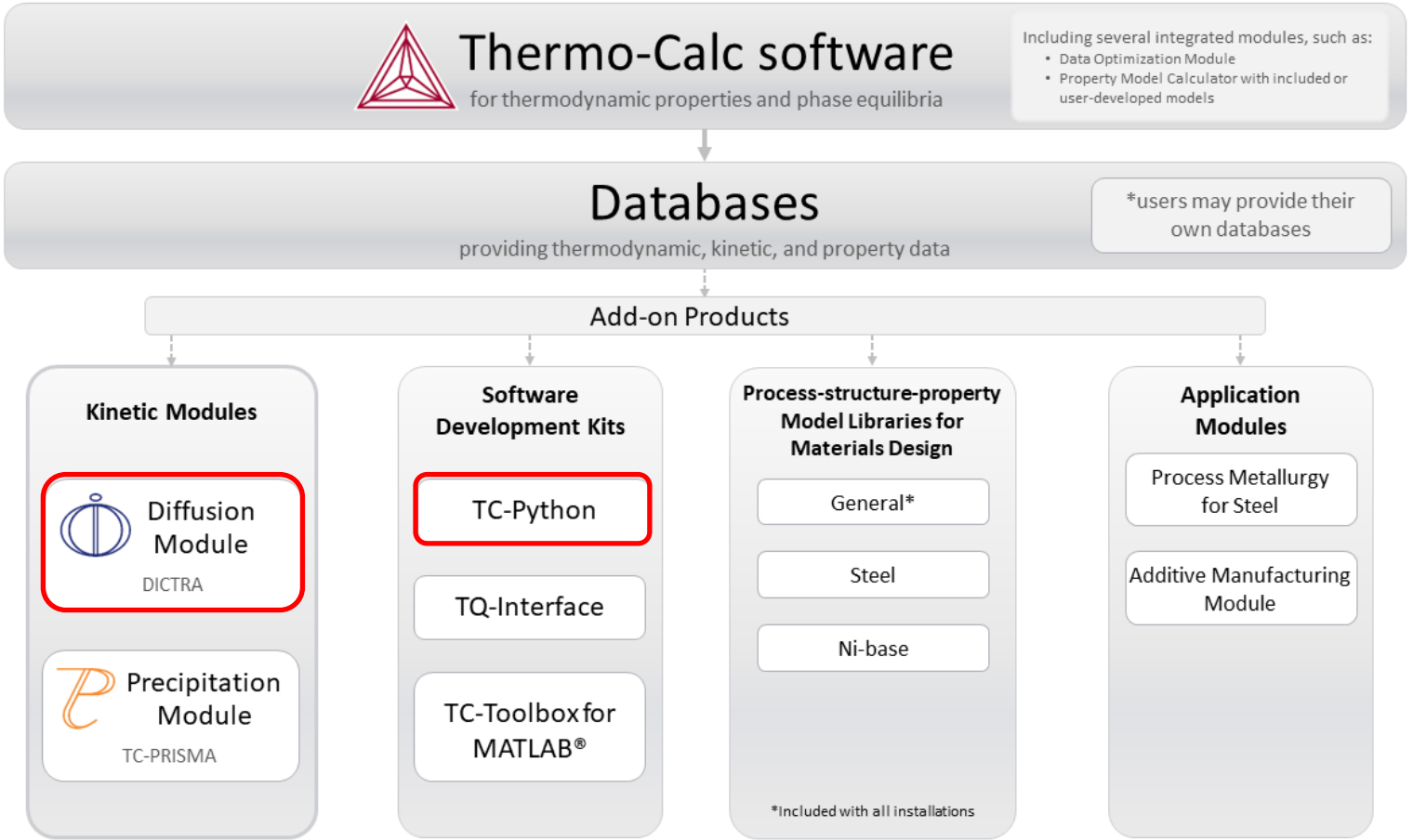
1. Introduction
    1. Thermo-Calc
    2. Thermodynamics: Calphad method
    3. Diffusion simulations (DICTRA)

2. Low Pressure Carburization framework
    1. Setup in DICTRA
    2. Results
    3. Future work

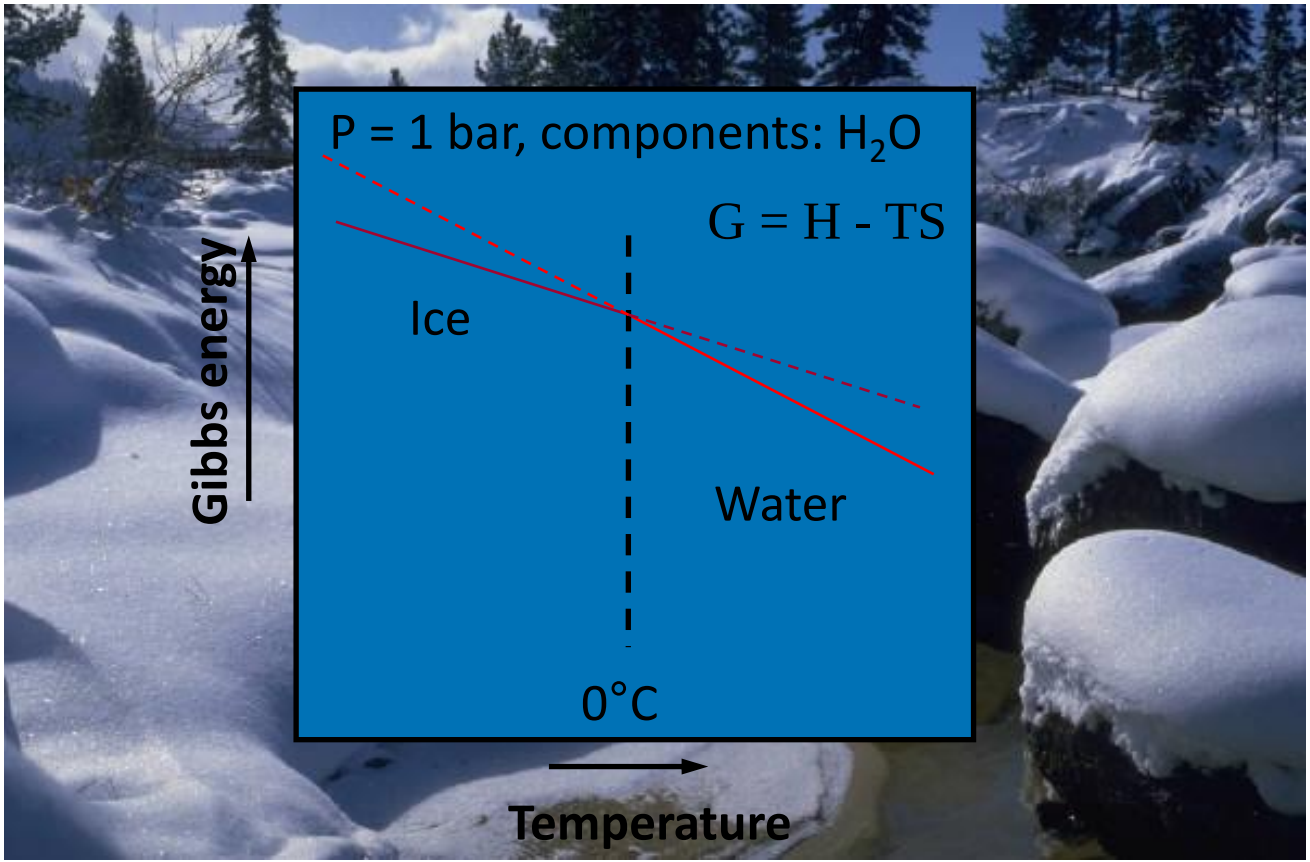
Thermo-Calc Software

- **Company dedicated to provide computational tools in the field of materials engineering**
- Originating at KTH Stockholm in late 70s, Company Founded in 1997
- Headquarters in Stockholm (45 employees)
- Subsidaries in US, Pittsburgh (8 employees) and South Korea (1 employee)
- Offices in Zurich, Düsseldorf, Gothenburg, Vancouver, São Paulo.
- Worldwide representation through local partners in Japan, China, India, Dubai, Australia, Brazil and Turkey
- > 1800 customers in 70+ countries

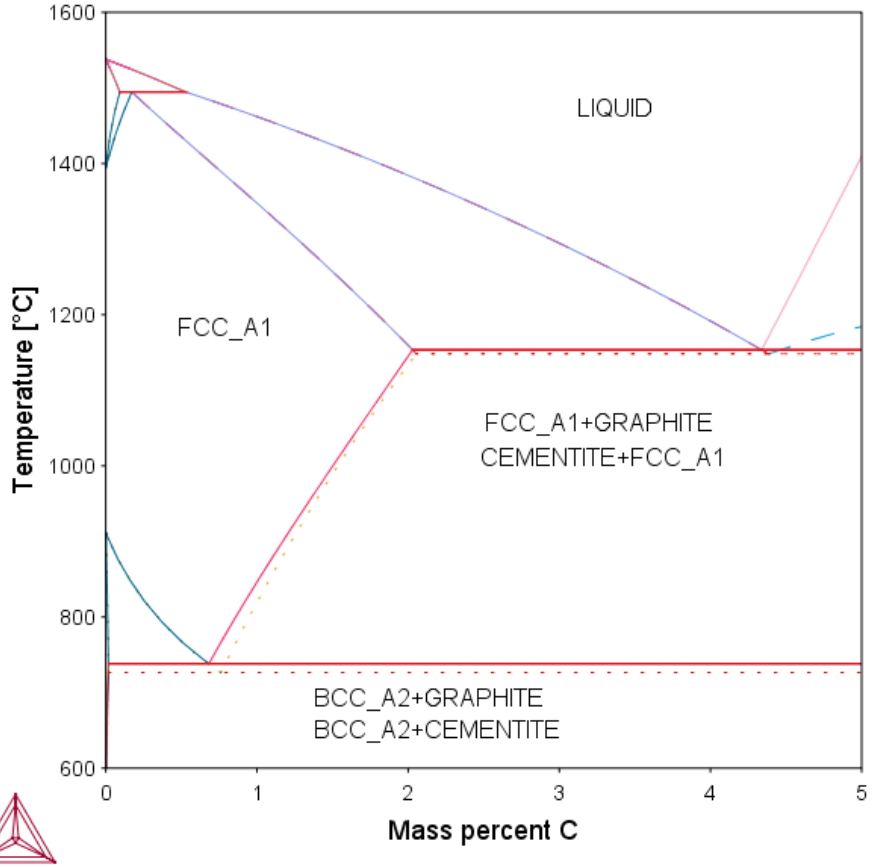
Product overview



Why does water melt at 0°C?

