INTERACTIVE COUPLING OF THERMAL PROPERTIES CALCULATED THERMO CHEMICAL RESULTS WITH FEM SOLIDIFICATION SIMULATION PROGRAM

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INTRODUCTION

- Thermo- physical and physical properties are critical data for solidification simulations.
- Latent heat release, solid fraction transformation, thermal conductivity, volume and density all as function of temperature are difficult to get experimentally.
- Lack of information → common to use binary alloy data to perform multi- component alloy calculations.
- Small variations in composition can have appreciable effects on properties. No sense to extrapolate from other alloys or binary alloy data.
- Cooling rate has also influence on those properties.
- Highly desirable to develop computer models for calculation of the thermo-physical and physical properties of multi- component alloys.
- Already some computational techniques available e.g. FactSage

OBJECTIVES

- Achieve a coupling of calculated thermo- physical properties with WinCast®.
- Study influence of changing cooling rates and alloying elements on thermo- physical properties of an alloy.
- Evaluate how can the simulation results change.
- Using ChemApp, a thermodynamic calculation interface, a couple of programs pretended to set to obtain thermo physical properties.

- Computer modelling tools based on the CALPHAD (CALculation of Phase Diagrams) method commonly used to predict thermo- physical properties and phase equilibriums in multi component alloys.
- Calculation methods:
  1. Enthalpy method
  2. Gibbs energy minimisation
  3. Modified specific heat method

$$\frac{1}{V}\cdot\frac{\partial\Phi}{\partial t} = -divJ_{\Phi}$$

$$c_p^* = \frac{dL(T)}{dT} + c_p$$

- Latent heat prediction
- Phase diagram prediction
- Physical property prediction
- Solute partition prediction

- Stoichiometric compounds $G_m - H_m^{SER} = a + bT + cT\ln T + \sum_2^n d_n T^n$
- Solution phases $\Delta G = \Delta G^0 + \Delta G_{mix}^{ideal} + \Delta G_{mix}^{xs}$
- Ideal solution model $\Delta G = \sum_i x_i \Delta G_i^0 + RT\sum_i x_i \log_e x_i$
- Nonideal solution model $\Delta G = \sum_i x_i \Delta G_i^0 + RT\sum_i x_i \log_e x_i + \sum_i \sum_{j>i} x_i x_j \sum_v \Omega_{ij}^v (x_i - x_j)^v$

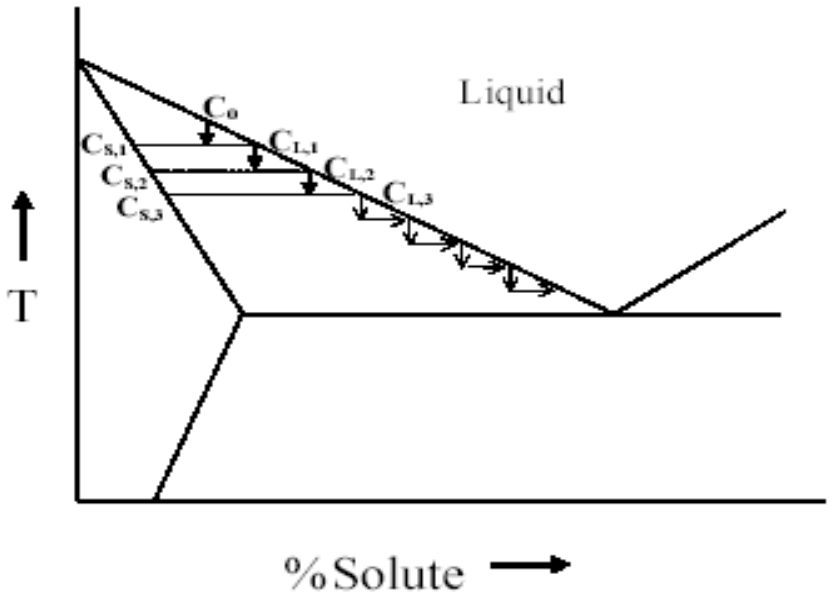
ChemApp

- Library of programmable subroutines to perform phase equilibrium calculation.
- Based on improved equilibrium routines of ChemSage, same data- file format and same comprehensive library of models for non-ideal solution phases.
- Can be programmed in FORTRAN, C, C++, Visual Basic® or Delphi®.
- Great flexibility to design and implement thermodynamic calculation techniques due to its modularity.
- To initialise and obtain results three simple programming stages are necessary:

