Coupling WinCast to ChemApp for the calculation of final microstructure distribution

Haritz Sarriegi Etxeberria Ph. D. student

Mondragon Unibertsitatea

Mechanical and Manufacturing Department

Arrasate-Mondragon, Basque Country, Spain

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Outline

- Introduction
- ChemApp coupled microstructure development model for AZ91 Mg alloy
  - ❑ Phase distribution depending on diffusion time
  - ❑ Al and Zn segregation in solid depending on diffusion time
  - ❑ Latent heat release depending on diffusion time
  - ❑ Solid fraction vs Latent heat
- Casting simulations with WinCast
- Summary and Future work

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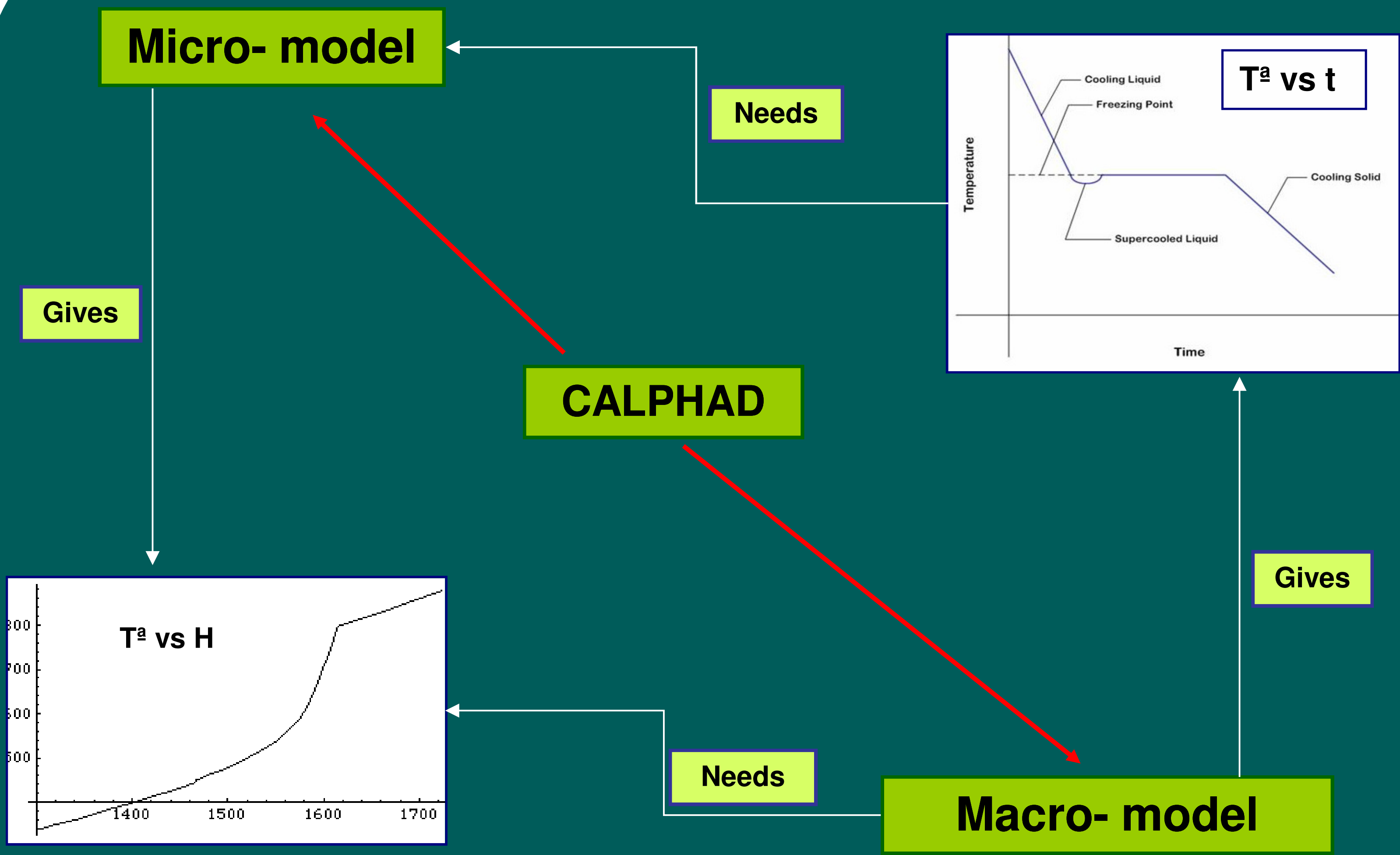

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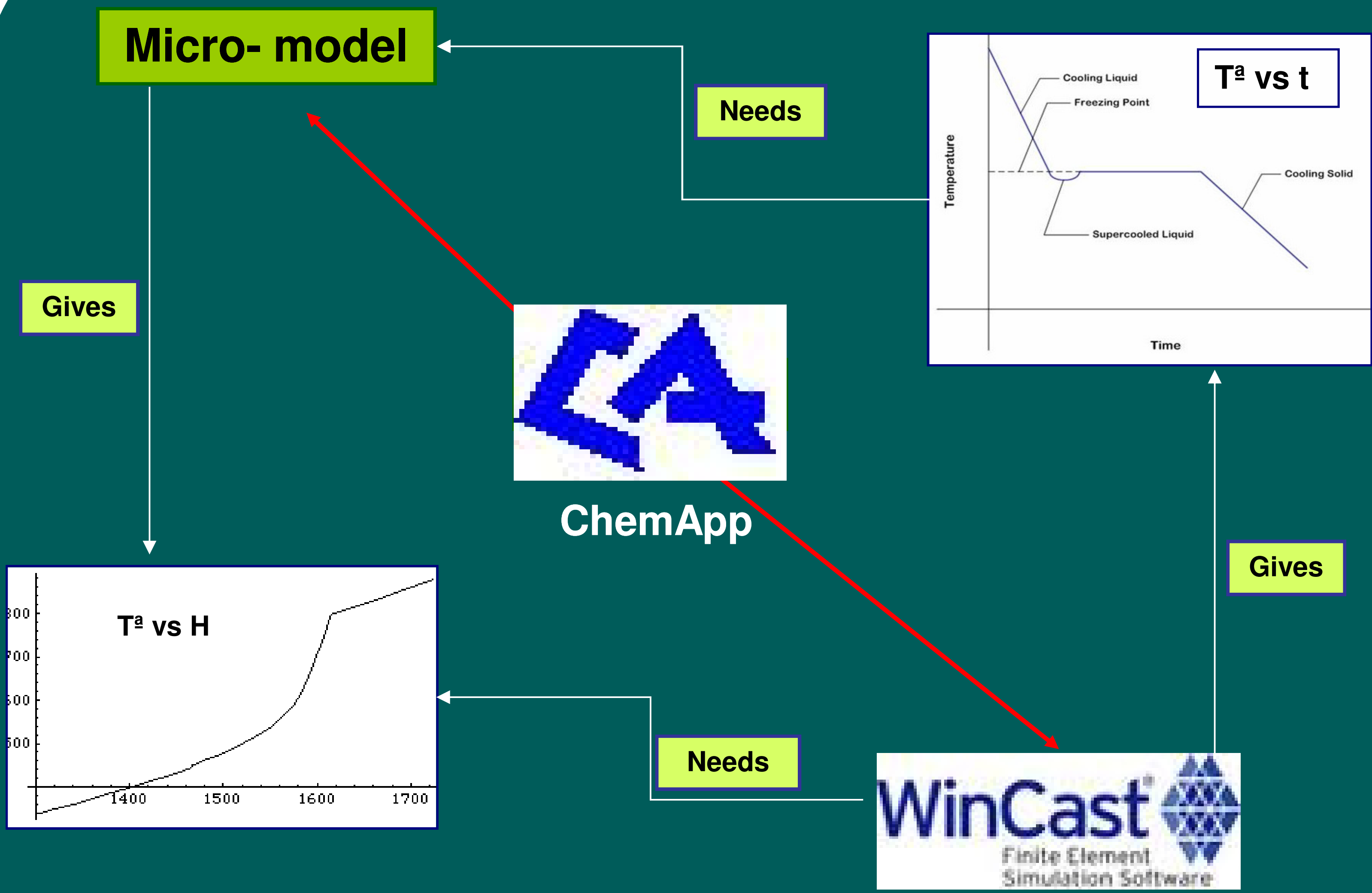