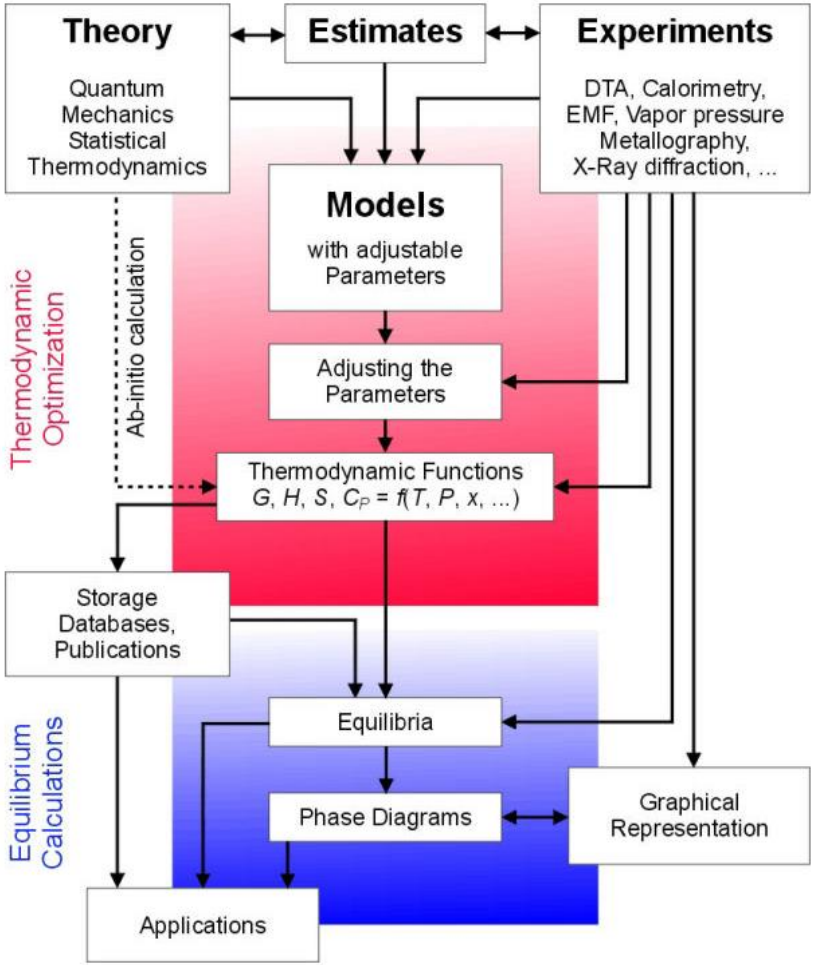


Example Fe-C


1600
1400
1200
1000
800
600
Temperature [°C]
0
1
2
3
4
5
Mass percent C
LIQUID
FCC_A1
FCC_A1+GRAPHITE
CEMENTITE+FCC_A1
BCC_A2+GRAPHITE
BCC_A2+CEMENTITE

Thermodynamic Databases (*The CALPHAD approach)*

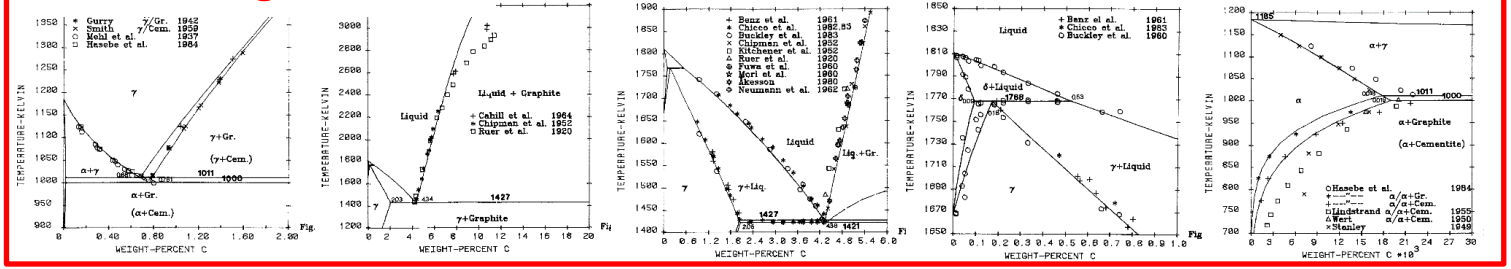
- Calphad: Calculation of Phase Diagrams
- Models describe Gibbs Energy of phases
- Optimize model parameters



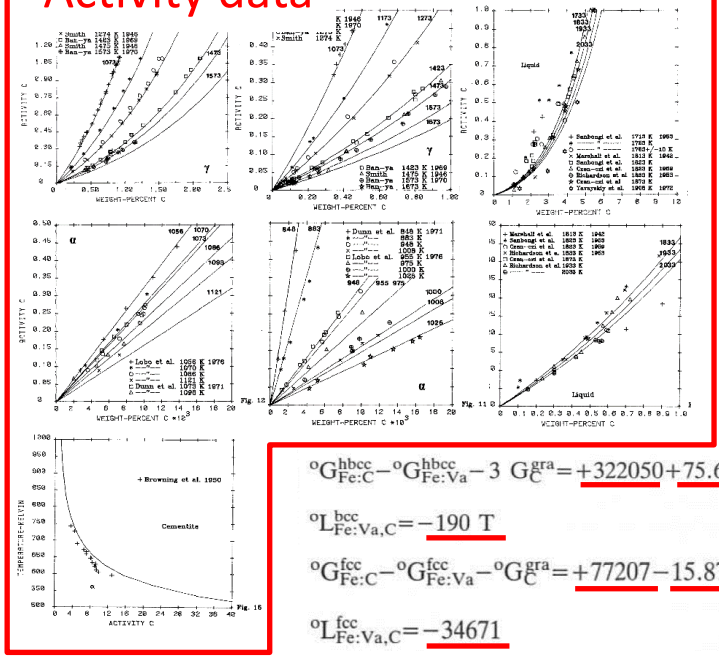
Example Fe-C Per Gustafson, 1985, *Scand. Journal of Metallurgy* **14**(5):259-267

Thermo-Calc Software

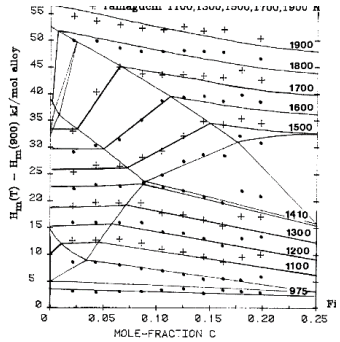
Phase diagram data

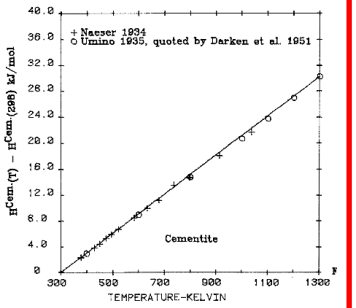


Activity data



Enthalpy data





$${}^{o}G^{hbcc}_{Fe:C} - {}^{o}G^{hbcc}_{Fe:Va} - 3\ G^{gra}_{C} = +322050 + 75.667\ T$$

$${}^{o}L^{bcc}_{Fe:Va,C} = -190\ T$$

$${}^{o}G^{fcc}_{Fe:C} - {}^{o}G^{fcc}_{Fe:Va} - {}^{o}G^{gra}_{C} = +77207 - 15.877\ T$$

$${}^{o}L^{fcc}_{Fe:Va,C} = -34671$$

$${}^{o}G^{cem}_{Fe:C} - H^{SER}_{C} - 3\ H^{SER}_{Fe} = -10745 + 706.04\ T - 120.6\ T\ \ln(T)$$

$${}^{0}L^{liq}_{Fe,C} = -124320 + 28.5\ T$$

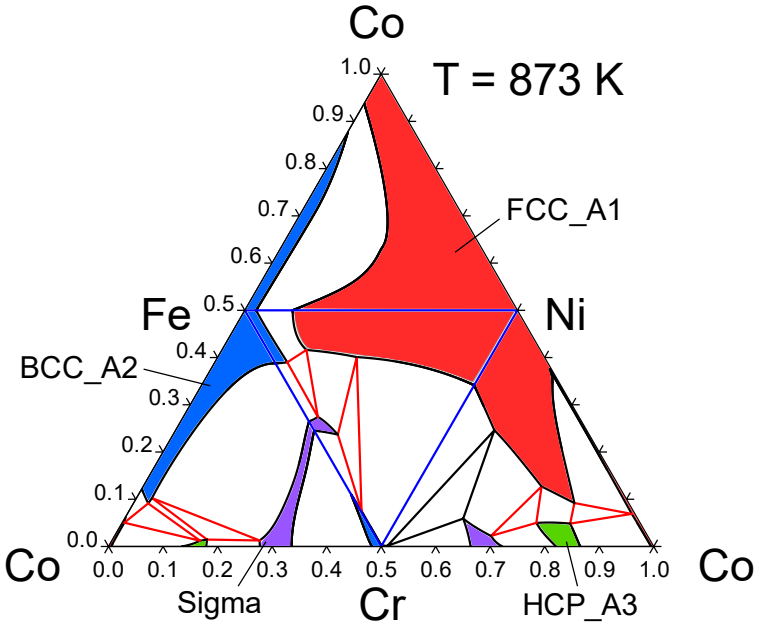
$${}^{1}L^{liq}_{Fe,C} = +19300$$

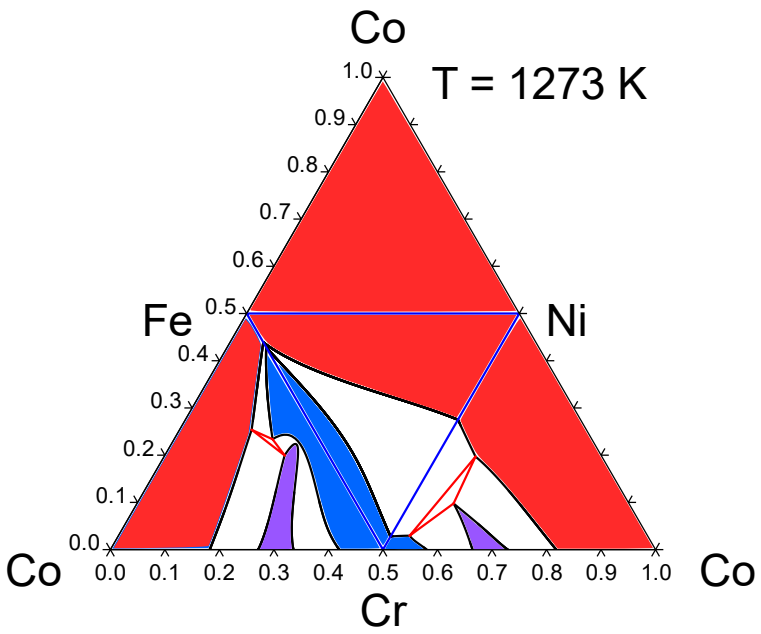
$${}^{2}L^{liq}_{Fe,C} = +49260 - 19\ T$$

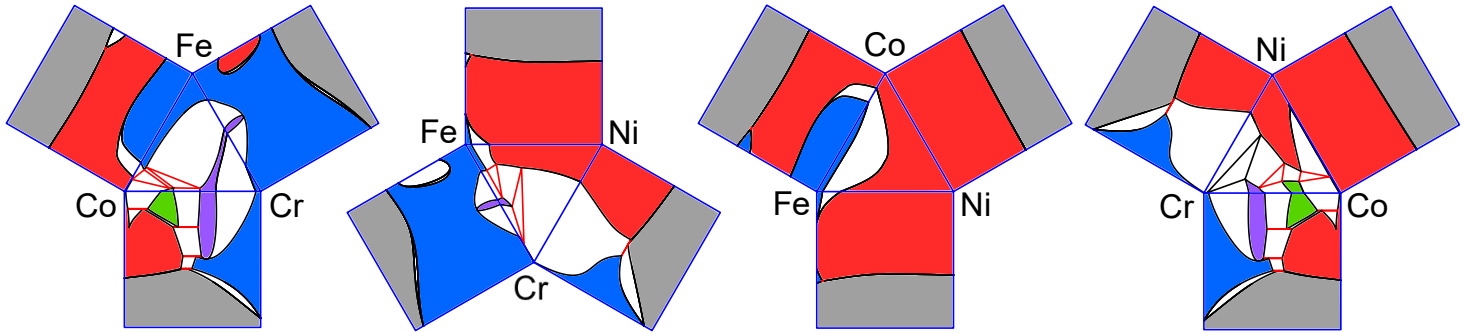
4 phases, >1000 experiments reproduced with 14 parameters

Extension: binaries → ternaries → quaternaries → further

2 elements 3 elements 4 elements

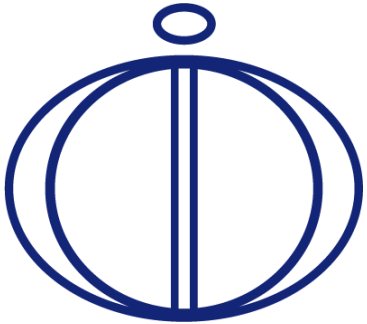






Not only thermodynamics

- Equilibrium Thermodynamics > Phase Diagram
- Many alloys / processes do not reach equilibrium!
  - Fe-C, Ni-base alloys, Al-alloys…
- Kinetics important
  - Diffusion module DICTRA