1. **Initialise interface, read a thermodynamic data-file and adjust the chemical system.**
2. **Set initial conditions for the equilibrium calculation, defining:** { Global conditions. / Streams.
3. **Perform the calculation and collect results.**

Scheil- Gulliver solidification model

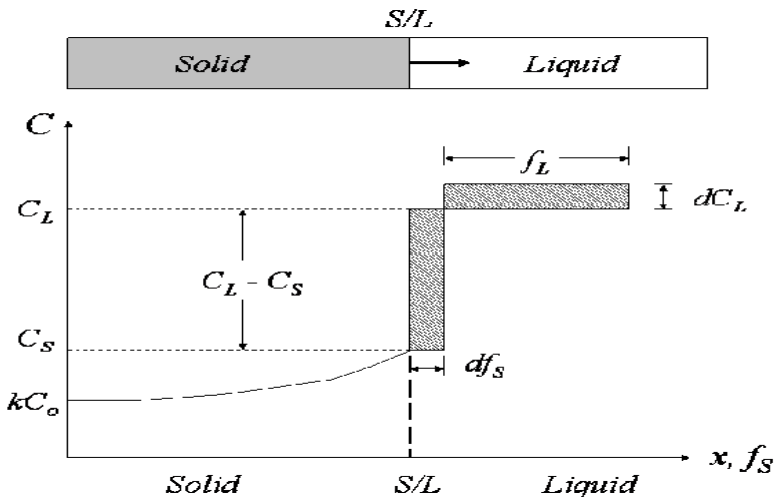
- No solute diffusion in solid phase and complete diffusion in liquid phase.



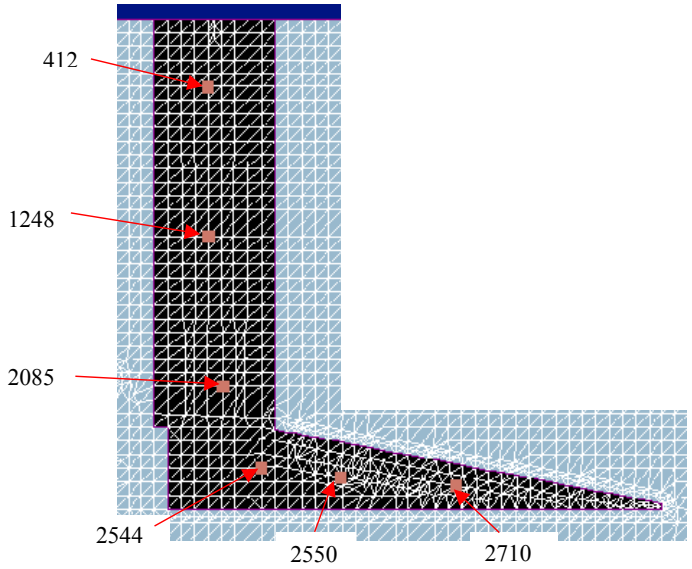
$$x_s = k \cdot x_0 (1 - f_s)^{(k-1)}$$

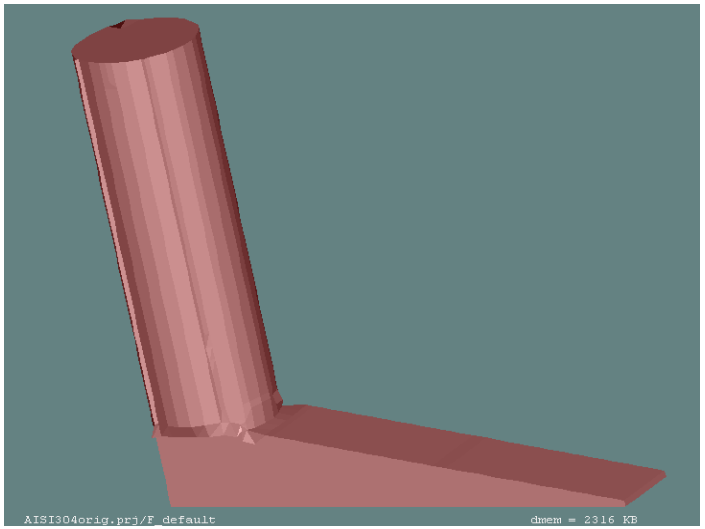
$$f_s = 1 - \left(\frac{T_s - T}{T_s - T_L} \right)^{\left[\frac{1}{k-1}\right]}$$