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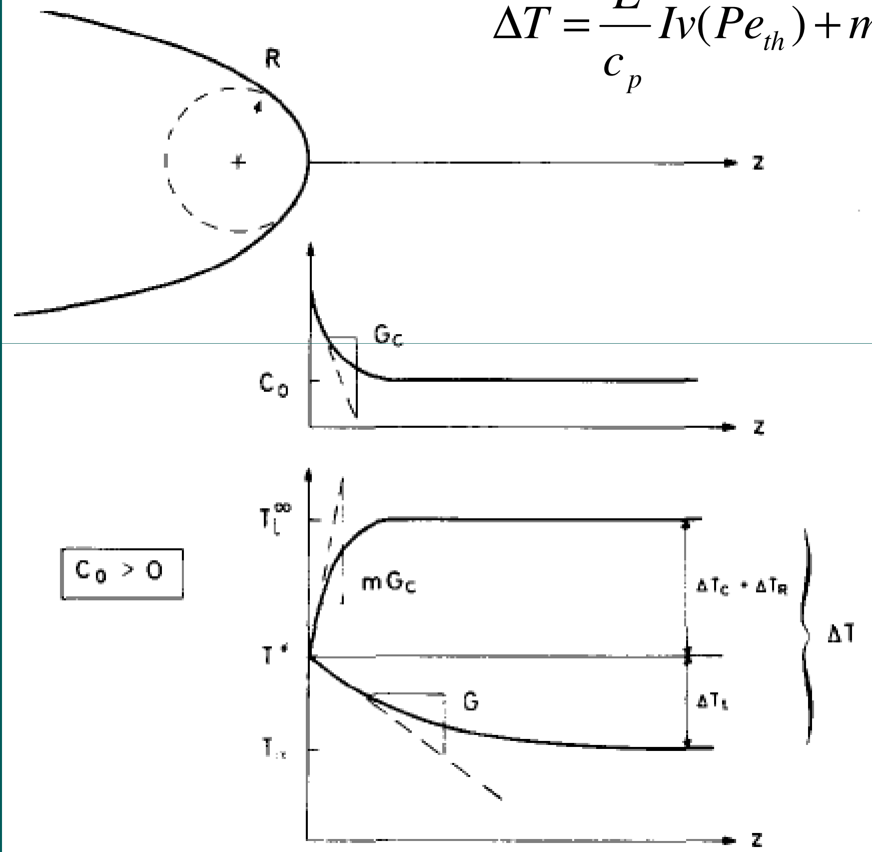
Dendritic Growth in an Undercooled Melt

$$\Delta T = \frac{L}{c_p} Iv(Pe_{th}) + m \cdot c_0 \left(1 - \frac{1}{1-(1-k)\cdot Iv(Pe_c)} \right) + \frac{2\Gamma}{R_d}$$



LGK model

- Thermal Undercooling
- Constitutional Undercooling
- Curvature Undercooling

↓

Operating point of the tip

V , R

Lipton, J., M. E. Glicksman, and W. Kurz. "Dendritic growth into undercooled alloy melts." Mat. Scie. and Eng. 65.1 (1984): 57-63.

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Introduction

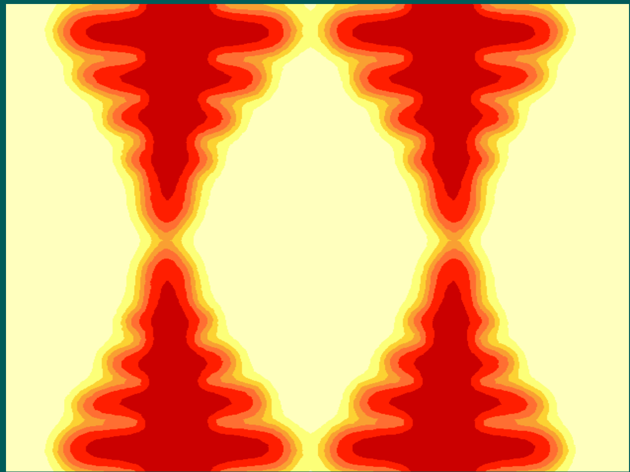
Micro+ChemApp Model

Micro+ChemApp Results

Casting Simulations

Summary

Solute Distribution - Diffusion effect in liquid



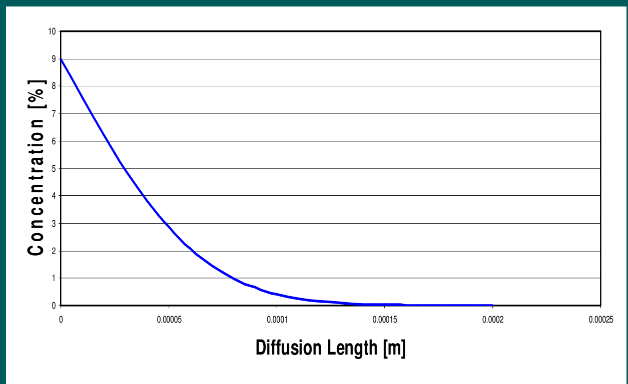
Error function based analytical diffusion equation

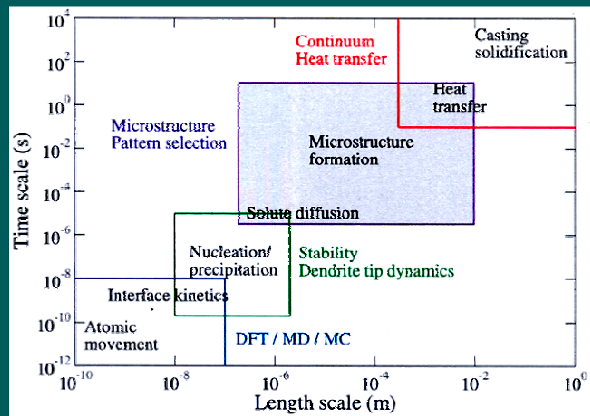
$$c = c_0 - c_0 \cdot erf\left(\frac{x}{\sqrt{D \cdot t}}\right)$$

D → Diffusion coef.

x → Diffusion length

t → Diffusion time





AZ91 Mg alloy (Ternary Mg-Al-Zn)

%	Al	Zn	Mn	Si	Cu	Ni	Other	Mg
AZ91	9	0.42	0.13	0.5	0.1	0.03	max 0.3	Balance

From 601.75 ℃ to 433.49 ℃

LIQUID -> HCP_A3 (α Mg)

From 433.49 ℃ to 430.13 ℃

LIQUID -> ALMG_GAMMA ($Mg_{17}Al_{12}$) + HCP_A3 (α Mg)