Outline

1. Introduction
    1. Thermo-Calc
    2. Calphad method
    3. **Diffusion simulations (DICTRA)**

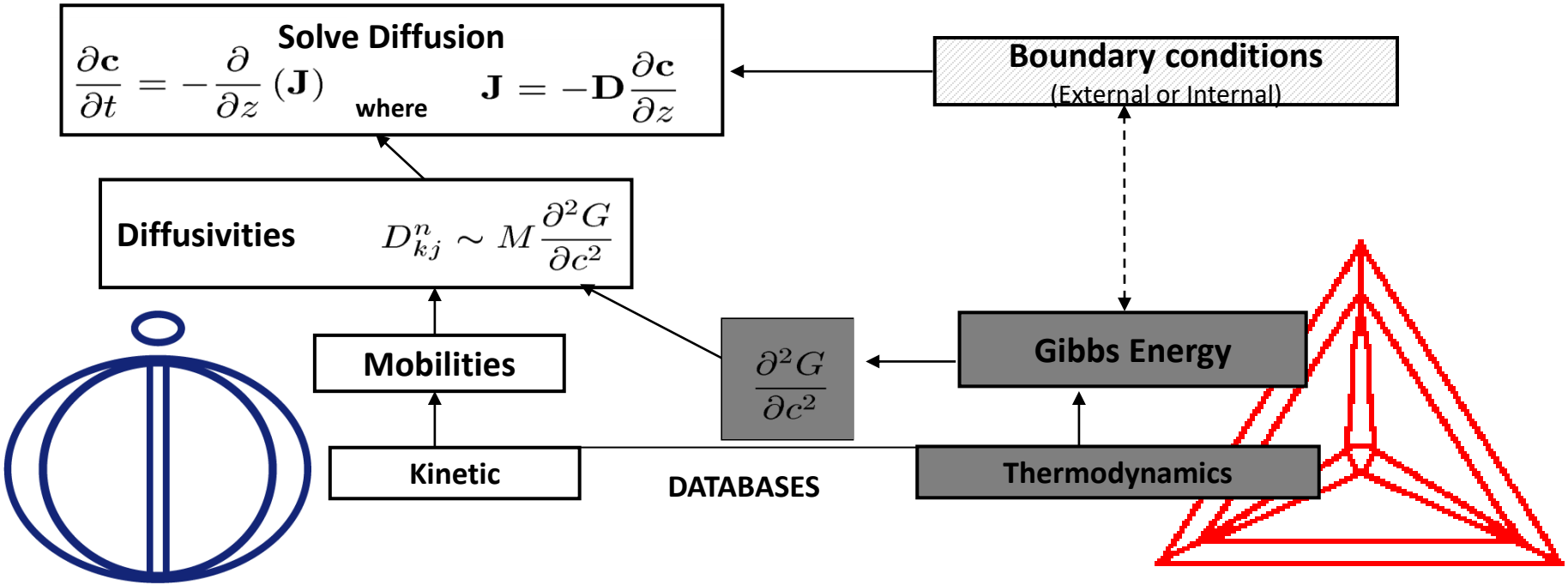
2. Low Pressure Carburization framework
    1. Setup in DICTRA
    2. Results
    3. Future work

Diffusion Module (DICTRA)

- Software package for simulation of diffusion controlled reactions in multi-component alloys.
- 1-dimensional simulation, with geometrical symmetry (planar, cylindrical or spherical)
- Linked to Thermo-Calc, which provides all necessary thermodynamic properties.
- The result of more than 30 years R&D at:
  - Royal Institute of Technology in Stockholm, Sweden
  - Max-Planck Institute für Eisenforschung in Düsseldorf, Germany
  - Thermo-Calc Software AB

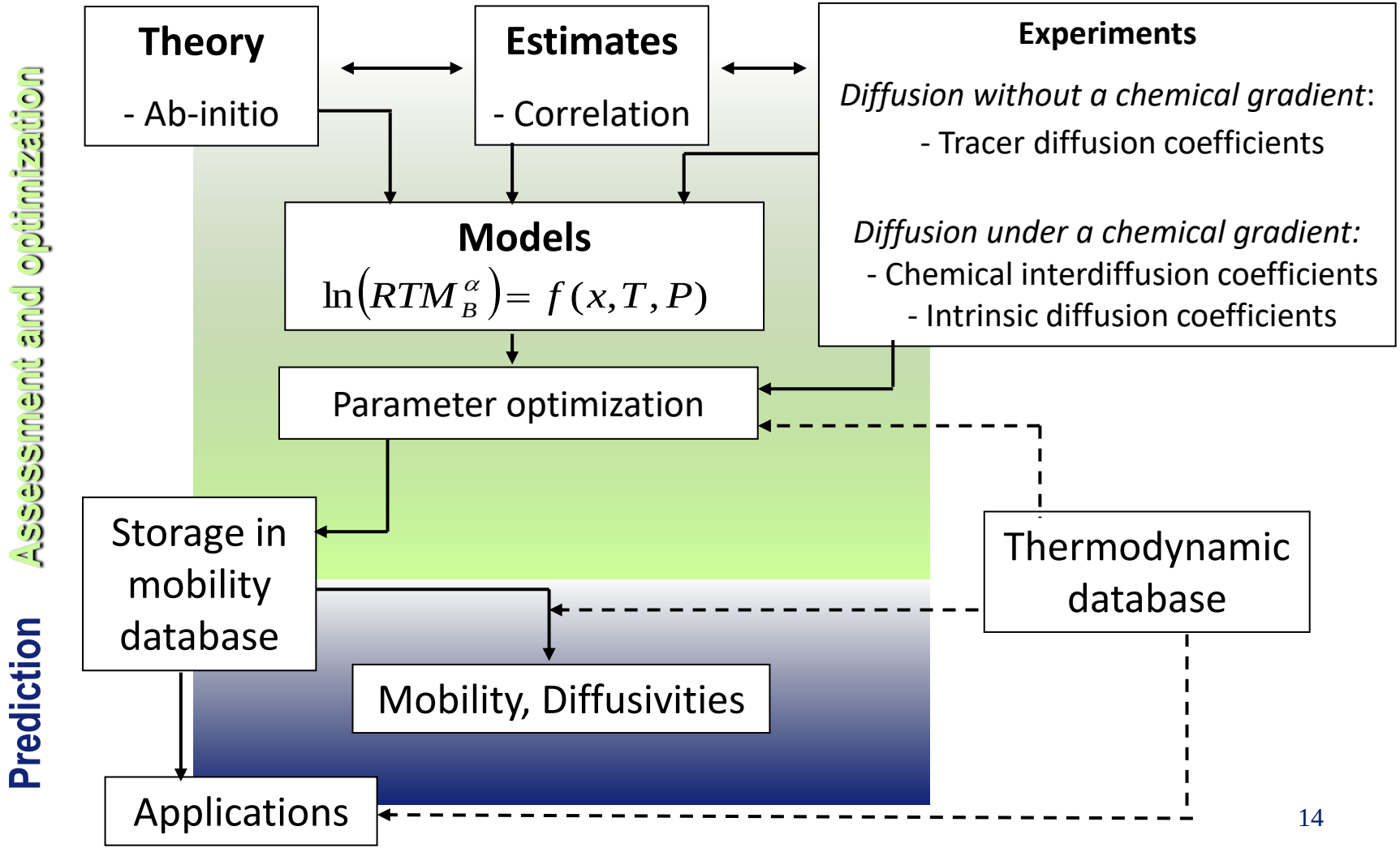
Basic calculation procedure

A numerical finite difference scheme is used for solving a system of coupled parabolic partial differential equations



All simulations depend on assessed kinetic and thermodynamic data, which are stored in databases

Kinetic Databases (*in a CALPHAD spirit*)



Modelling of the atomic mobility

From absolute reaction-rate theory arguments Andersson and Ågren[1] suggested:

$$M_B = M_B^0 \exp\left(\frac{-Q_B}{RT}\right)\frac{1}{RT}$$

M_B *Mobility for element B*
M_B^0 *Frequency factor*
Q_B *Activation energy*

When treating the composition dependency of the mobility, Jönsson[2] found it superior to expand the logarithm of the mobility rather than the value itself, i.e.

$$RT\ln\left[RTM_B\right] = RT\ln M_B^0 - Q_B$$

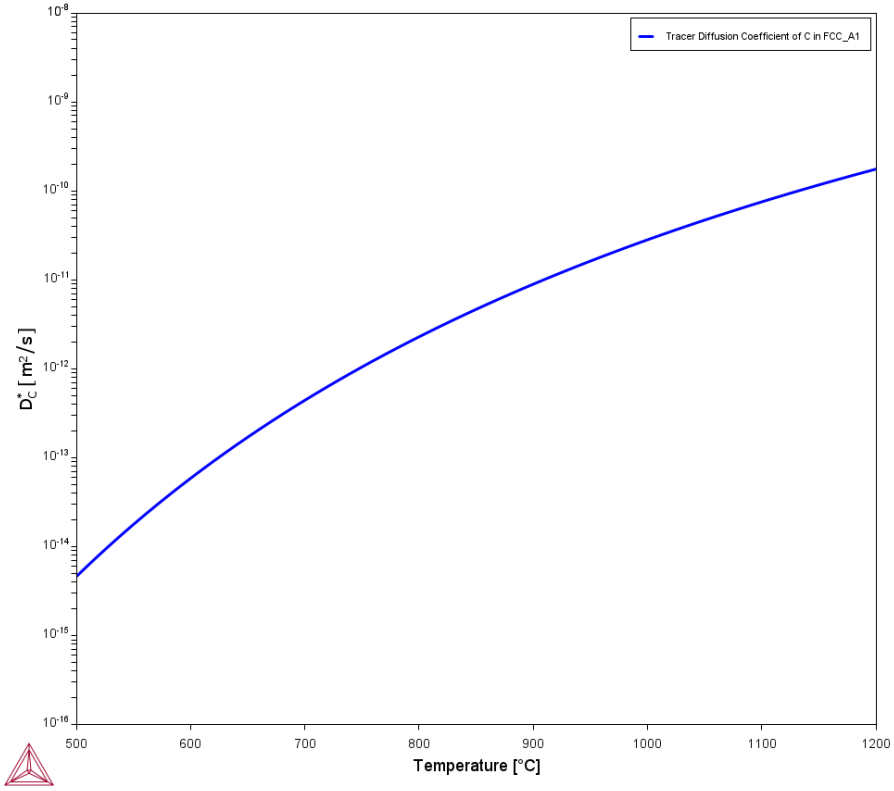
Because $\ln[RTM_i]$ is often found to have a fairly linear composition dependency

1. Andersson, Ågren, J Appl Phys 72(1992)1350
2. Jönsson, Scand J Metall 24(1995)21

Composition dependency

How does this then affect the Carbon diffusion?

Example, Carbon diffusion in Austenite:
Fe-0.5C



Composition dependency

How does this then affect the Carbon diffusion?

