



COST 526
"Automatic Process Optimization in Materials Technology"
(APOMAT)

Half-Yearly Report

1. Reporting Period	1.7.2004 – 31.12.2004
Project title	Optimisation of casting of corundobaddeleyit material EUCOR
Project leader Organization	Prof.Dr.Frantisek Kavicka
Main collaborators involved	Dr.J.Heger, Prof.K.Stransky, Prof.J.Dobrovska, Dipl.Ing.P.Ramik,Dipl.Ing.J.Stetina, Prof.V.Dobrovska,Dr.Sekanina,

2. Funding Situation	
Amount of money received specifically for COST	7 kEuros
Other resources partially used for the project	0 kEuros

3. International Collaboration (mention group and type of work done in collaboration during the reporting period)
Participation in the Working Group Meeting in Brno (Czech Rep.) + project progress report YES

4. Industry participation (mention name of companies and work done in collaboration during the whole project)
EUTIT, L.t.d., Stara Voda, Czech Republic, TU-VSB Ostrava, Czech Republic

5. Meetings, visits, exchange of scientists, short-term scientific missions	Location, date
COST 526 APOMAT 5th Joint Working Group	Brno, Czech Rep., November, 2004

6. Progress within the reporting period

Application of the model of the temperature field

The application of the 3D numerical model on a transient temperature field requires systematic experimentation, including the relevant measurement of the operational parameters directly in the foundry. A real 350 x 200 x 400 mm EUCOR block had been used for the numerical calculation and the experiment (Figure 1). Temperature measurement (using thermocouples) and its successive confrontation with the calculation proved that it is possible to apply the numerical model on basic calculations of solidification and cooling of EUCOR. It is also possible to determine the temperature gradients, the rate of solidification and the local solidification times (i.e. the time for which the given point of the casting finds itself between the liquidus and solidus temperatures). The local solidification time θ significantly affects – according to the analogy from steels – the forming of the pouring structure of the given material.

Since the research also covered measurement of chemical heterogeneity of the oxides of EUCOR, the previous conclusion was used to develop the numerical model of chemical heterogeneity.

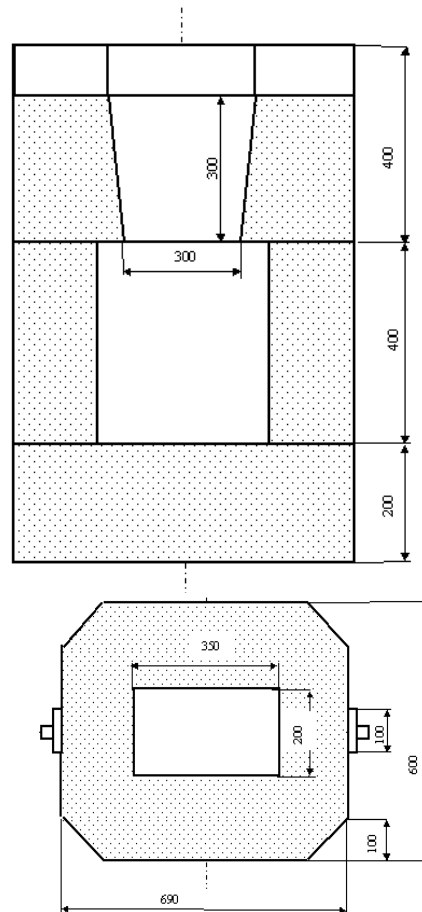


Figure 1 The casting-riser-mould system

The model of chemical heterogeneity of corundobaddeleyit material EUCOR

The principle of the model of chemical heterogeneity has been described in detail and explained in the publication concerning the solidification of steels [1], and its utilisation for the description of chemical heterogeneity of EUCOR is based on the analogy of the laws of solidification of this material with the solidification of steels. The preconditions for the application of the model of chemical heterogeneity on EUCOR are:

If the analytical distribution of micro-heterogeneity of the oxides of the ceramic material are available, if their effective distribution coefficient is known and it is assumed that it is possible to describe the solidification of the ceramic material via analogical models as with the solidification of metal alloys, then it is possible to conduct the experiment on the mutual combination of the calculation of the temperature field of a solidifying ceramic casting with the model describing the chemical heterogeneity of the oxides.

If the Brody-Flemings model [2] is applied for the description of the segregation of oxides of the solidifying ceramic material and if an analogy with metal alloys is assumed, then it is possible to express a relationship between the heterogeneity index I_{het} of the relevant oxide, its effective distribution coefficient k_{ef} and the dimensionless parameter α using the equation

$$\ln(2\alpha k_{ef}) / (1 - 2\alpha k_{ef}) = [\ln(1 + nI_H^{(m)}) / k_{ef}] / (k_{ef} - 1) \quad (1)$$

whose right side, based on the measurement of micro-heterogeneity, is already known and through whose solution it is possible to determine the parameter α , which is also on the left hand side of the equation in $2\alpha k_{ef} = X$. The quantity n has a statistical nature and expresses what percentage of the measured values can be found within the interval $x_s \pm ns_x$ (where x_s is the arithmetic mean and s_x is the standard deviation of the set of values of the measured quantity). If $n = 2$, then 95 % of all measured values can be found within this interval.