Equilibrium Latent Heat → 442.63 J/g

Scheil Latent Heat → 494.43 J/g

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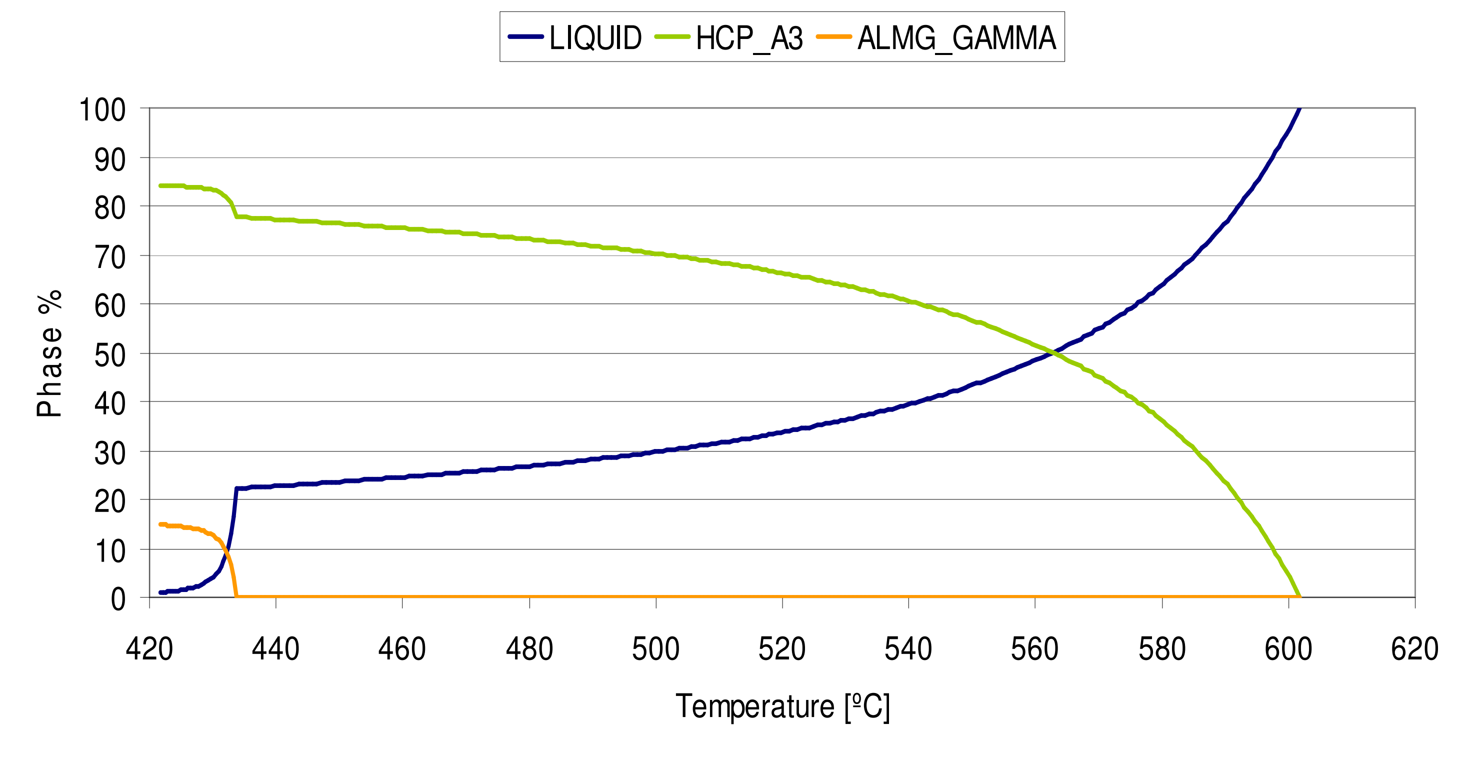
Phase distribution for a 5 ºC/s cooling rate



Diffusion length → 1E-7 m

Diffusion time → 1E-5 s

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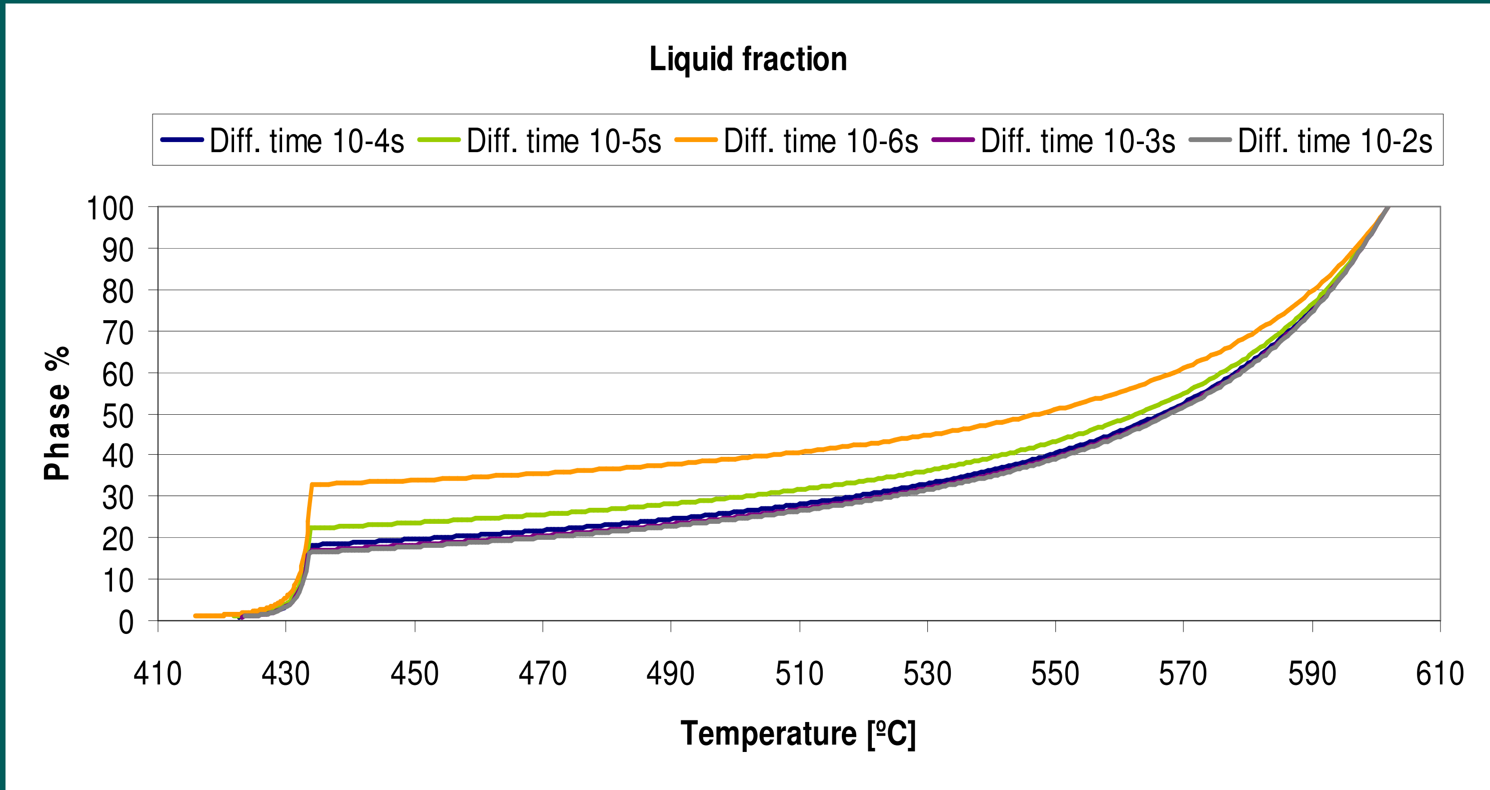
Liquid Fraction variation depending on the diffusion time