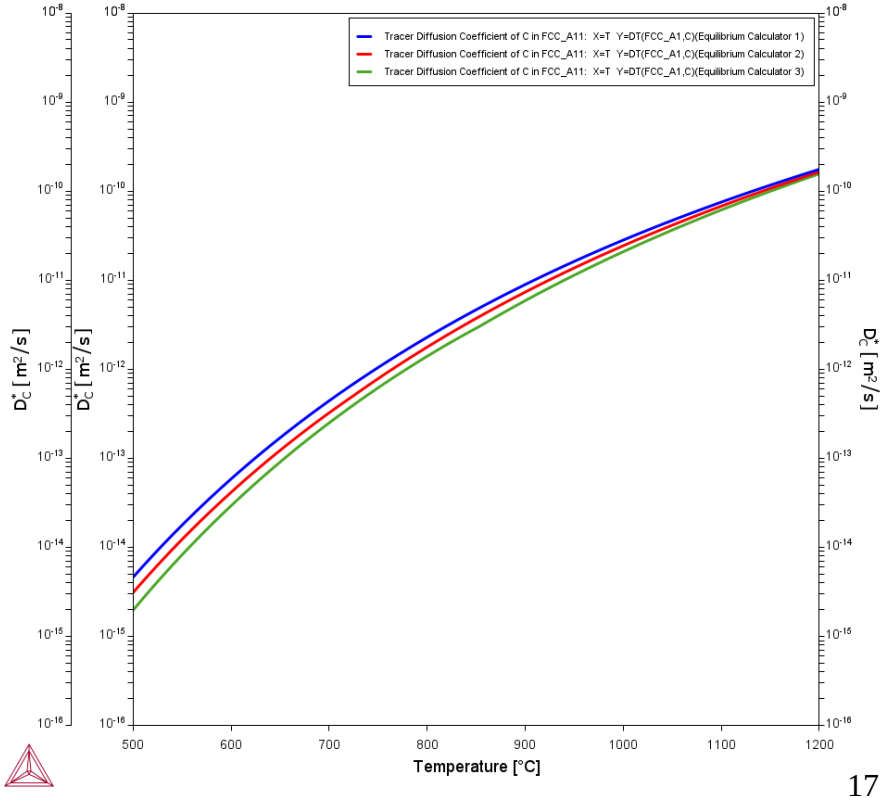
Example, Carbon diffusion in Austenite:

Fe-0.5C

Fe-2Cr-0.5C

Fe-5Cr-5Ni-0.5C

Note: Also ferromagnetic and chemical ordering is considered

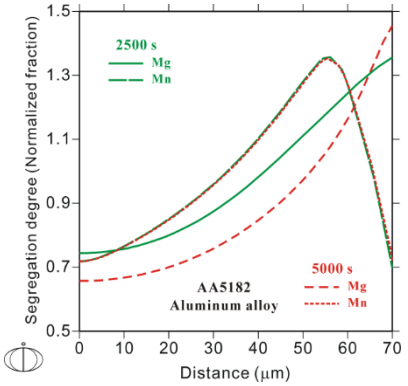


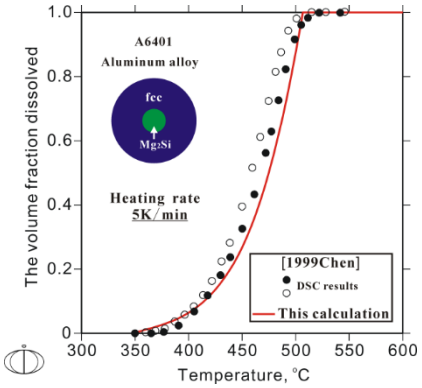
Diffusion Module (DICTRA)

Example of applications:

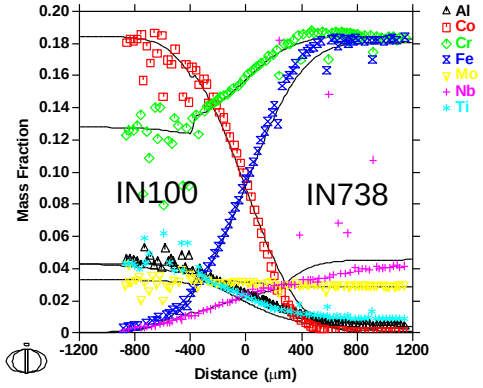
- ❑ Microsegregation during solidification
- ❑ Homogenisation treatment
- ❑ Precipitate growth and dissolution
- ❑ Carburization- Nitriding
- ❑ Interdiffusion in coating/substrate systems
- ❑ TLP bonding of alloys and much more…

Micro-segregation during solidification in alloy AA5182

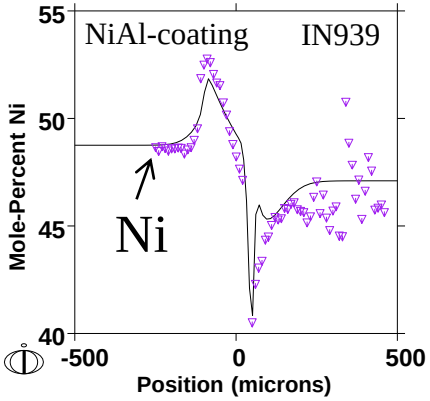




Dissolution of Mg_2Si precipitate in alloy A6401



Multicomponent diffusion couple

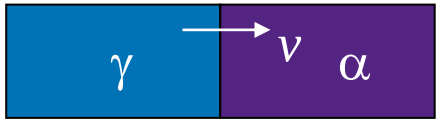


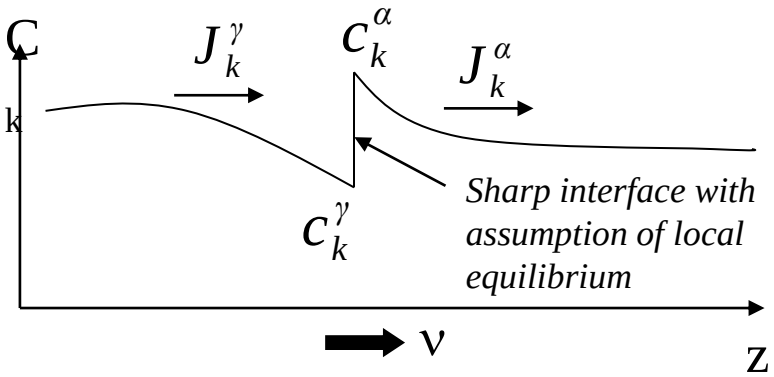
Interdiffusion between NiAl coating and Ni-base superalloy

Diffusion Module (DICTRA)

Two proven models for dealing with situations that involves more than a single phase. Program may switch automatically between them.

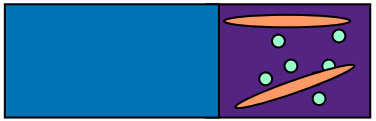
Moving boundary problems with sharp interface



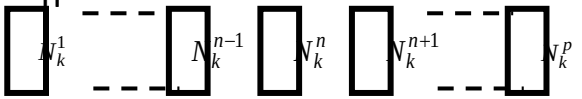


$$\sum_{k=1}^{n-1}\left[v\left(c_k^{\alpha}-c_k^{\gamma}\right)-\left(J_k^{\alpha}-J_k^{\gamma}\right)\right]^2<\varepsilon$$

Multiphase problems with/without finite interface



Flux between slices "n-1" and "n"



$$J_k=\frac{-1}{V_m}\sqrt{[M_k x_k]_{n-1}^{eff}[M_k x_k]_n^{eff}}\,\frac{\Delta\mu_k}{\Delta z}$$

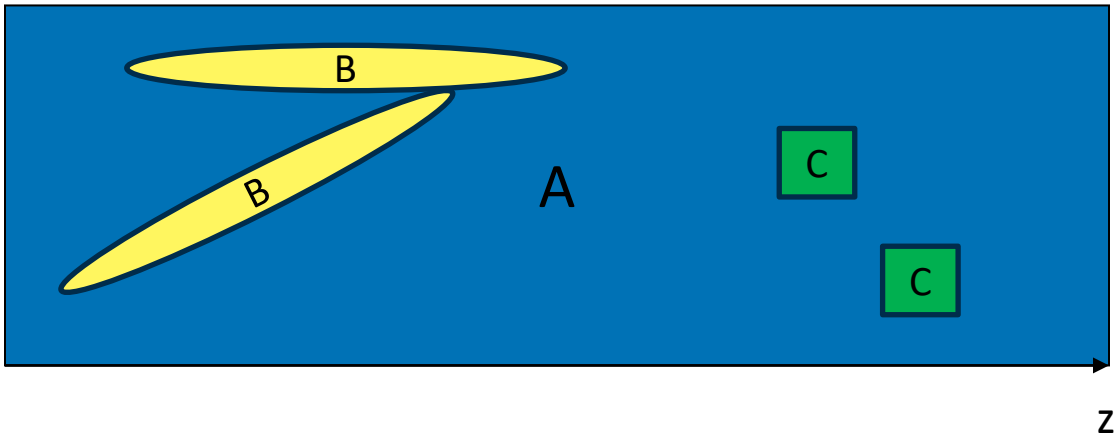
"Effective" $[M_k x_k]$ from combining rules

Outline

1. Introduction
    1. Thermo-Calc
    2. Calphad method
    3. Diffusion simulations (DICTRA)

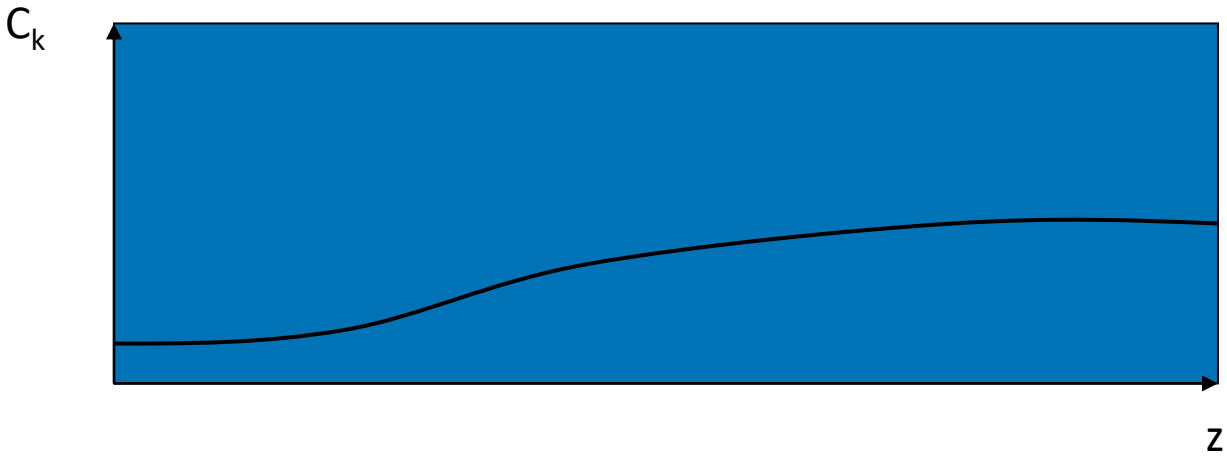
2. **Low Pressure Carburization framework**
    1. **Setup in DICTRA**
    2. Results
    3. Future work

Basic setup, Carburization - Nitriding



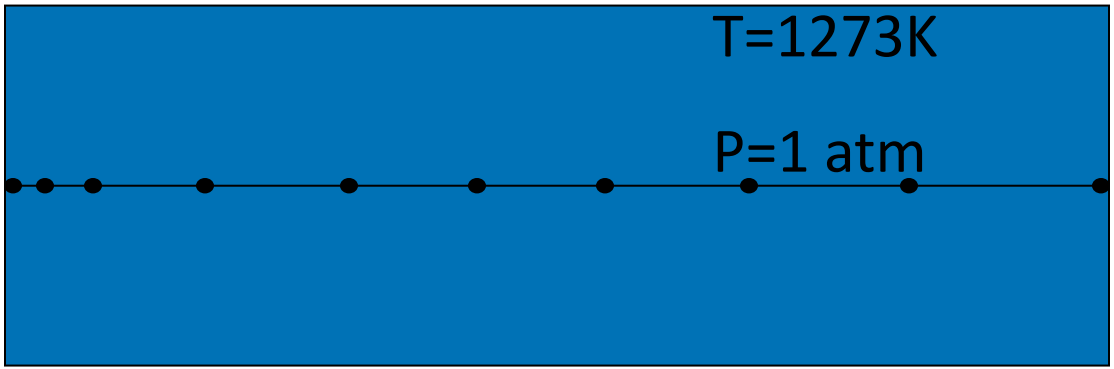
Region with a length z, and with phases A, B, C