$$x_L = x_0 \cdot f_L^{(k-1)}$$



SENSITIVITY ANALYSIS





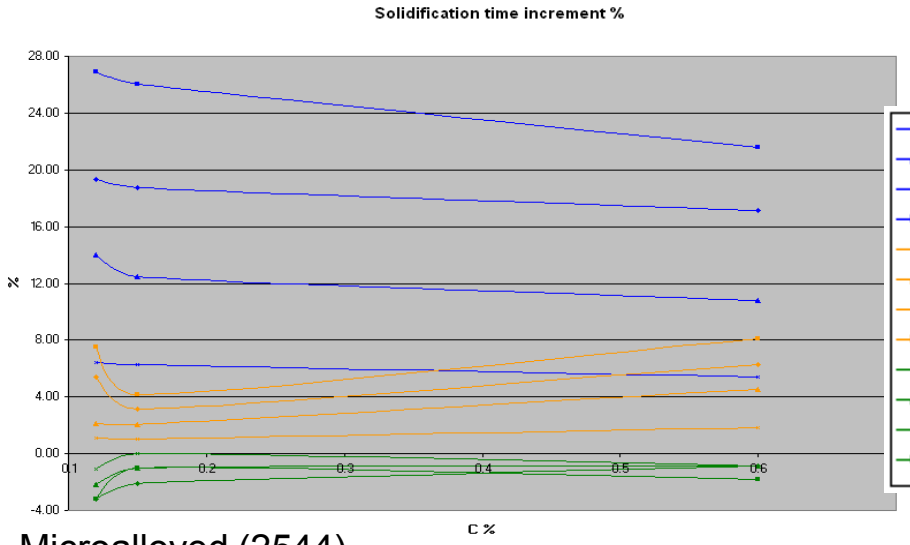
Analysed alloys: for the geometry wedge

- 1.1201
- 1.6740
- AISI430
- AISI304
- Microalloyed steel
- DP500
- AZ91E
- MRI207S (Mg- Zn- Zr- Nd- Y- Gd)
- Al Si Alloys