Diffusion length → 1E-7 m

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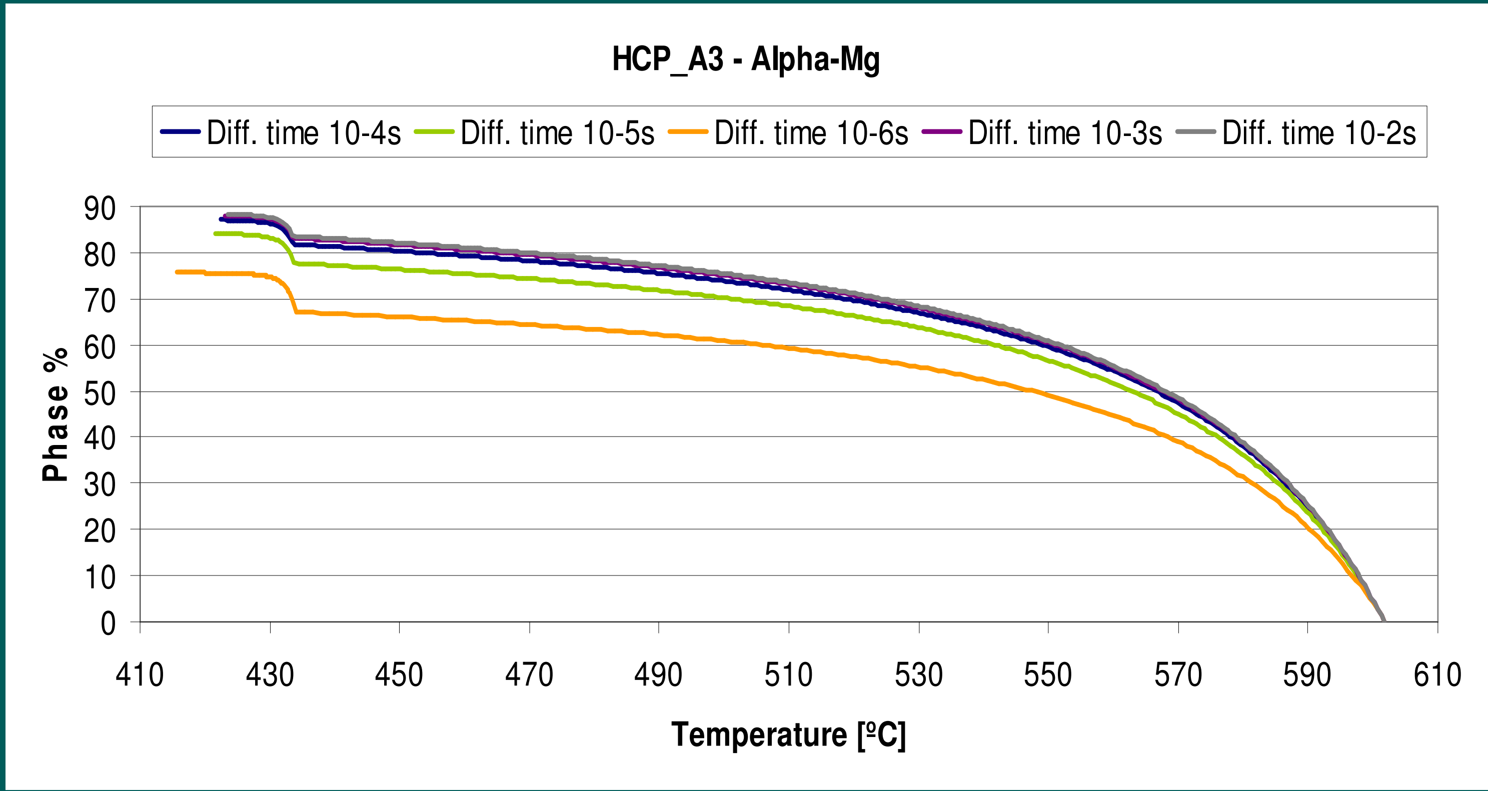
HCP_A3 (α-Mg) fraction variation depending on the diffusion time



Diffusion length → 1E-7 m

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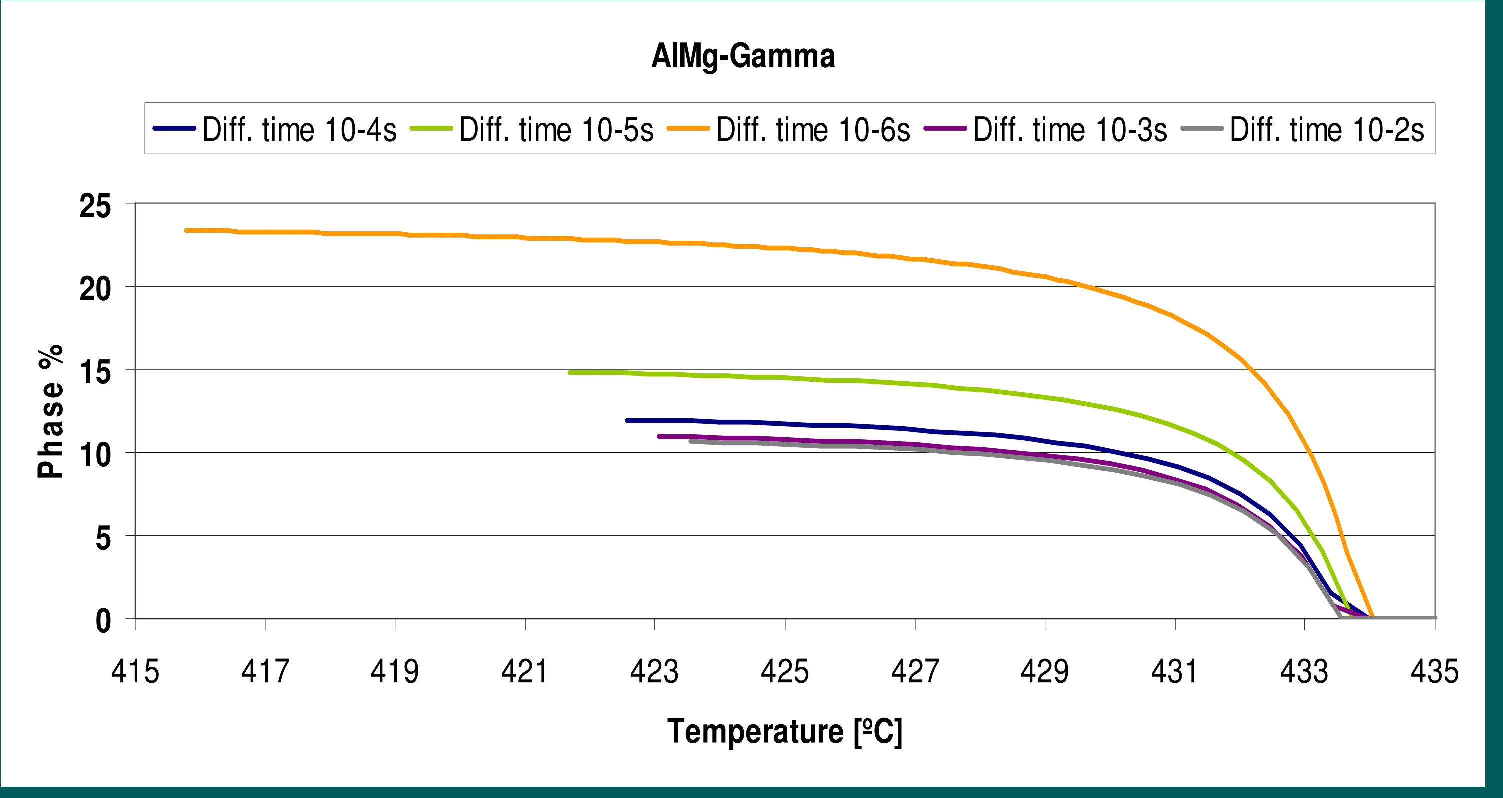
AlMg-Gamma (Mg12Al17) fraction variation depending on the diffusion time