Concentration Profile



Concentration, C_k of an element as a function of distance z

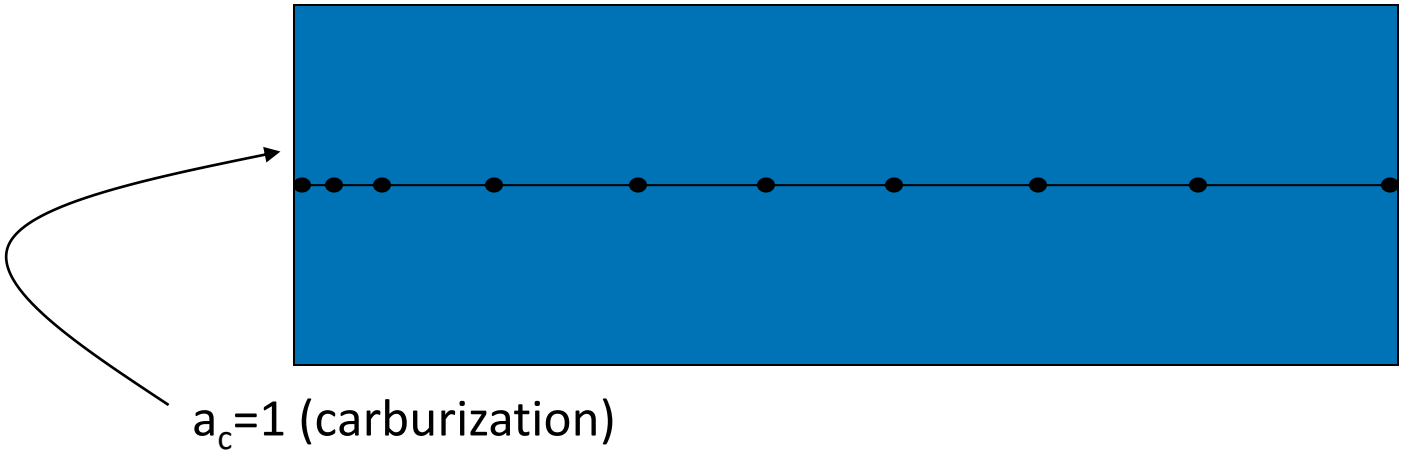
Global Conditions



Conditions valid for entire system, T and P

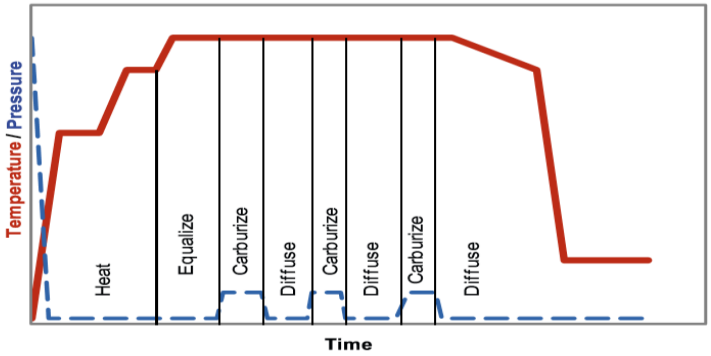
Define grid point distribution

Boundary Conditions



Conditions that apply to region boundaries (could be functions of time and temperature)

LPC setup in DICTRA



General conditions:

- Temperature
- Geometry (cylinder ∅25cm)
- Initial composition
- Austenite matrix, carbides can form

Boost step:

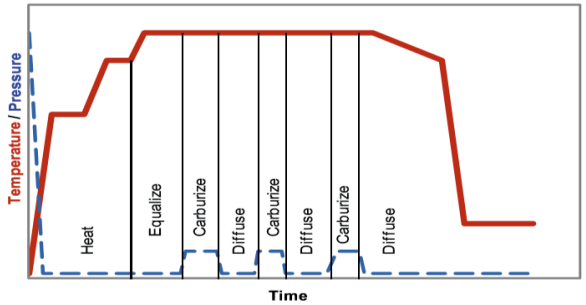
- Activity of carbon on surface=1 (pure graphite)

Diffusion step:

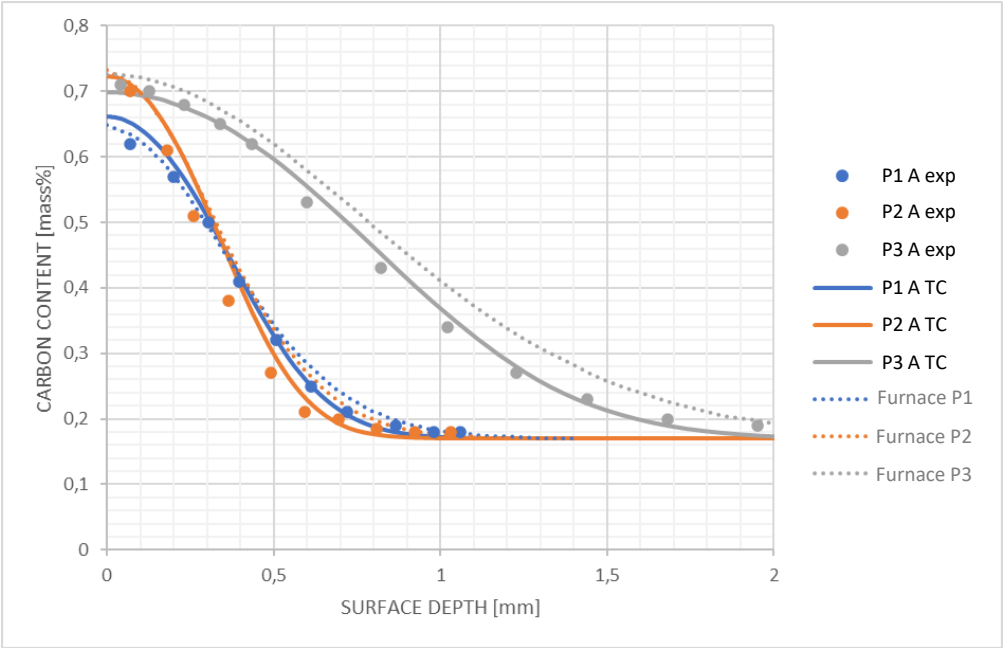
- Closed system (No elements can enter or leave system)

LPC validation

Run DICTRA simulations to reproduce LPC recipes from furnace programs, on 3 Steels A, B, C



3 different recipes for Steel A

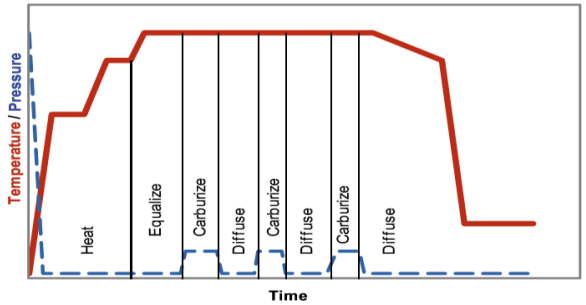


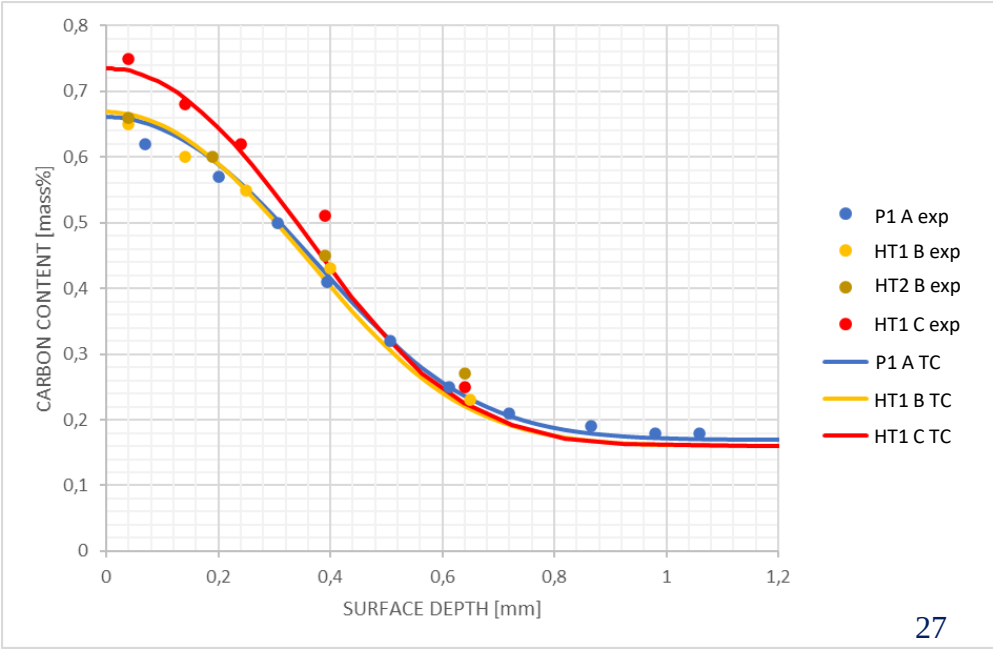
P1: 6 + 6
P2: 3 + 3
P3: 12 + 12

LPC validation

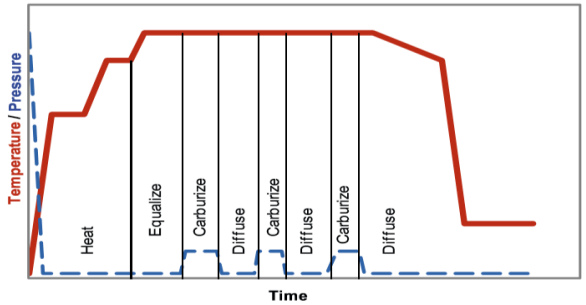
Same recipe
3 different Steels

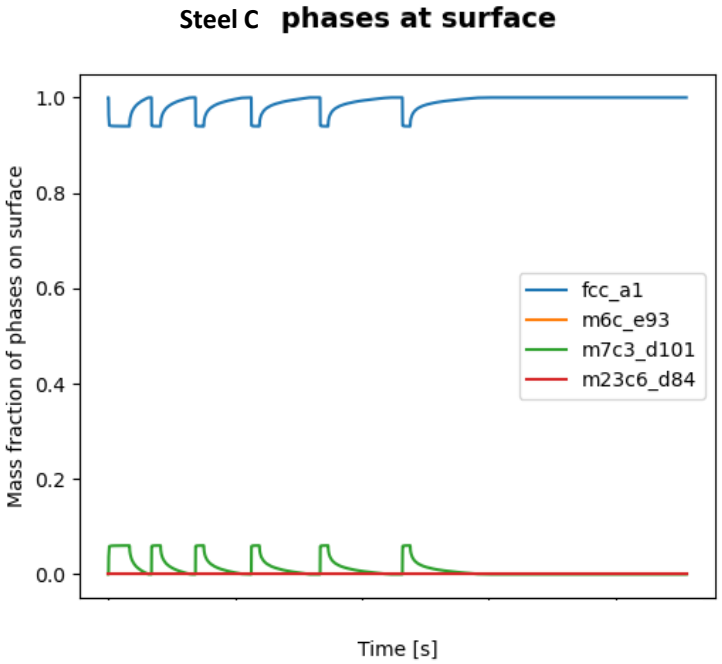
Steel A
Steel B
Steel C

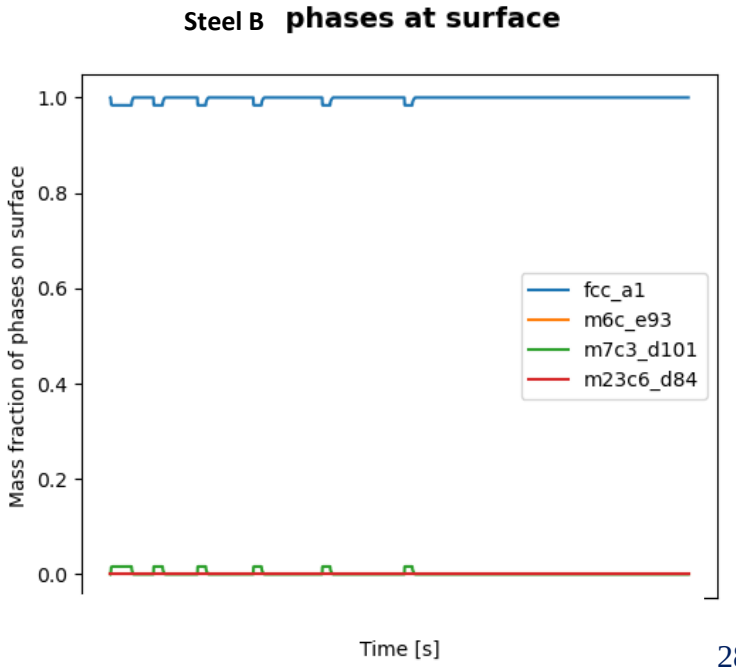




LPC validation



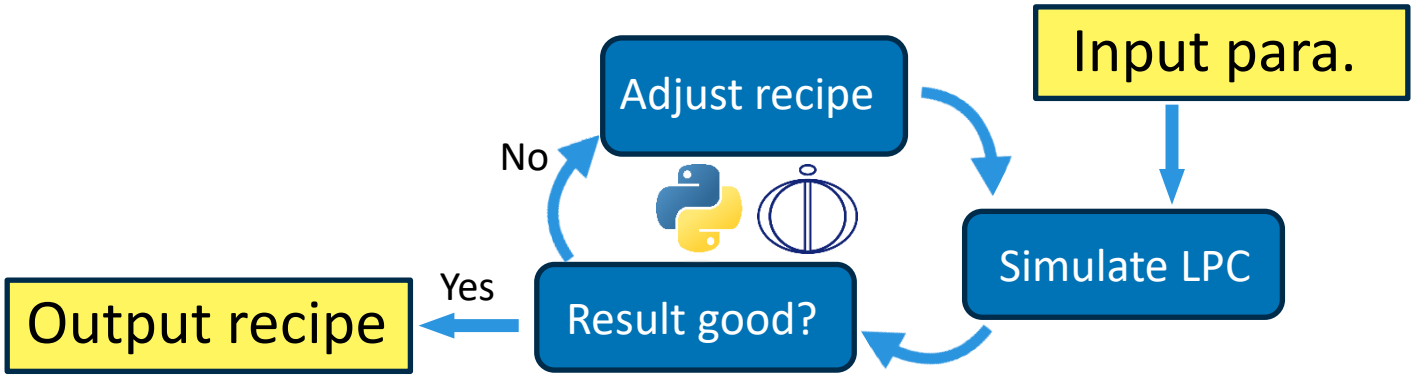




LPC Optimization framework

Since we have proven that DICTRA gives good results of Carbon profiles, we can use a TC-Python framework to “optimize” a LPC-recipe for any steel and hardening depth.

