Experimental Verification of Hematite Ingot Mould Heat Capacity and its Direct Utilisation in Simulation of Casting Process

Bedřich Smetana[1], Monika Žaludová[1], Markéta Tkadlečková[2], Jana Dobrovská[1], Simona Zlá[1], Karel Gryc[2], Petr Klus[2], Karel Michalek[2], Pavel Machovčák[3], Lenka Řeháčková[1]

[1]*VŠB-TU Ostrava, Faculty of Metallurgy and Materials Engineering, Department of Physical Chemistry and Theory of Technological Processes, Regional Materials Science and Technology Centre, 17. listopadu 2172/15, Ostrava-Poruba, Czech Republic*

[2]*VŠB-TU Ostrava, Faculty of Metallurgy and Materials Engineering, Department of Metallurgy and Foundry, Regional Materials Science and Technology Centre, 17. listopadu 2172/15, Ostrava-Poruba, Czech Republic*

[3] *VÍTKOVICE HEAVY MACHINERY a.s. (VHM), Ruská 2887/101, Ostrava-Vítkovice, Czech Republic*

00420 597 321 594

00420 597 323 396

bedrich.smetana@vsb.cz

XXXXXXX URL
Article note

Heat capacity of alloys (metals) is one of the crucial thermo-physical parameters used for process behaviour prediction in many applications. Heat capacity is an input variable for many thermo-dynamical (e.g. Thermocalc, Pandat, MTData,...) and kinetic programs (e.g. IDS-Solidification analysis package,...). The dependences of heat capacity on common variables (temperature, pressure) are also commonly used as the input data in software packages (e.g. ProCast, Magmasoft, ANSYS Fluent...) that are applicable in the field of applied research for simulations of technological processes. It follows from the above that the heat capacities of materials, in our case alloys, play a very important role in the field of basic and applied research. Generally speaking, experimental data can be found in the literature, but corresponding (needed) data for the given alloy can very seldomly be found or can differ from the tabulated ones. The knowledge of proper values of heat capacities of alloys at the corresponding temperature can be substantially used for addition to and thus towards the precision of the existing database and simulation software. The paper presents the values of C_p measured for the hematite ingot mould and comparison of the measured data with the C_p obtained using the software *CompuTherm* with respect to simulation of technological casting process.

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heat capacity, DTA, 3D DSC, phase transition temperatures, computation, simulations, real process

Abbreviations

Introduction

Heat capacity [1] and other material properties (phase transition temperatures, latent heats, surface tension, interface tension,...) [2–9] of alloys (metals) are crucial thermo-physical quantities for many applications. Many of these data are accessible in the literature, but it is very often difficult to find data for a given material (with exact chemical composition), as well as for the required temperature interval. The data found for given material in different literature resources sometimes even differs [2, 3, 7].

Heat capacities are typically used as basic data in many calculating software packages (SW), e.g. Thermocalc, MTData, PANDAT, IDS and others. Proper thermo-physical and thermo-dynamic data are used (necessary for simulations) also in SW, such as Magmasoft and ProCAST.

This paper deals with the investigation of heat capacity (C_p) of a hematite ingot mould, Fig. 1, used in VÍTKOVICE HEAVY MACHINERY a.s. for casting of steel ingots. This kind of mould is used for the production of heavy steel forging ingots that are used for the production of many products in the assortment of VÍTKOVICE HEAVY MACHINERY a.s. (steam generators, heat exchangers, collectors for conventional and nuclear power engineering,...). Constantly increasing demands on higher quality of products lead to the necessity of optimization of technological processes. The best way to optimize the production process is to have proper data from operation, proper material data and simulation SW. In this paper the measured values of heat capacity C_p of a hematite mould are compared with C_p values calculated using CompuTherm. Both experimental and

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calculated dependences of C_p were used for the simulation of process of casting of a steel ingot with use of ProCAST SW, and the obtained results are discussed.