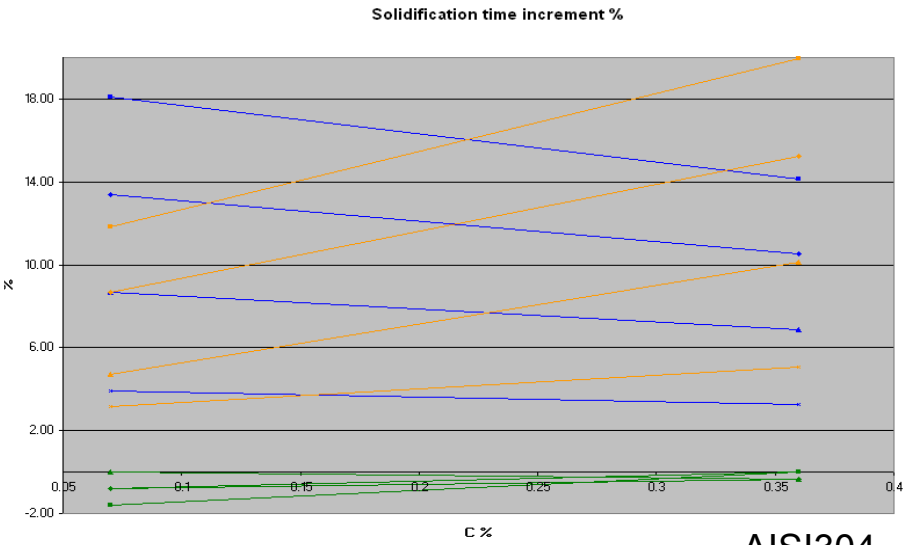
Sand casting simulations

Changing GE, RO, LA
5%, 10%, 15%, 20%

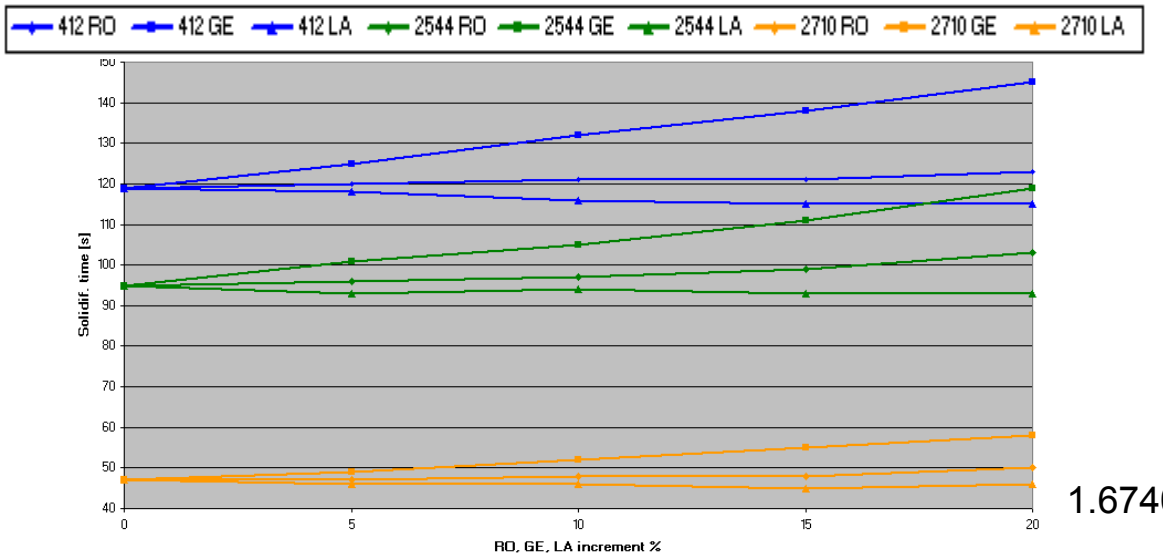
SENSITIVITY ANALYSIS



Microalloyed (2544)



AISI304 (2544)



1.6740 (0.33 %C)

CONCLUSIONS

- C % variations can alter pretty the latent heat of solidification within the composition range for a microalloyed steel.
- According to IDS cooling rate variations do not change thermo-physical properties at liquidus temperature, ChemApp demostrates that it is not true.
- When C, Cr and Ni % and casting simulation input properties vary, solidification times increment.
- Latent heat release augmented 20% respect the original increments 25% solidification time.

CONCLUSIONS

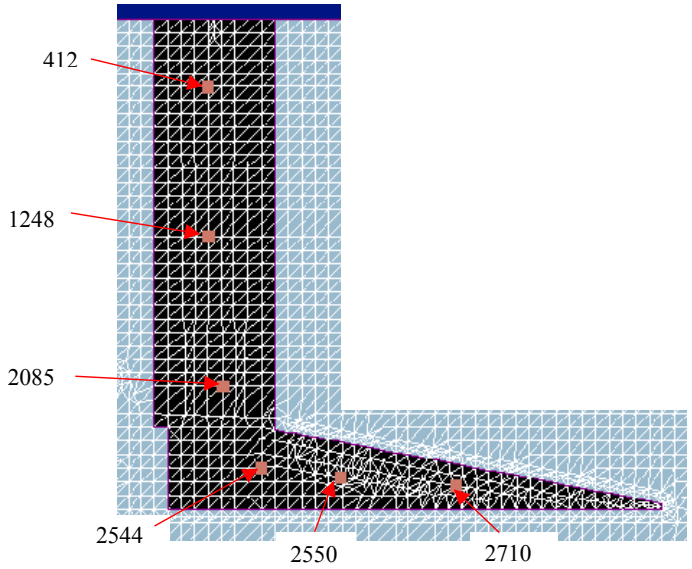
- Density and specific heat values increment solidification time, but as latent heat release except for stainless steels. Increments on thermal conductivity reduce solidification time.

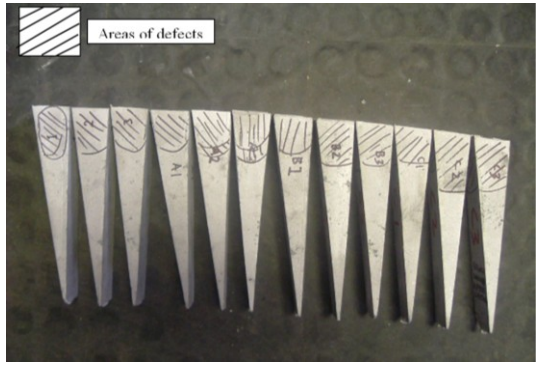
- Two programs created from ChemApp programmed subroutines to achieve a coupling of calculated thermo- physical properties with WinCast.