The output of the algorithm is a recipe that contains a sequence of boost and diffusion steps with calculated lengths that will result in the specified carbon profile, within the tolerances.



LPC Optimization framework

Mandatory input to the algorithm

Material_name

The name of the material
Example:
‘Steel 18-8'

Initial_composition

The material in mass%
Example
{“C": 0.08, “Cr”: 18, “Ni”: 8}

Radius

The radius of the cylindrical material in m
Example 12.5e-3

LPC Optimization framework

Optional input to the algorithm

hardening_depth
Hardening depth in m, measured from the centre of the cylindrical material.
Default value: 12.1e-3

done_when_c_at_hardening_depth
The carbon content to achieve at hardening depth when done, in mass fraction
Default value: 0.0035

done_when_c_at_surface
The carbon content to achieve at surface when done, in mass fraction.
Default value: 0.007

temperature
The temperature in Kelvin.
Default value: 1233

min_frac_fcc_at_surface_when_done
The minimum phase fraction of FCC on the surface that is allowed after the **last** diffusion step. (this is for dissolving carbides e.c.t.)
Default value: 0.999

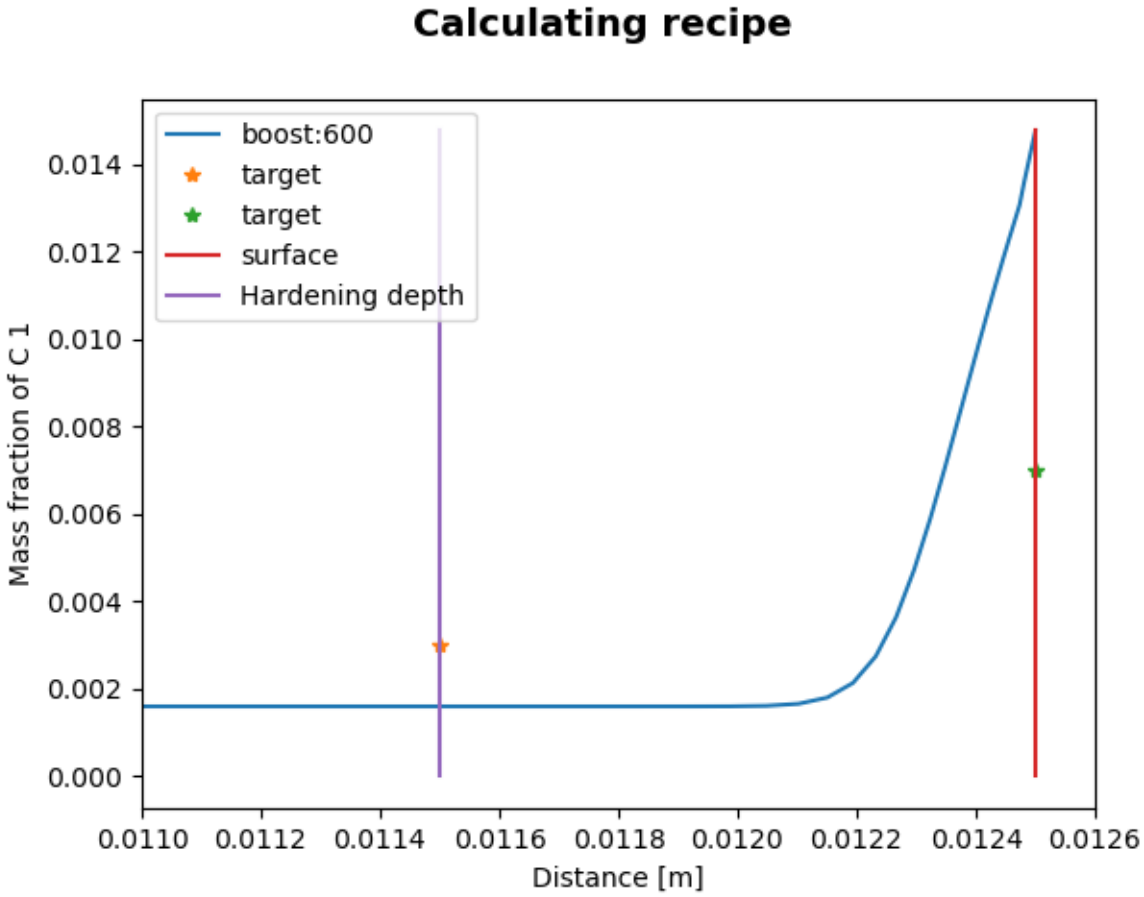
LPC Optimization framework

Internal parameters

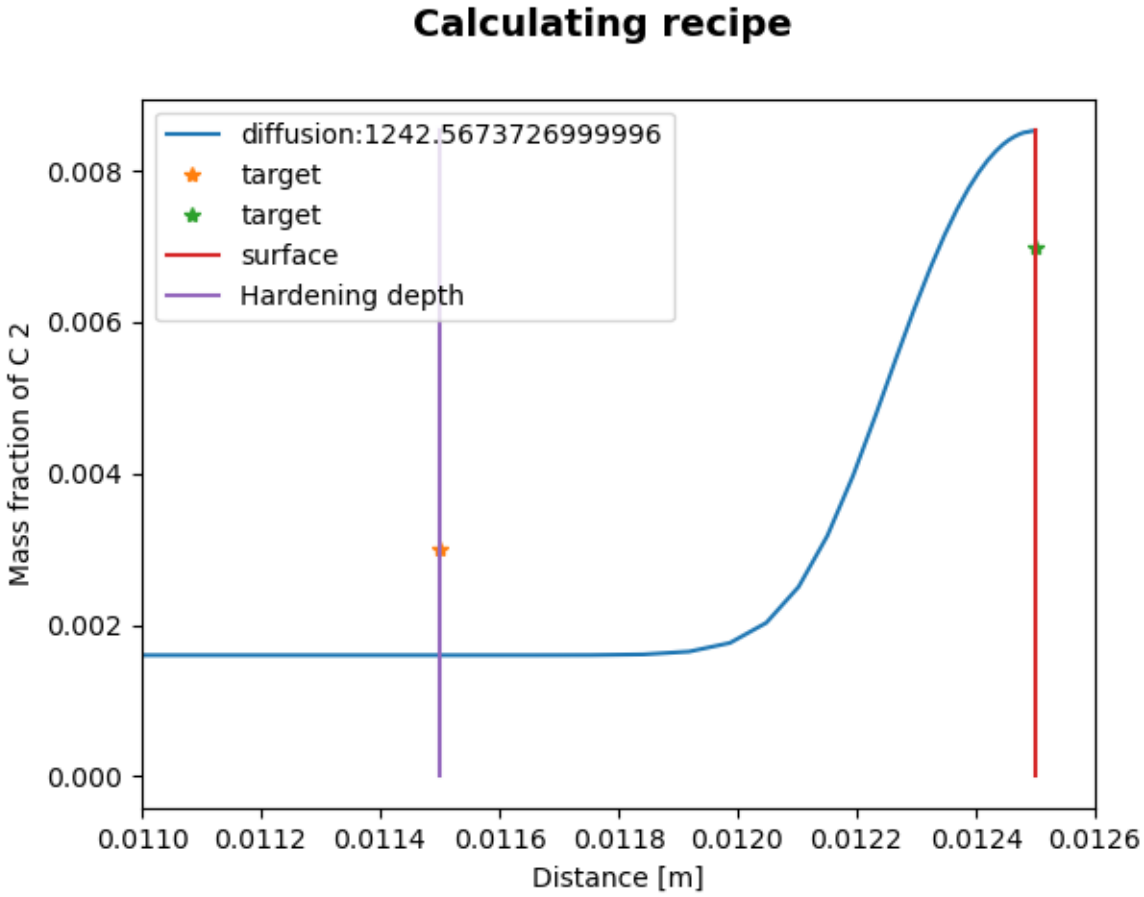
base_diffusion_step_in_s = 3600
max_boost_step_in_s = 600
min_boost_step_in_s = 50
tolerance_c_at_solution = 0.03 (in percent)

These numerical parameters are internal and not exposed to the user right now.
That could easily be changed.