Diffusion length → 1E-7 m

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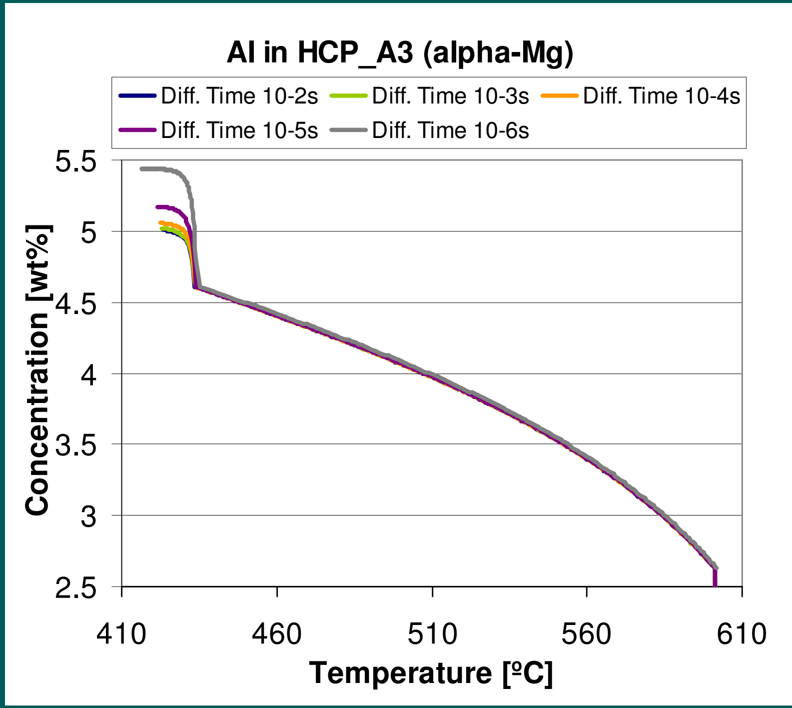
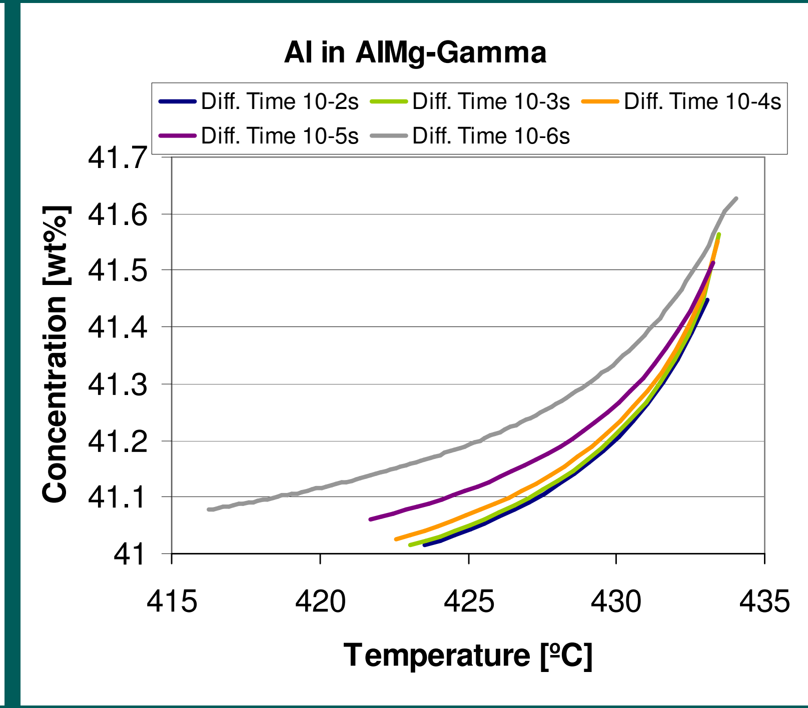
Al segregation in the solid phases





Diffusion length → 1E-7 m

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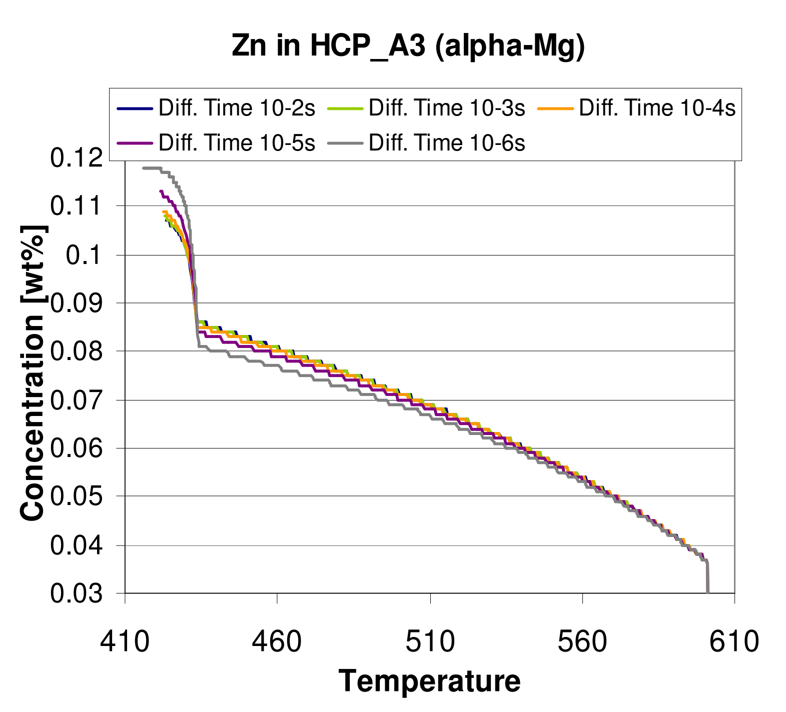
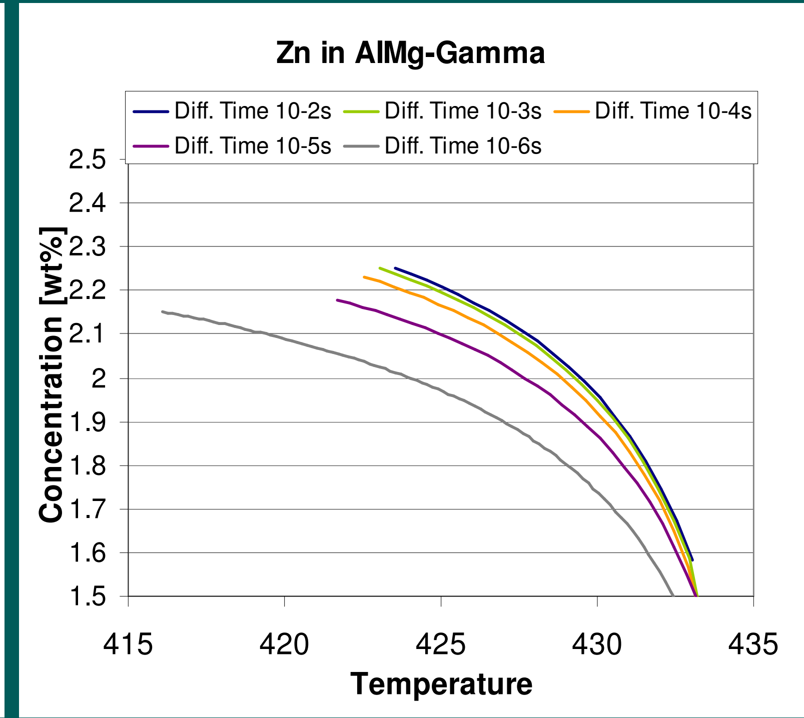
Zn segregation in the solid phases