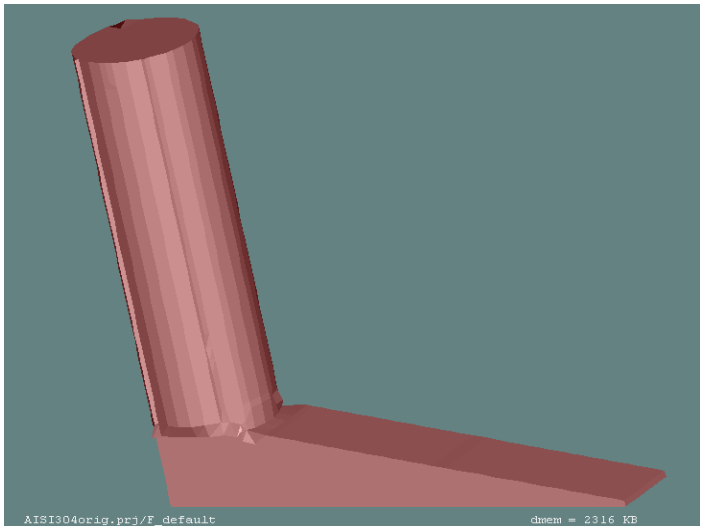
- Calculation accuracy improved since four different latent heat releasing and density- cp modes can be computed.

- Availing ChemApp subroutines phase diagrams, solid and liquid fractions, phase names, phase composition, specific heat capacities or remaining liquid fraction's liquidus and solidus temperatures can be achieved.

REAL CASTINGS







The real castings are carried out during the IDEA project. Here some investment castings.

Solidification calculation

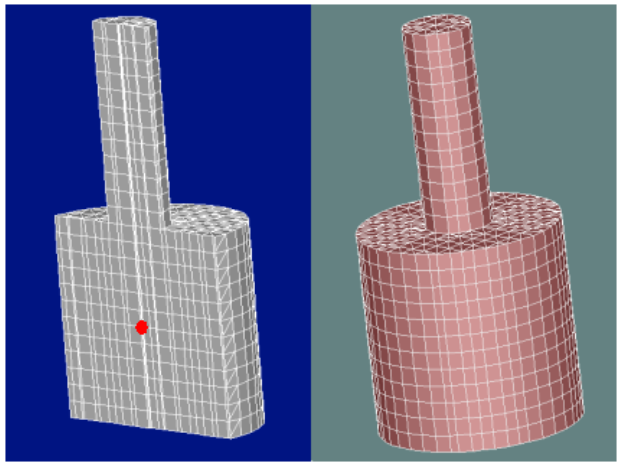
```
Alloy composition in weight %: Si=  7.00   Al= 92.70   Mg=  0.30

 - The liquidus temperature is          615.39 °C
 - The solidus temperature is           567.66 °C
 - The eutectic temperature is          557.43 °C
 - The nominal fusion temperature is    858.21 °C


n° of phases: 11

Equilibrium latent heat=  454.55 J/g

Temperature= 570.84 °C       Specific heat(cp)= 1.155 J/gC

Latent heat=   38.81 J/g

Phase 1:           LIQUID:  7.70 %      Si= 12.81 %   Al= 85.71 %   Mg=  1.48 %

 - The liquidus temperature is     570.84 °C
 - The solidus temperature is      557.43 °C

Phase 2:       DIAMOND_A4:  4.72 %      Si=100.00 %   Al=  0.00 %   Mg=  0.00 %
Phase 3:           FCC_A1: 87.58 %      Si=  1.48 %   Al= 98.31 %   Mg=  0.21 %
Phase 4:       ALMG_GAMMA:  0.00 %      Si=  0.00 %   Al=  0.00 %   Mg=  0.00 %
Phase 5:           HCP_A3:  0.00 %      Si=  0.00 %   Al=  0.00 %   Mg=  0.00 %
Phase 6:        Mg_hcp_a3:  0.00 %      Si=  0.00 %   Al=  0.00 %   Mg=  0.00 %
Phase 7:        Al_fcc_a1:  0.00 %      Si=  0.00 %   Al=  0.00 %   Mg=  0.00 %
Phase 8:     Al30Mg23_eps:  0.00 %      Si=  0.00 %   Al=  0.00 %   Mg=  0.00 %
Phase 9:   Al140Mg89_beta:  0.00 %      Si=  0.00 %   Al=  0.00 %   Mg=  0.00 %
Phase10:    Si_diamond_a4:  0.00 %      Si=  0.00 %   Al=  0.00 %   Mg=  0.00 %
Phase11:           Mg2Si:  0.00 %      Si=  0.00 %   Al=  0.00 %   Mg=  0.00 %
```