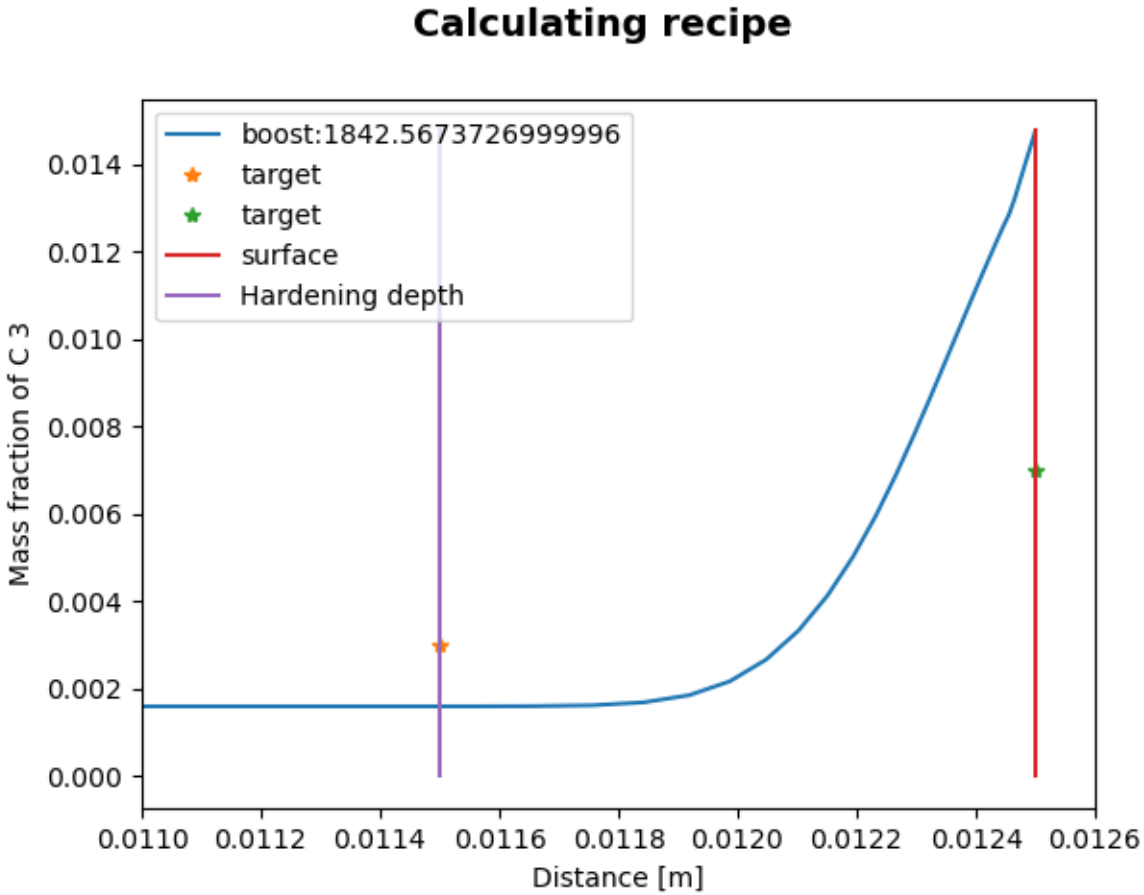
LPC Optimization framework: Result



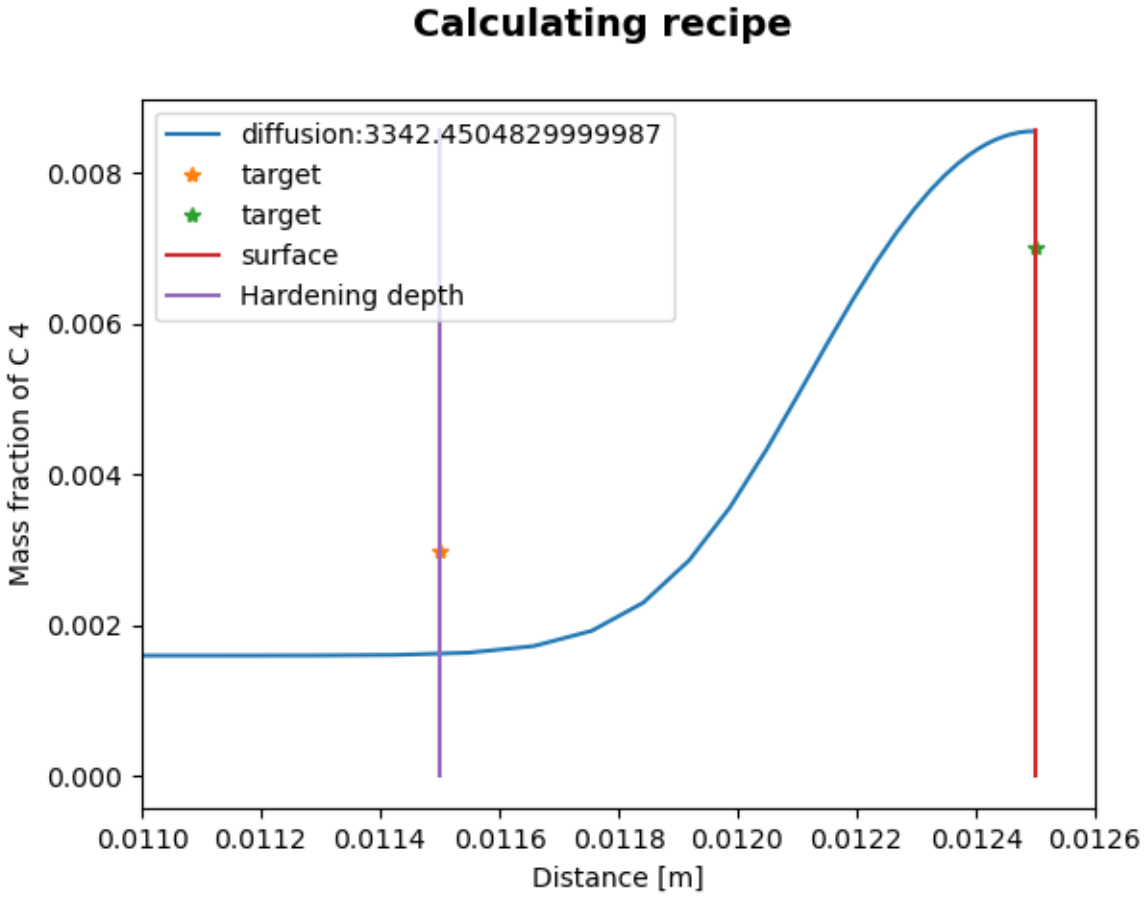
LPC Optimization framework: Result



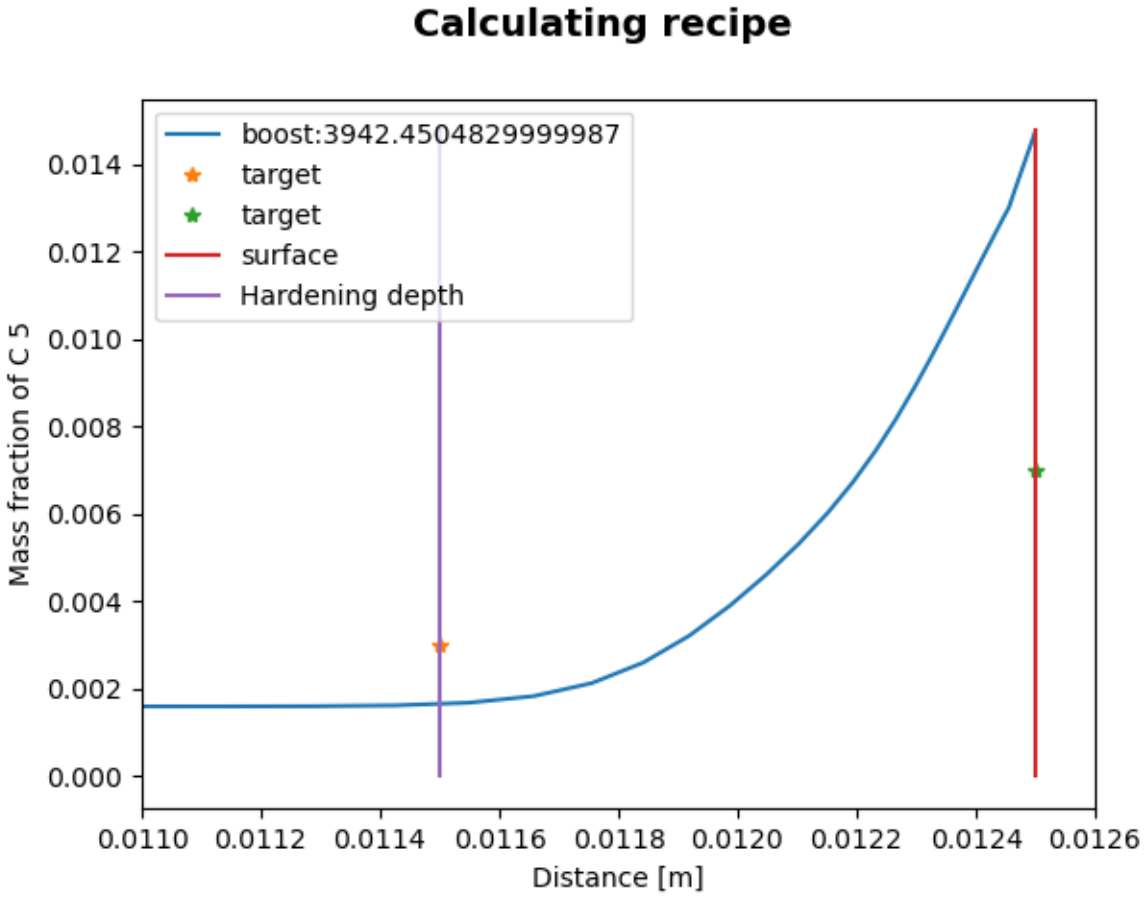
LPC Optimization framework: Result



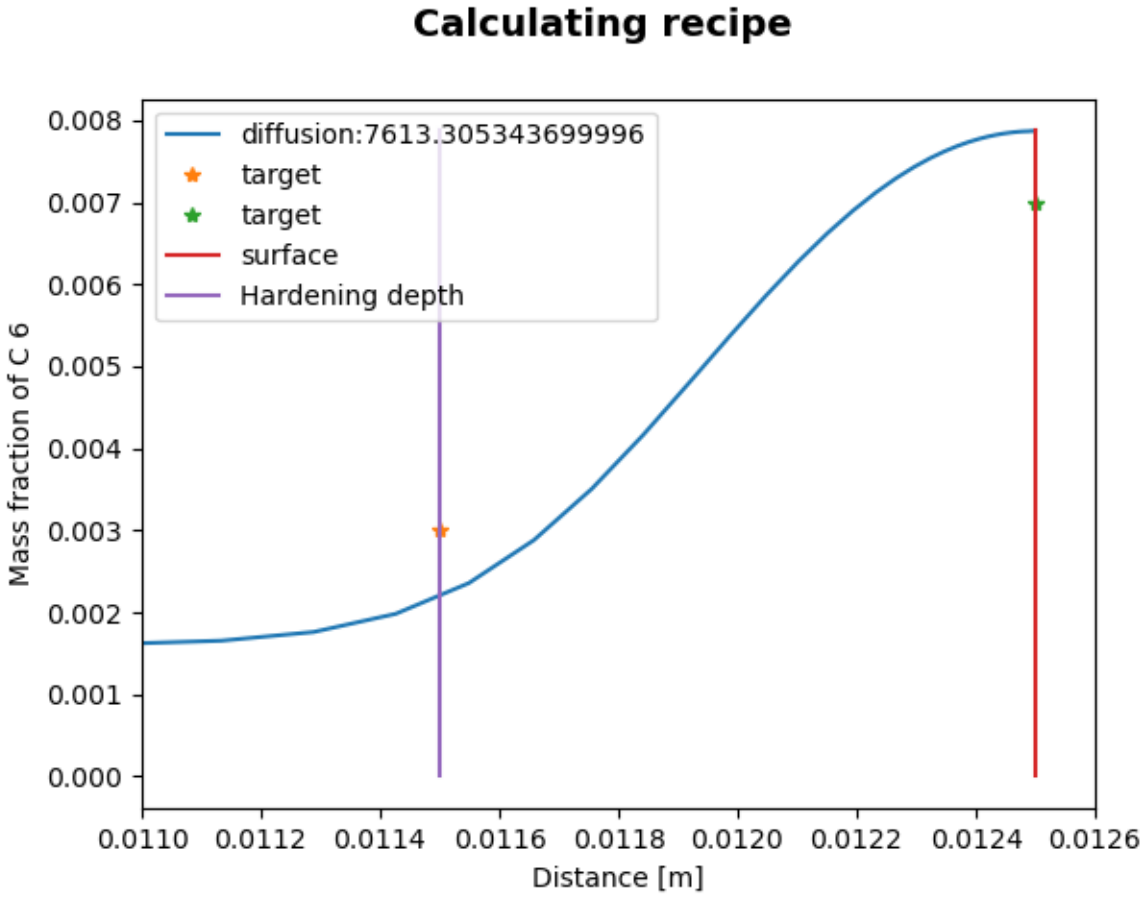
LPC Optimization framework: Result



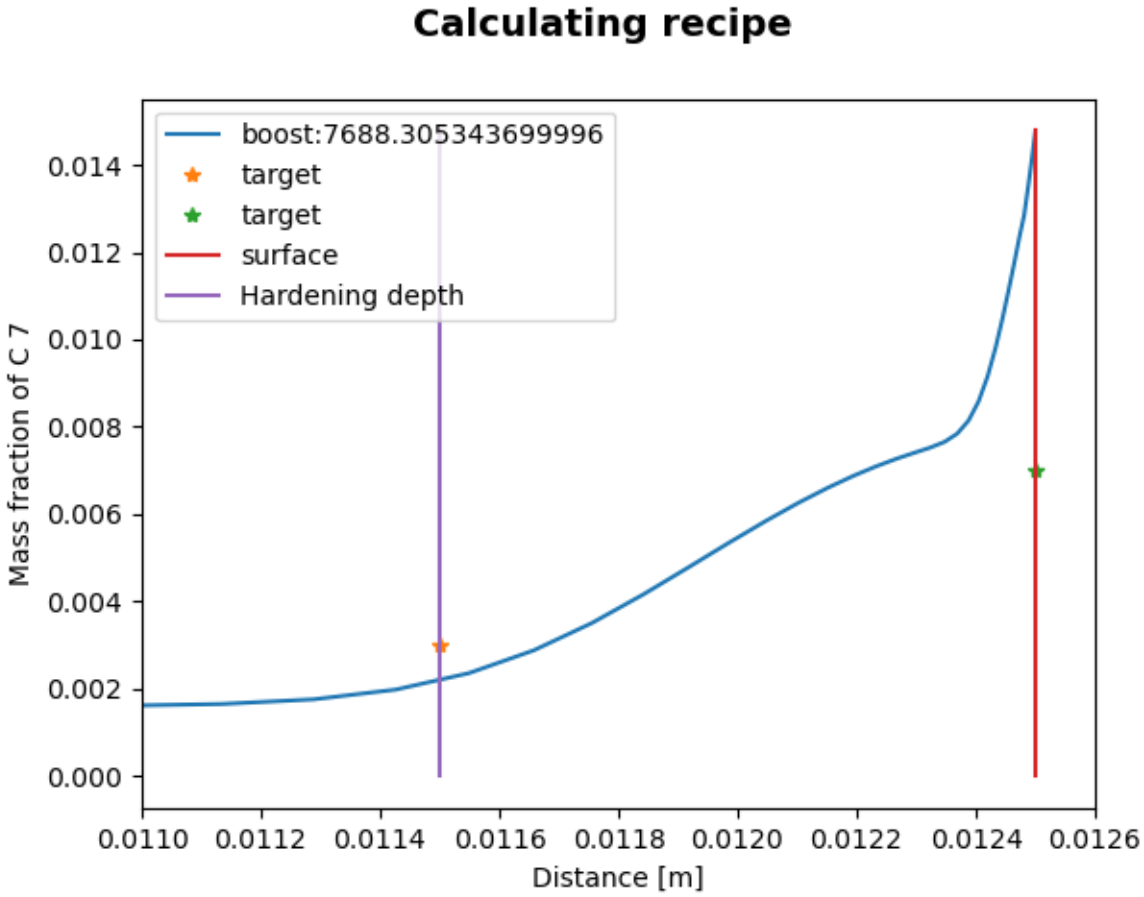
LPC Optimization framework: Result



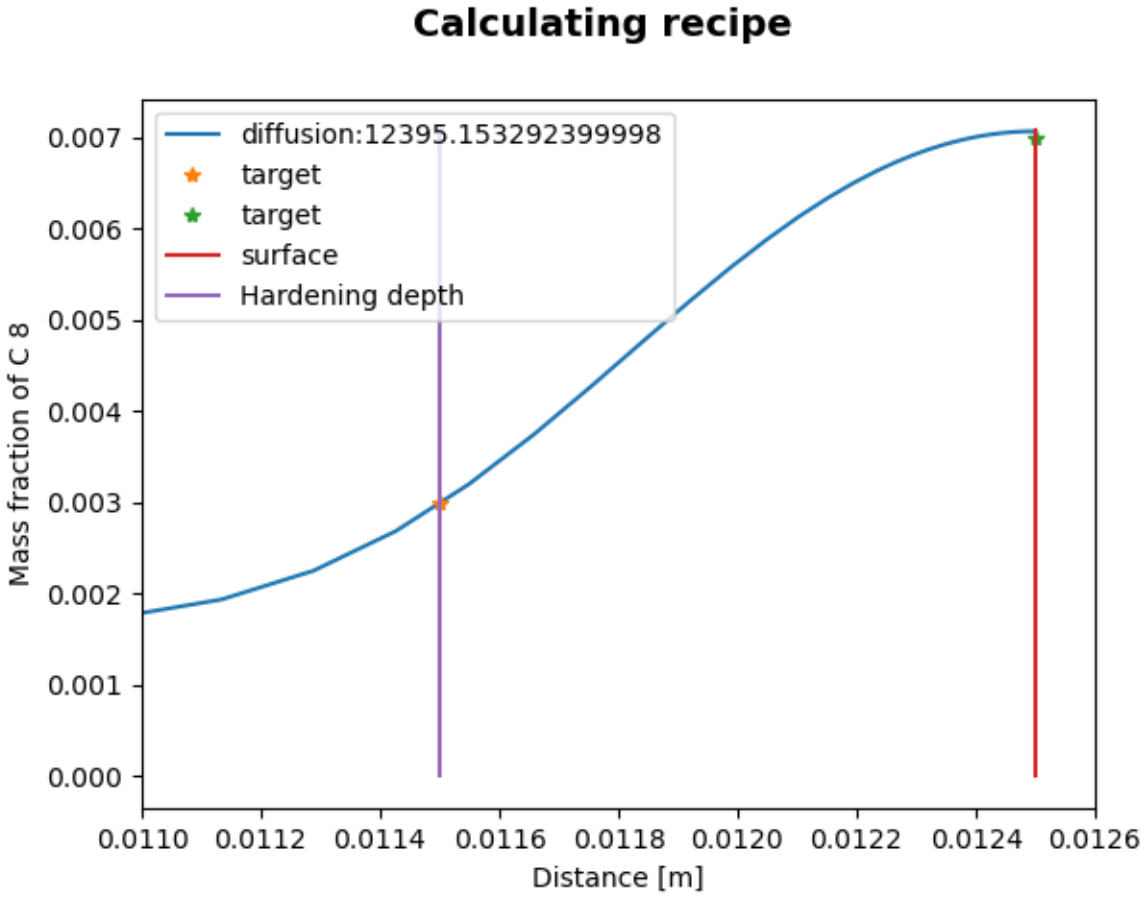
LPC Optimization framework: Result



LPC Optimization framework: Result

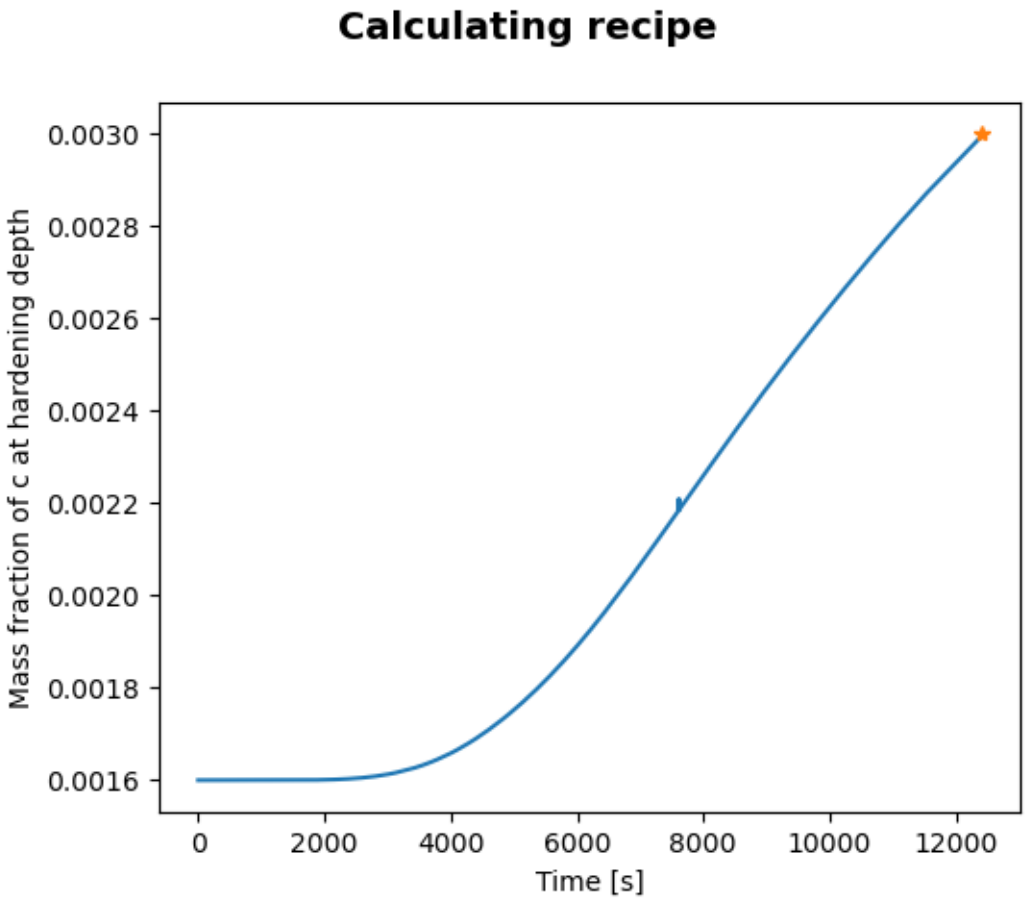


LPC Optimization framework: Result



LPC Optimization framework: Result