Diffusion length → 1E-7 m

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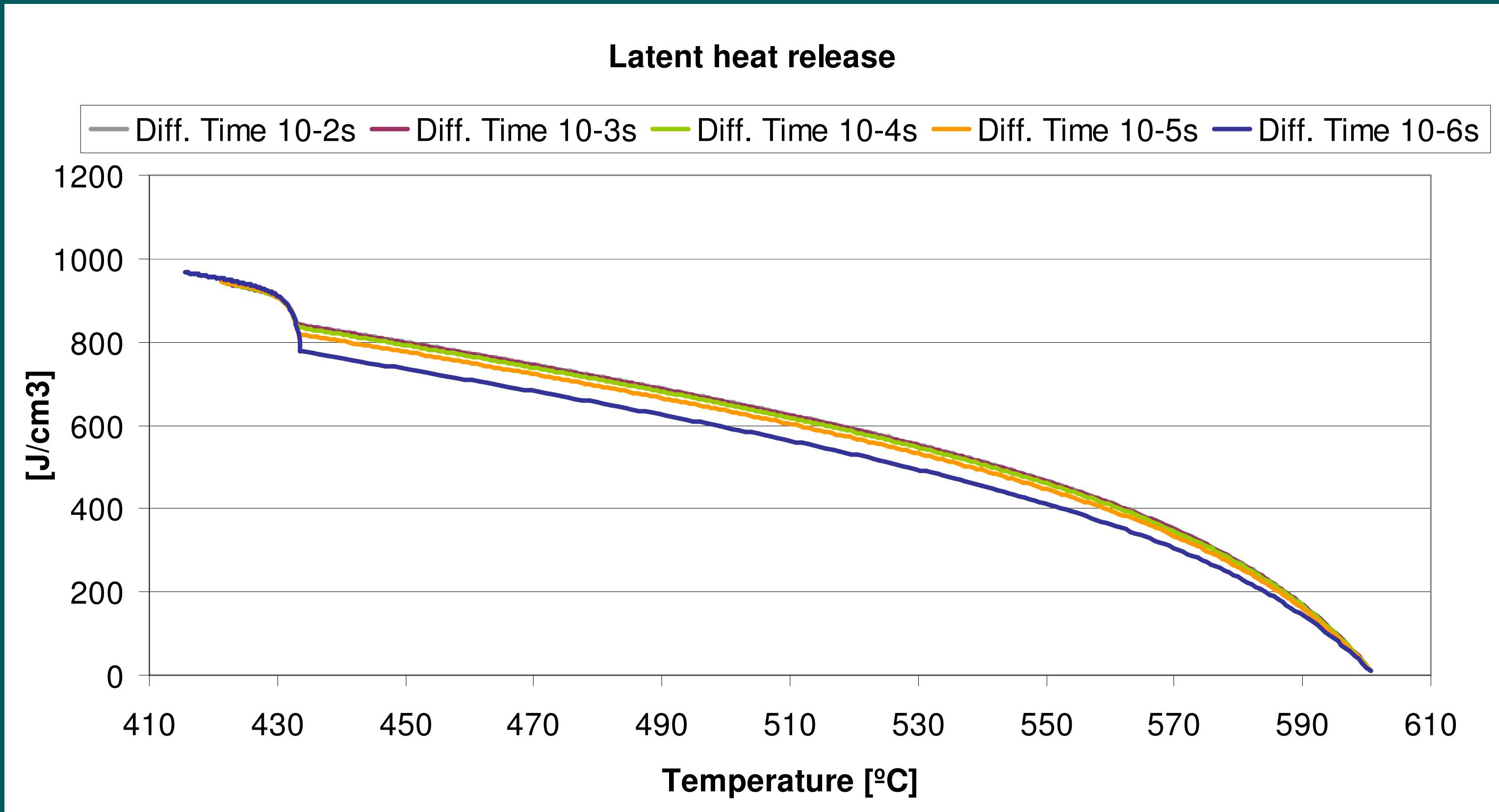
Latent heat release depending on the diffusion time



Diffusion length → 1E-7 m

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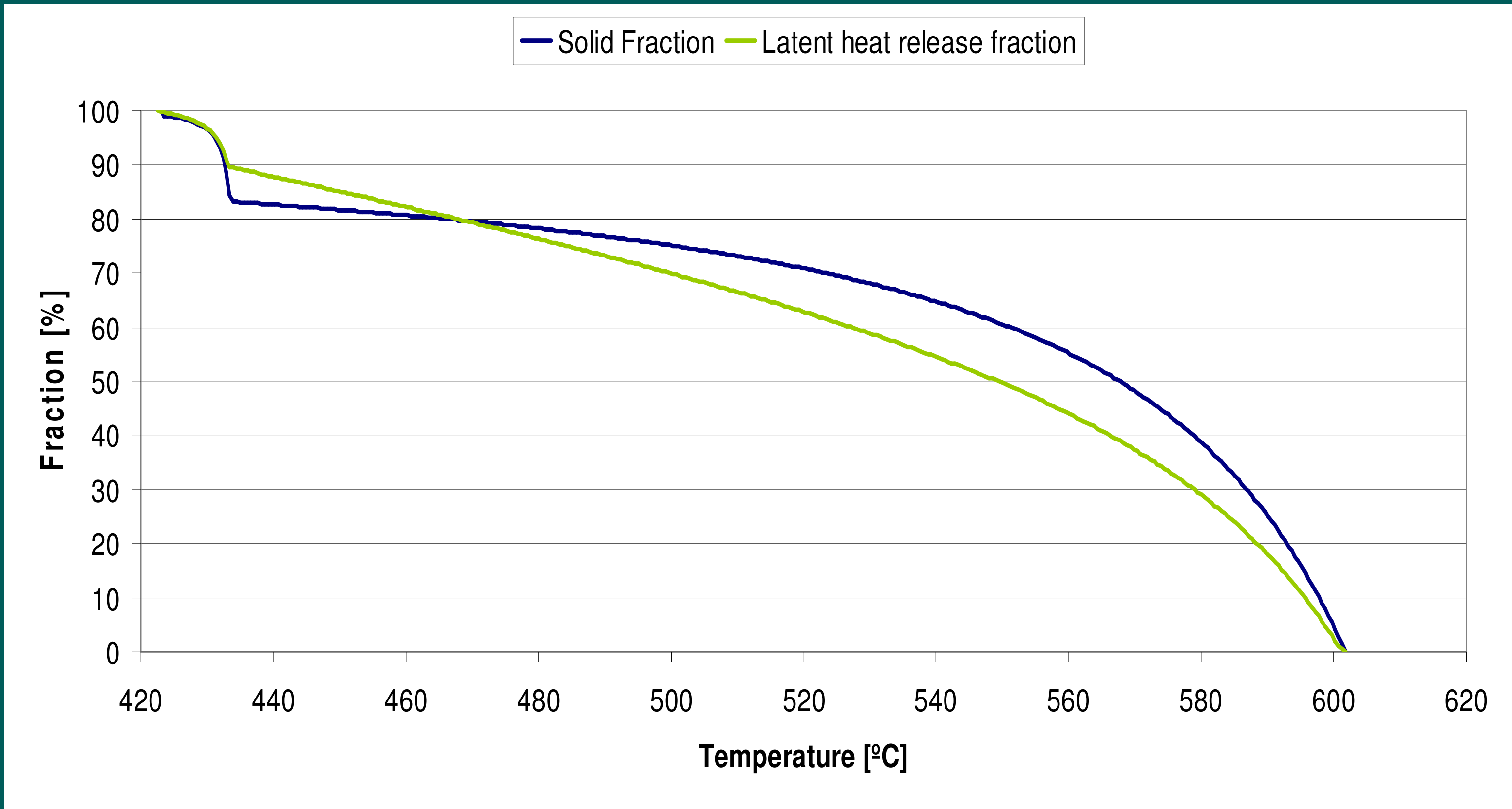
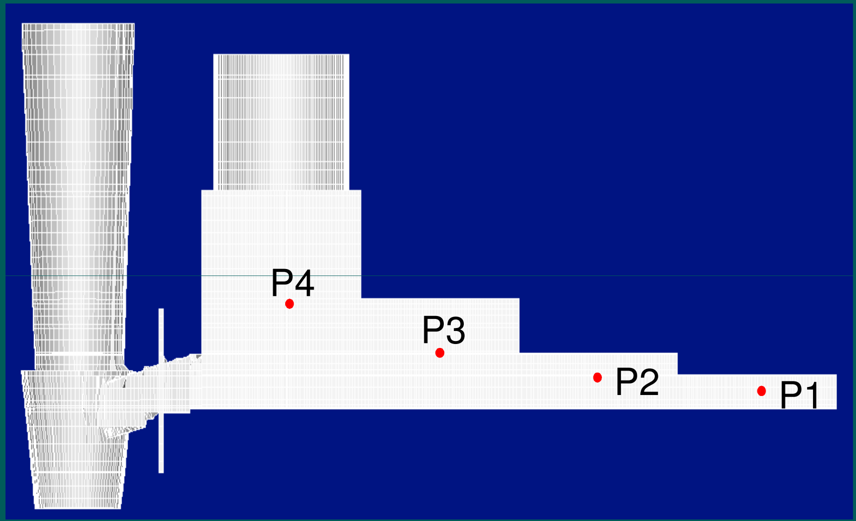
The solid fraction and the heat release fraction are not proportional