Theory

Heat capacity can be expressed as heat (Q) absorbed/released by the sample (material) during its heating or cooling between the temperatures T_1 and T_2 [1]:

Mean value of C_p at constant pressure can be expressed by the equation (1):

$$\overline{C} = \frac{Q}{T_2 - T_1} \tag{1}$$

For comparison of the heat capacity of different materials it is necessary to relate this quantity to the amount of material. If the C_p is related to the (sample) mass then the so-called specific heat capacity at constant pressure is defined [1].

The fastest way to obtain the values of heat capacity is the utilization of calculation relation(s) or calculation SW. Considering the multi-component alloys (steels and other alloys) it is possible to use the Neumann-Kopp rule to calculate C_p dependence on temperature [1].

Secondly, it is possible to use SW for calculation of C_p. JmatPro, IDS or CompuTherm (ProCast sub module) are very often used for calculation of temperature dependence of C_p. Although utilization of the calculation SW is very comfortable and fast, this procedure is mostly based on theoretical assumptions, limitations and approximations connected with the composition of the alloy, temperature interval, calculation model limitations and others. C_p values are mostly calculated only with respect to the chemical composition, but the C_p value (dependence) may be influenced by structure, phases present in the sample and influence of the deformational state. Therefore, the best way to obtain proper data for the system under investigation is by carrying out an experiment.

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Almost all classical DSC devices make it possible to perform two basic methods for heat capacity determination. The first is the continuous method and the second is the so-called stepwise method. Special equipment is used for the so called DROP method. General description of these three methods can be found e.g. in [10].

Continuous method is the fastest method for C_p determination and was used for experimental measurements in this work. The scheme of the continuous method is shown in Figure 2.

The heat capacity determined on the basis of DSC experiment comprises three main sequences: 1st sequence - adjusted isothermal dwell, 2nd sequence - linear heating in the whole measured temperature interval and the 3rd sequence is isothermal dwell at the temperature that makes it possible to cover the desired temperature interval. All three sequences must be performed with empty crucibles (B), with the sample (S) and with the reference sample (C). Consecutively, the heat capacity can be calculated according to the following formula [10]:

$$C_p = C_{pC} \times \frac{m_C \times (A_S - A_B)}{m_S \times (A_C - A_B)} \tag{2}$$

where, A_B, A_S, A_C in [mW] are segments corresponding to the heat effects detected for the measurement of blank (empty crucibles), measurement with the sample and the reference sample, C_{pC} [J K^{-1} g^{-1}] is the heat capacity of the reference sample, C_p [J K^{-1} g^{-1}] is the heat capacity of the measured sample, m_S [mg] and m_C [mg] are masses of the sample and the reference sample.

Numerical simulation of real casting process

The principle of numerical simulation, as published in [11–17], is the numerical solution of each task divided into the three stages: pre-processing, processing and post-processing.

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Pre-processing includes the geometric modelling and the computational mesh generation process, and definition of calculation. The whole 3D ingot mould geometry was created in the CAD system SolidWorks. Comparison of the real and CAD geometry of the casting system is shown in Figs. 1 A and B. The computational mesh was generated in Visual-Mesh, which is a part of the packet of ProCAST software. Figure 1C presents the final computational mesh of the casting system. Figure 1 D shows the final 3D ingot geometry.

Determination of some boundary, operating and initial conditions is not usually difficult. The quality of the results of the numerical simulation of the temperature field, volume defects in ingots, especially macro-segregation of elements, is mainly determined by the quality of the thermo-dynamic and thermo-physical properties of steel and of ingot mould material. In the simulation section this paper is focused on comparison of temperature fields in an ingot mould obtained using the values of C_p calculated using CompuTherm (Computherm enables calculation only of the enthalpy dependence on the temperature, not the specific heat temperature dependence, not the separately specific heat temperature dependence and latent heats of the running phase transitions. Therefore, the dependence of enthalpy on temperature was recalculated to the heat capacity dependence including the latent heat of the phase transition in the investigated region. So, the so-called apparent heat capacity was obtained [18, 19]) with the values of C_p (apparent C_p) obtained experimentally using the DSC measurements, other conditions (parameters) during simulation were unchanged.