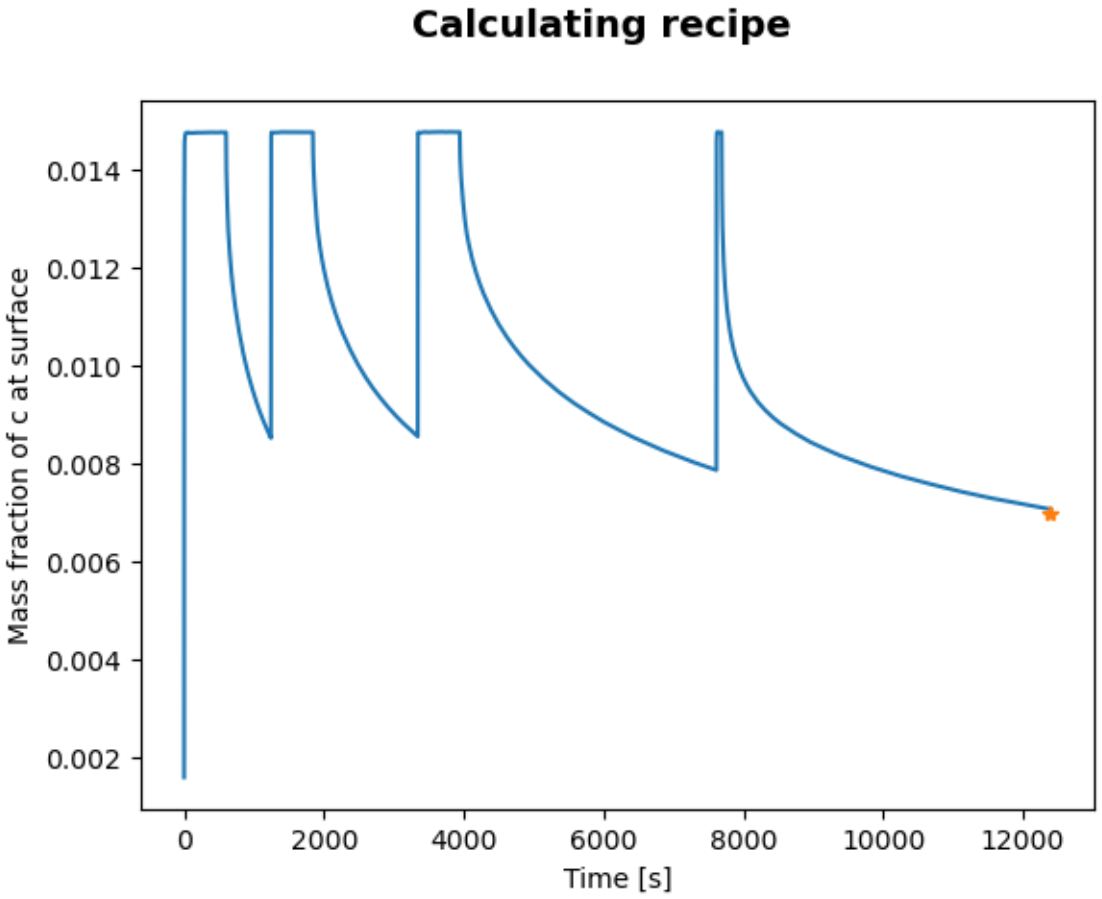
Hardening depth
C-content
vs Time



~3 hours

LPC Optimization framework: Result

Surface
C-content
vs Time



~3 hours

Summary

- DICTRA has proven to accurately predict the LPC process for varying recipes and alloys.
- TC-Python can be used as an “Optimization Framework” for developing new recipes.

- More experimental verification is needed for more high alloyed steels (Ongoing) and for validating the recipes from the optimizer.
- Optimize for other criterions?
- Future product model: package this as a specific software/service?

Tack för att ni lyssnade!