Diffusion length → 1E-7 m

Diffusion time → 1E-3 s

Gravity Die Casting simulations with WinCast



Casting material: AZ91 Mg alloy

Mould material: GGG40

Melt temperature: 720 ºC

Mould temperature: 230 ºC

Filling time: 3 s

Part dimensions:

Each step is 70 mm long by 110 mm wide

8, 12, 20 and 40 mm thick respectively

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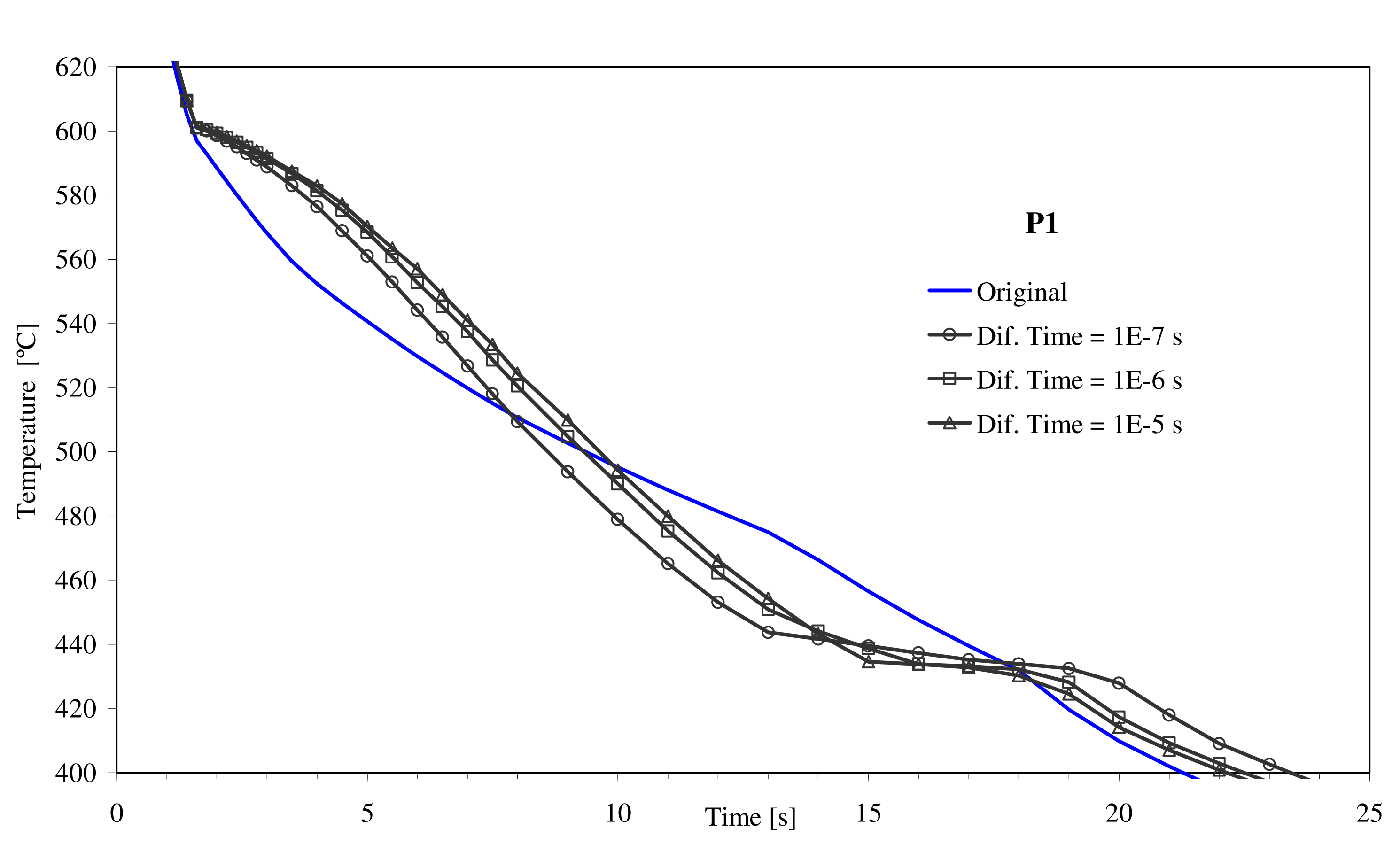
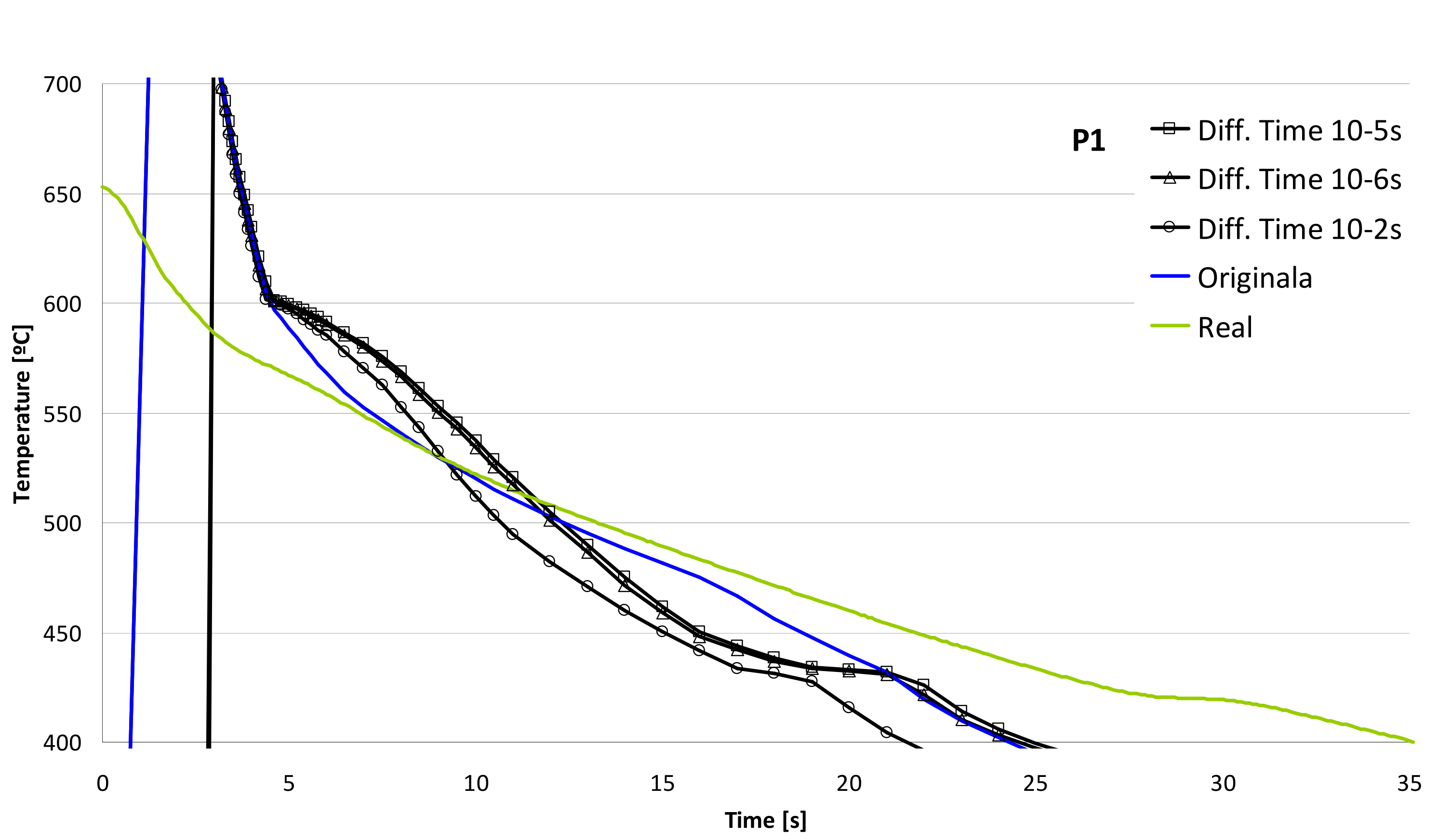
Comparing cooling curves before and after calculating energy release with ChemApp in function of diffusion time