WinCast

```
16       438.14       628.39       435.60
 435.60           0.000
 445.80           0.021
 458.84           0.022
 471.88           0.023
 484.93           0.025
 497.97           0.027
 511.01           0.029
 524.05           0.031
 537.09           0.034
 550.14           0.038
 563.18           0.043
 576.22           0.058
 589.26           0.086
 602.30           0.144
 615.34           0.309
 628.39           1.000
    Latente Waerme     438.14(J/cm3)
    Stoff              <MgAl2.2Si1>
    Quelle             ChemApp calculation
```

- Latent heat release: GE
- Density x Cp: RO

Results and discussion

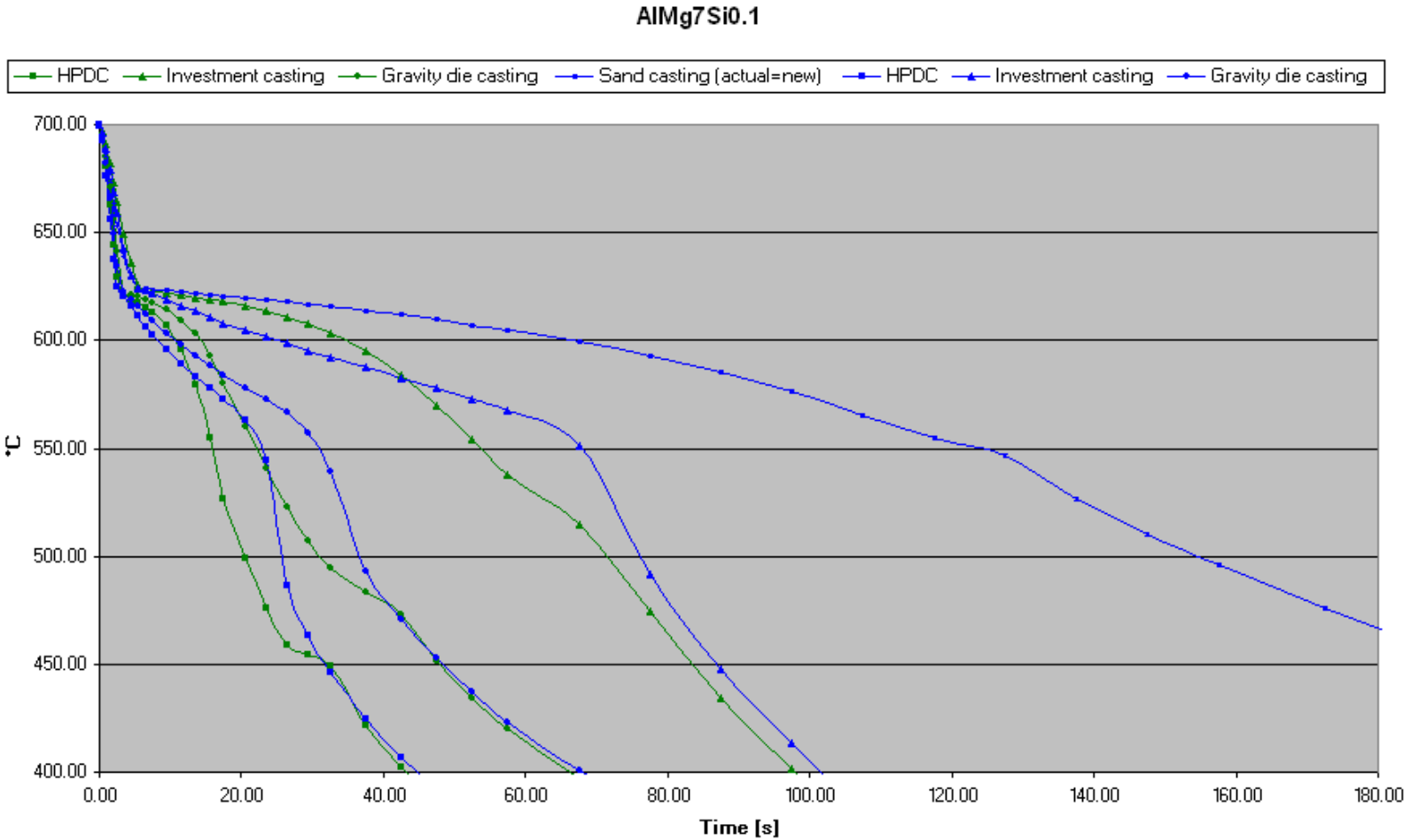


Casting technology	Mould material	Initial mould temp. [ºC]
Sand casting	Sand	25
Investement casting	Mullit	280
Gravity die casting	1.2343 steel	340
High pressure die casting	1.2343 steel	400