If the dimensionless parameter α is known for each oxide, then there exists a key to the clarification of the relationship between the local solidification time θ of EUCOR, to the diffusion coefficient D of the relevant oxide within the solidifying phase and to the structure parameter L , which characterises the distances between individual dendrites. The equation of the dimensionless parameter α is

$$\alpha = D\theta / L^2 \quad (2)$$

Application of the model of chemical heterogeneity

The verification of the possibility of combining both methods was conducted on samples taken from the EUCOR blocks – from the edge (sample B) – and from the centre underneath the riser (sample C).

Both the measured and computed parameters of chemical micro-heterogeneity and the computed parameters of the local solidification time θ (according to the temperature-field model) were calculated. The local solidification time of sample B is $\theta_B = 112.18$ [s] and of sample C is $\theta_C = 283.30$ [s].

The computed values of parameter α and the local solidification time θ determine, via their ratio, the quotient of the diffusion coefficient D and the square of the structure parameter L , which means that the following relation applies:

$$\alpha / \theta = D / L^2 \quad [1/s] \quad (3)$$

The calculated values of relation (10) for oxides of samples B and C are arranged in the following table I together with parameters α :

Oxide	Sample B: α	$\alpha / \theta_B \cdot 10^4$ [1/s]	Sample C: α	$\alpha / \theta_C \cdot 10^4$ [1/s]
Na ₂ O	0.0732	6.53	0.0691	2.44
Al ₂ O ₃	0.0674	6.01	0.0662	2.34
SiO ₂	0.0741	6.61	0.0663	2.34
ZrO ₂	0.00035	0.0312	0.00008	0.0028
K ₂ O	0.0721	6.43	0.0665	2.35
CaO	0.075	6.69	0.0703	2.48
TiO ₂	0.0759	6.77	0.0757	2.67
Fe ₂ O ₃	0.0732	6.53	0.0711	2.51
HfO ₂	0.0165	1.47	0.00017	0.006

Table I Calculated values of equation (3)

It comes as a surprise that the values of the parameter $\alpha/\theta = D/L^2$ of the oxides Na, Al, Si, K, Ca, Ti and Fe differ by as much as an order from the value of the same parameter of the oxide of zirconium and hafnium. This could be explained by the fact that zirconium contains hafnium as an additive and, therefore, they segregate together and the forming oxides of zirconium and hafnium have the highest melting temperature. From the melt, both oxides segregate first, already in the solid state. Further redistribution of the oxides of both elements runs on the interface of the remaining melt and the successive segregation of other oxides only to a very limited extent. It is therefore possible to count with the fact that the real diffusion coefficients of zirconium and hafnium in the successively forming crystallites are very small (i.e. $D_{Zr} \rightarrow 0$ a $D_{Hf} \rightarrow 0$). On the other hand, the very close values of the parameters $\alpha/\theta = D/L^2$ of the remaining seven analysed oxides: $D/L_B^2 = (6.51 \pm 0.25) \cdot 10^{-4}$ and $D/L_C^2 = (2.45 \pm 0.12) \cdot 10^{-4}$ [1/s] indicate that the redistribution of these oxides between the melt and the solid state runs in a way, similar to that within metal alloys, namely steels.

It would be possible to count – in the first approximation – with the diffusion coefficients of the oxides in the slag at temperatures of 1765 °C (solidus) and 1775 °C (liquidus) with an average value of $(2.07 \pm 0.11) \cdot 10^{-6}$ cm²/s (the data refers to the diffusion of aluminium in the slag with a composition of 39% CaO-20% Al₂O₃-41% SiO₂). For these cases, and using Eq. (3), it is possible to get the magnitude of the structure parameters that govern the chemical heterogeneity of the values:

$$L_B = \sqrt{(2.07 \cdot 10^{-6}) / (6.51 \cdot 10^{-4})} = 0.5639 \cdot 10^{-3} \text{ [m] and}$$

$$L_C = \sqrt{(2.07 \cdot 10^{-6}) / (2.45 \cdot 10^{-4})} = 0.9192 \cdot 10^{-3} \text{ [m]}$$

which corresponds to 564 μm in sample B and 919 μm in sample C.