Experimental

Samples characterisation

Samples of the ingot mould were supplied by VÍTKOVICE HEAVY MACHINERY a.s. Samples were machined into the form of cylinders (5 mm in diameter and 17 mm in height with a mass of ~2100 mg for DSC analysis and 3.5 mm in diameter and 3 mm height with mass of ~160 mg for TG/DTA analysis), chemical composition is shown in Table 1 (supplied by VÍTKOVICE HEAVY MACHINERY a.s., the analyses were performed with use of spectroscopy with glow discharge and combustion analysers). Prior to the performed TG/DTA and DSC analyses the samples were ground in order to remove a possible oxidation layer, then cleaned in acetone by simultaneous ultrasound impact.

Simultaneous TG/DTA analysis

Alloys containing carbon are predisposed to the decarburisation at higher temperatures (due to the high carbon diffusivity) [20]. Therefore, simultaneous thermal analysis (TG/DTA) was performed in order to check the possible decarburisation (mass loss) of an ingot mould sample during the analysis. The TG/DTA was performed in the temperature interval of 300–1700 K in an inert atmosphere of Ar (6N). Analyses were performed for two heating rates, 10 and 20 K min^{-1}. Simultaneous TG/DTA analyses were performed in corundum crucibles.

TG and DTA curves obtained for different heating rates are presented in Figure 3. According to the obtained DTA curves the running phase transitions were checked and compared with the DSC results. The observed TG curve, in dependence on temperature, showed whether the mass of sample was changed during the experiment or not.

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TG/DTA analyses were performed until the complete melting of the sample. During the heating rate of 10 K min^{-1} mass loss was observed, which corresponded with high probability with the decarburisation degree of the sample. The start of the carbon loss was observed at around 950 K. The constant trend in the mass loss of carbon was observed up to the temperature of ~1300 K. Then the mass loss was substantially faster than between the temperatures of 950–1300 K. Over 1300 K the sample melting was observed and therefore also the faster decarburisation, as observed from the TG curve(s). The sample mass loss was 1.9 %. Assuming that the sample mass loss is 1.9 wt %, then the carbon content decrease is more than 50 %. On the basis of the preliminary TG/DTA analyses (at 10 K min^{-1}) it was necessary to modify the conditions of thermal analyses experiments in order to avoid possible decarburisation that might have corresponding influence on the values of heat capacity. Another heating rate was set to be 20 K min^{-1}. The mass loss of the sample was not observed (Figure 3) at such a fast heating rate in the temperature region from 300–1300 K. In the melting region the decrease of mass was approx. 0.1 %. That means that the maximum reduction of the carbon content was no more than 4 % (if complete melting of the sample was realised).

With respect to the observed facts, the heating rate of 20 K min^{-1} was chosen as suitable for the performed DSC analyses (blank, calibration with corundum, analysed sample).

Moreover, the temperature calibration was performed with use of standard metals (Sn, Al, Ag, purity 5N) at corresponding heating rates.

DSC analysis

Heat capacity (apparent heat capacity, heat capacity including latent heat of the phase transition) of the ingot mould was measured with use of the Setaram MHTC 96 Line (Multi High Temperature Calorimeter) equipped with 3D heat flux DSC B-type measurement sensor making it possible to perform experiments up to 1823.15 K. Measurements were performed in the temperature interval between 500–1100 K in an inert atmosphere of He (6N, flow rate 20 ml min^{-1}; helium is more suitable for obtaining the C_p values using scanning methods because of a substantially high thermal conductivity in comparison with Ar). The resulting value of heat capacity dependence was obtained from three measurements. The prepared cylinders of the samples were put into the corundum sleeve (shut by corundum lid), the sleeve was inserted in to the Pt–crucible and shut by the Pt–lid, and consequently the Pt crucible was inserted into the 3D DSC sensor and covered by the corundum plate.

The temperature programme started from 300 K by linear heating (5 K min^{-1}) of the sample up to the temperature of 423.15 K. At this temperature the first isothermal dwell was realised. Subsequently the linear heating (20 K min^{-1}) to the second isotherm (1373.15 K) followed. Experimental values of C_p were obtained from the temperature interval of 500–1300 K (temperature interval without disturbing effects caused by change of isotherms and heating mode, Figure 3). The same temperature programme was set for calibration measurements with corundum (purity 4N8) and for the blank.