	Mg%	Al%	Si%
AlSi7Mg0.3	0.3	92.7	7
AlMg7Si0.1	7	92.9	0.1
MgAl2.2Si1	96.8	2.2	1
MgAl9.7Si0.3	90	9.7	0.3

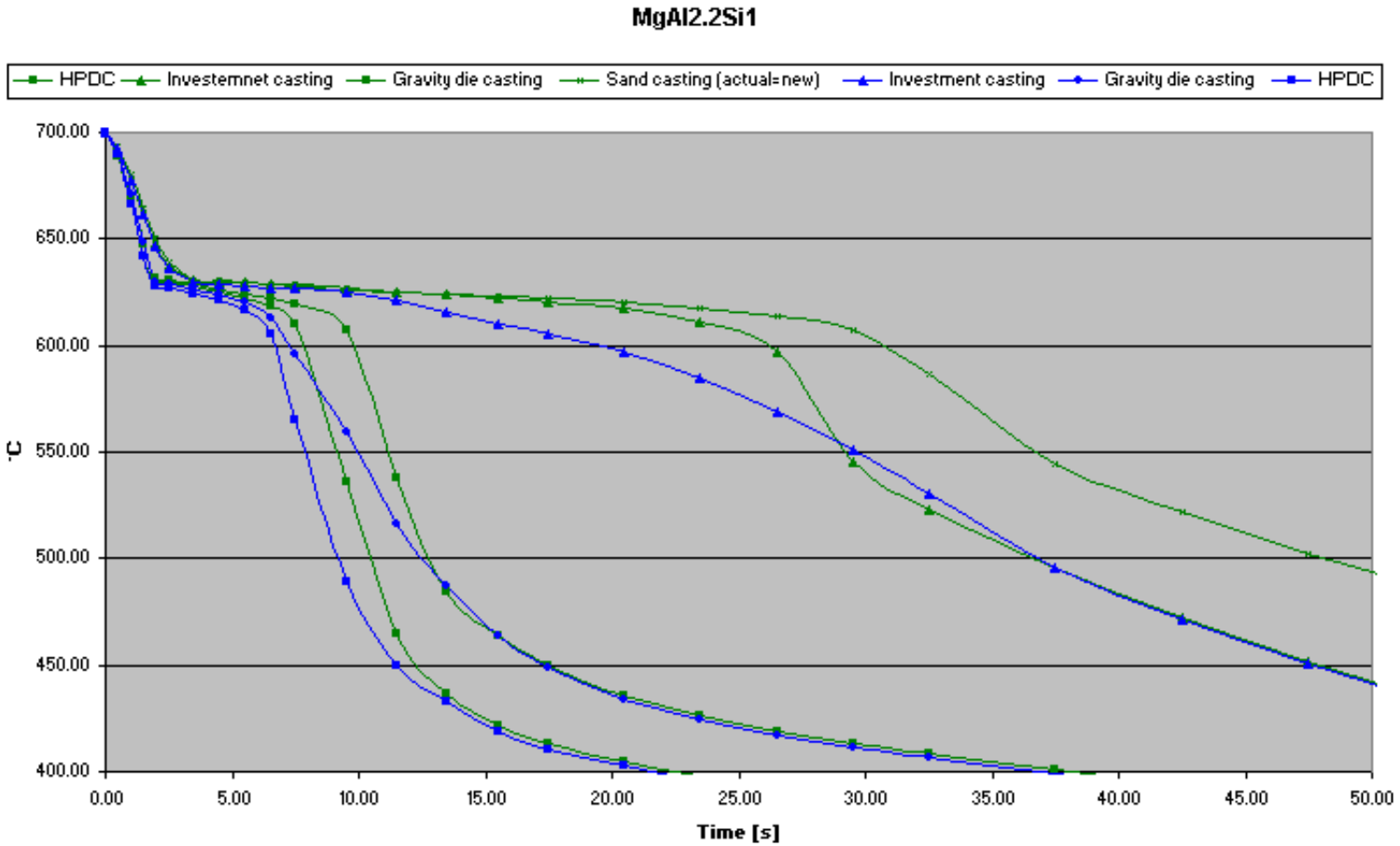
- Feeder covered with ***kal80*** sleeve at initial temp.: ***25ºC***
- Initial melt temperature: ***700ºC***

Results and discussion



HPDC new solidification temperature interval 100% greater than actual.