From the comparison of the micro-structures of the analyses samples B and C (Figs. 2 and 3) it is obvious that the micro-structure of sample B (L_B) is significantly finer than the micro-structure of sample C (L_C), which semi-quantitatively corresponds to the qualified estimate of the structure parameters L , conducted on the basis of calculations from the data obtained from both models.

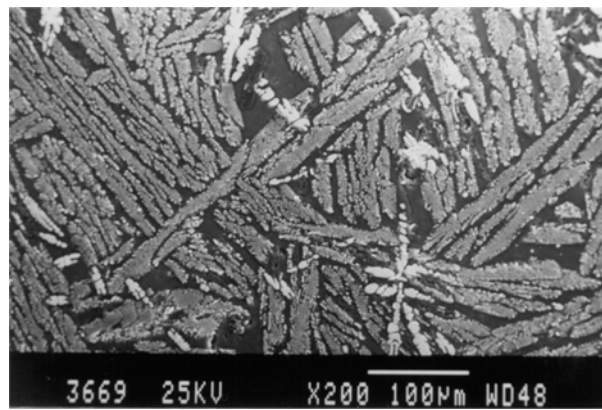


Figure 2 The structure of sample B ($L_B = 564 \mu\text{m}$)

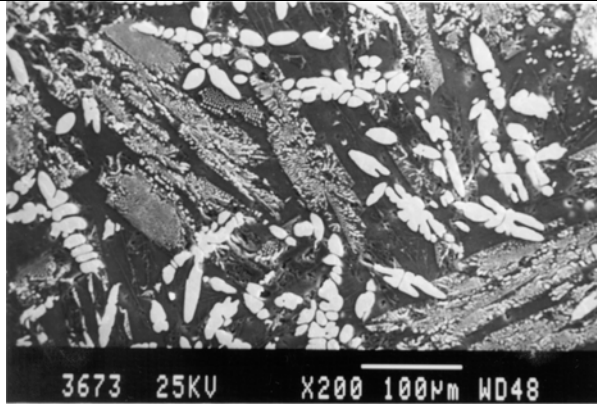


Figure 3 The structure of sample C ($L_c = 919 \mu\text{m}$)

- [1] DOBROVSKÁ, J. - DOBROVSKÁ, V. - REK, A. - STRÁNSKÝ K.: Possible ways of prediction of the distribution curves of dendritic segregation of alloying elements in steels. Scripta Materialia, vol. 18, 1998, No. 10, pp. 1583-1598.
- [2] BRODY, H. D., FLEMINGS, M. C.: Trans. AIME, 1966, vol. 236, p. 615-624.

List of publications

Dobrovská J., Kavická F., Stránský K., Dobrovská V., Stetina J.: Two numerical models for optimization of the foundry technology of the ceramics EUCOR. Proceedings and CD ROM of the 2004 ASME Heat transfer fluids engineering summer conference, Charlotte, North Carolina, USA, July 11-15, 2004, p. 30

Kavická F., Stetina J., Sekanina B., Stránský K., Dobrovská J., Heger J.: Model of solidification of a massive casting from malleable cast-iron. Proceedings of the 2004 ASME/JSME pressure vessels and piping conference, San Diego, California, USA, July 25-29, 2004, p.249-255

Kavická F., Stetina J., Sekanina B., Ramík P., Heger J. : Simulation of heat transfer under air-water cooling jets. Proceedings and CD ROM of the 16th international congress of chemical and process Engineering, Prague, Czech Republic, August 22-26, p. 1634

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Stránský K., Bazan J., Kavická F., Buchal A., Janová D. : On the composition of the blast furnaces slag from Ustron in district Tesin. Proceedings of the XIV. International scientific conference, Mala Lucivna, Slovakia, October 13-15, 2004, (at the printers)

Senberger J., Musilová I., Bazan J., Million B., Dobrovská J., Kavická F., Stránský K. : The modelling of the ductile iron structures. Proceedings of the XIV. International scientific conference, Mala Lucivna, Slovakia, October 13-15, 2004, (at the printers)

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Stetina J., Kavicka F., Sekanina B., Stransky K., Dobrovska J., Cemek L., Masarik M.: Optimization of a concasting technology via a dynamic solidification model of a slab caster. Proceedings of the XIV. International scientific conference, Mala Lucivna, Slovakia, October 13-15, 2004, (at the printers)

Stetina J., Kavicka F., Dobrovska J., Cemek L., Masarik M.: Optimization of a concasting technology via a dynamic solidification model of a slab caster. Proceedings of the 5th Pacific International Conference on Advanced Materials and Processing, Peking, China, Part 5, p.3831-3834

Stetina J., Kavicka F., Dobrovska J., Cemek L., Masarik M.: Optimization of a concasting technology via a dynamic solidification model of a slab caster. Material Science Forum, Vol. 475-479, pp.3831-3834, Switzerland