Heat capacity measurements were checked with respect to the known heat capacity of corundum. The relative standard deviation from three measurements (computed from three runs performed with corundum) for the temperature interval between 500–1300 K was ± 0.2 %. Comparison with the generally accepted C_p

values of corundum was performed. The standard deviation (mean value)

calculated from experimentally obtained values and from the generally accepted

C_p for the specific temperature is 5 % (in the measured temperature interval).

The temperature calibration was performed also with use of standard metals (Sn,

Al, Ag, purity 5N) at the heating rate of 20 K min^{-1}.

Results and discussion

Phase transitions

DTA and DSC analysis also revealed two thermal effects, see Figs. 3 and 4. The

first thermal effect corresponds with the change of magnetic properties

(ferromagnetic to paramagnetic, temperature of the Curie point was evaluated,

T_C = 1019 K (DTA, 20 K min^{-1}). The second heat effect (DTA, 20 K min^{-1}) can

be, with high probability, attributed to the transition $\alpha + C_{grafitic} \rightarrow \gamma$ [6] (α –

ferrite, $C_{grafitic}$-graphitic carbon, γ-austenite). This transition takes place between

the temperatures of 1071–1108 K. Identical thermal effects were observed during

the DSC analysis, T_C = 1036 K and $\alpha + C_{grafitic} \rightarrow \gamma$ takes place between 1079–

1131 K. Transition temperatures obtained using DSC are shifted to the higher

temperatures, whereas the main reason for this phenomenon is the amount of the

sample used for the DSC analysis. The bigger the mass, the longer the time

needed for heat transfer (the transitions must not take place in each part of the

sample at the same time) within the whole volume of the sample. The shift of

temperatures might have been caused also by the detection limit of the sensor. In

the case of large samples and at relatively high heating rates, the beginning and

termination of the heat effect followed by the phase transition can be very often

more unclear in comparison with the experiments with small samples and lower

heating rates (this fact might have also influenced the results).

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Enthalpy and consequently the apparent heat capacity C_p of the hematite ingot mould was calculated using the CompuTherm SW, Fig. 4. When using this SW only one phase transition can be observed (1007-1067 K), which is in contrast with the real DSC and DTA experiments, when two transitions were observed. Probably, the authors of CompuTherm SW suppose, that the peak (heat effect) includes both the magnetic transition and transition of $\alpha + C_{grafitic} \rightarrow \gamma$ in close proximity (heat effects could overleap over each other). The authors of this SW do not present the models used for thermo-physical and thermo-dynamic quantity calculations in their instruction manuals and thus it is not clear which algorithm the authors used for the C_p calculation. So in fact it is not clear, whether the received C_p (enthalpy respectively) is just calculated, calculated and corrected with respect to the experiment or whether it is only experimental. Probably the calculation model with its limitations and simplifications may give somewhat different results in comparison with the experiments.

Heat capacity

Experimentally obtained and calculated values of apparent heat capacity are presented in Table 2 and graphically shown in Figure 4.

The experimentally obtained C_p values (on the basis of three measurements) are very close to the values calculated with use of the Computherm SW in the temperature interval of 500–1000 K, and in the interval of 1175–1300 K. The differences between experimental and calculated values are also presented in Table 2. The C_p dependence trends are the same. The experimentally obtained dependence shows mild curvature in the observed intervals. Heat capacity values significantly differ between the temperatures of 1000–1175 K due to running phase transition(s). The differences could probably be attributed to the simplifications and limitations that are implemented in the calculation models.

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The calculating relations and models are also often derived on the basis of experimental data (that are at present insufficient) and theoretical assumptions, which are valid most often for a certain interval of chemical composition. The data obtained by extrapolation beyond this interval (e.g. concentration interval) can be less relevant.