Diffusion length → 1E-7 m

Comparing calculated cooling curves to experimental casting curve



Diffusion length → 1E-7 m

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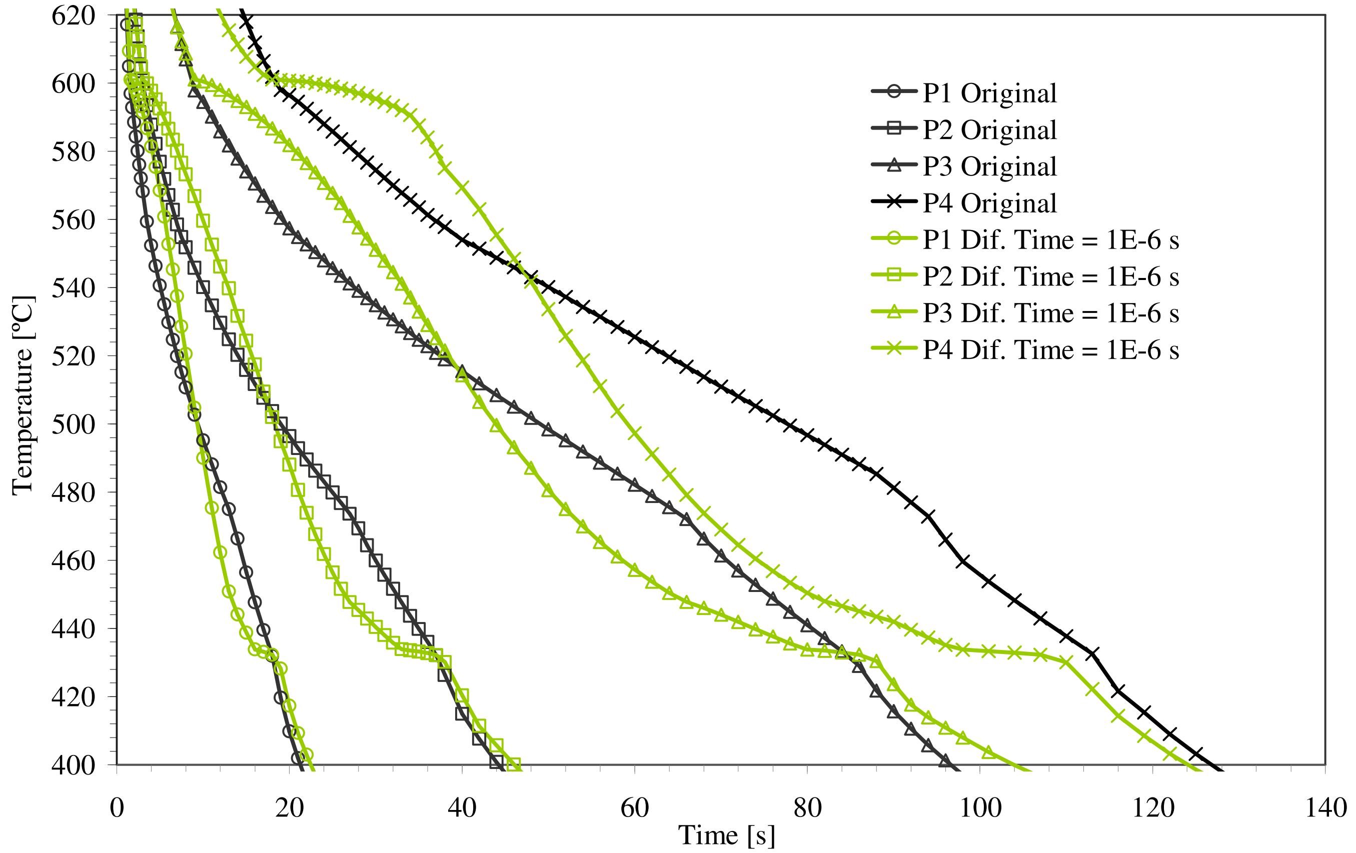
Comparing cooling curves before and after calculating energy release with ChemApp in function of cooling rate



Diffusion length → 1E-7 m

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SUMMARY AND FUTURE WORK

• A microstructure growth model has been modelled, supported by Calphad-ChemApp calculations to handle multi-component alloys.

• ChemApp calculates the appearance of phases and their temperature path. Released heat is also computed.

• Unlike diffusion times during calculations result in different amount of the solid phases and heat release, approaching to Scheil solidification (perfect solute mixture in liquid) as the diffusion time increases.

• The temperature where solidification finishes also varies with changing the diffusion time.

• Alloying element segregation is also computed in function of diffusion time.

• It is proved that using Calphad based tools, it is no longer accepted that solid fraction and latent heat release are proportional.

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CONCLUSIONS AND FUTURE WORK

- Casting simulations carried out with WinCast using ChemApp provided heat release data, improve the resulting calculation in comparison to DSC data for latent heat.

- A better description of the primary α-Mg phase and eutectic transformation is also obtained.

- **Future work:**

  - ❑ To achive full coupling of the micro-model and ChemApp calculations to WinCast.

  - ❑ Improve calculations to approach the calculated curves to the experimental ones.

Thank You For your Attention !!

Danke Für Ihre Aufmerksamkeit !!