Results and discussion



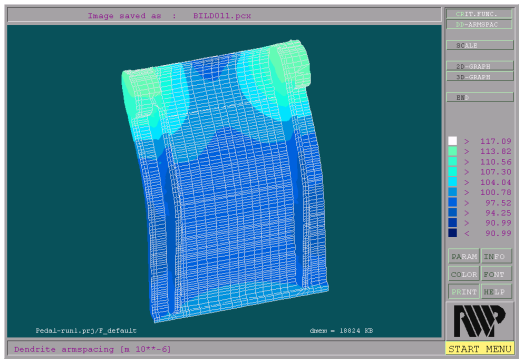
HPDC new temp. Gradient about 27ºC/s, actual about 8ºC/s.

Reference part “Pedal”

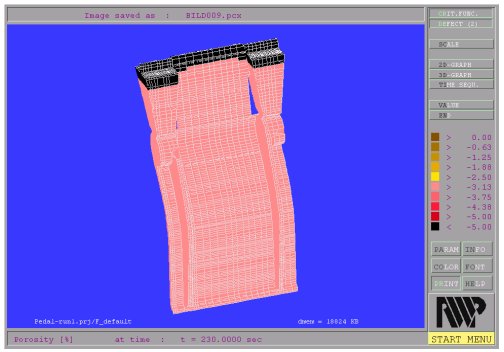
design for HPDC

design investment Casting

design for gravity die Casting

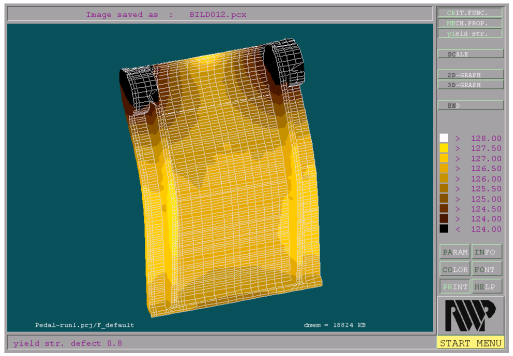


grain size Gs

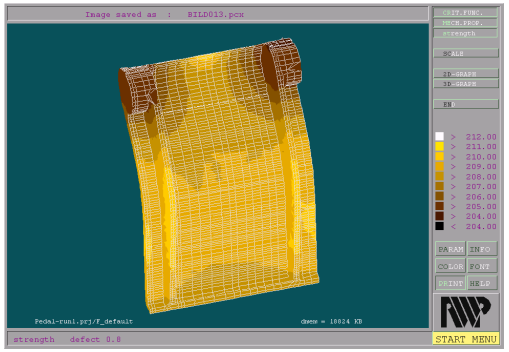


porosity P

form factor of 0.8



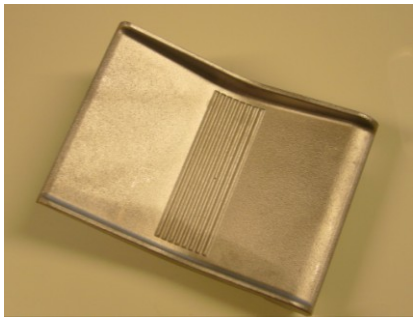
yield strength TYS



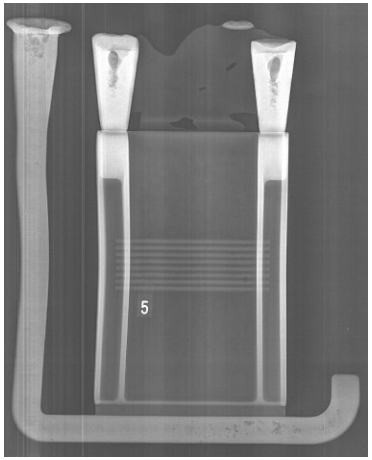
tensile strength UTS

Reference part “Pedal”

first trials



final test



X-ray test

FUTURE WORK

- Diffusion conditions are known only for two of the four cooling velocities. Equations that can describe diffusion would be good to be available as input.

- Data- bases which content material and phase related thermodynamic data must be increased.

- Thermal conductivity values must also be computed to perform as accurate casting simulations as possible.


Questions and discussion