Comparison of simulation results using calculated and experimental C_p values

Simulations were performed with use of the ProCAST SW. Comparison of the calculated results with the experimental and theoretical results are presented in Figure 5. A very important parameter was observed: the temperature field in the hematite ingot mould, which defines, together with the heat flux, also the heat transfer coefficients and ambient temperature, and also the character of the solidification, as well as the size of the volume defects, such as shrinkage or porosity. Figure 5 presents the temperature fields of real mould acquired with thermo-vision measurements compared with the results obtained with calculated and experimental C_p dependences after one hour, 2 hours and 3 hours and 20 minutes after the casting process. The temperature fields (real, calculated by the CompuTherm C_p and experimental C_p) are identical for the observed times: 1 hour and 3 hours and 20 minutes after the casting process. Only at the time of 2 hours after the end of the casting process was a mild deviation observed in the temperature interval 684.15–744.15 K between simulation results based on theoretical and experimental C_p. The differences can be seen at a border of concave regions of the mould, where the more distinct warming is evident. This feature, obtained by experimental C_p dependence, is very similar (more close) to the results obtained by real thermo-vision measurements in comparison with the results obtained with calculated C_p. Furthermore, a very important fact is that the

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temperature field on the ingot surface, after stripping, is identical with the calculated temperature field using the dependence of C_p on the temperature obtained by the DSC experiment.

It is possible to state from the obtained results that the experimental value of C_p temperature dependence in the observed temperature interval contributed to the results (simulations) that were more accurate and closer to the results obtained by real thermo-vision measurements. Although the differences in C_p dependences in the region of phase transitions significantly differ, the simulation results are very close (in majority the same). It is possible to state that a lack of proper basic experimental data still persists and that there are differences between the used data. More precise data are necessary for improvement of simulations and consequently for more precise setting of real conditions of technological processes leading to the improvement of properties of the final product.

Conclusions

The following conclusions were formulated on the basis of the obtained experimental results from DTA, DSC analyses and from comparison of real thermo-vision measurements and simulations using heat capacity calculated by the CompuTherm and experimental heat capacity measured using continuous method and SETARAM MHTC (Multi High Temperature Calorimeter) equipped with the 3D DSC sensor:

- The experiments must be performed very carefully with respect to the possible massive decarburisation.

- Two running phase transitions were detected by DTA and DSC analyses in the studied ingot mould.

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- Temperature of the Curie point was found to be 1019 K (DTA) and 1036 K (DSC) respectively.

- The second one is the transition $\alpha + C_{grafitic} \rightarrow \gamma$, which takes place between the temperatures 1071–1108 K (DTA) and 1079–1131 K (DSC) respectively.

- The heat capacity dependence obtained by the CompuTherm shows only one running phase transition (peak). It is not clear, to which phase transition this peak is related to. Probably, the authors of the CompuTherm suppose that the peak includes both: magnetic transition and transition of $\alpha + C_{grafitic} \rightarrow \gamma$.

- The experimental C_p values are very close to the calculated values in the temperature interval of 500–1000 K and in the interval of 1175–1300 K. More distinct deviations are in the temperature interval of 1000–1175 K.

- The results of simulations of casting process using experimental and calculated C_p values differed slightly after only 2 hours after the end of casting process. The results obtained by experimental C_p dependence (after 2 hours) are closer to the results obtained using thermo–vision measurements.

- The simulation results obtained using experimental C_p dependence seem to be more precise in comparison with the calculated C_p dependence.

- Despite relatively significant differences in the C_p dependence in the phase transition region it seems that these differences have no considerable impact on the simulation results (it is possible to use the calculated and measured C_p dependence also for obtaining very close–almost the same results).

Experimental measurements were performed in order to obtain our own data of the temperature dependence of C_p on the temperature for a hematite ingot mould. Simulations leading to description of temperature fields in the ingot mould were performed. The obtained results showed the necessity of experimental

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measurements and consequently improvement of present databases, as well as SW used for thermo–dynamical calculations and simulations.

Future work is planned and will be focused on the study of the origin of possible defects and on segregation processes that are strongly dependent on the changes of the temperature field in the ingot alone, and in the ingot mould as well.

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Figure Captions

Fig. 1 Ingot mould, A-real ingot mould, B-CAD geometry of ingot mould, C-final computational mesh of ingot mould, D-final computational mesh of ingot

Fig. 2 Scheme of continuous C_p method, X - section of values used for C_p evaluation

Fig. 3 Comparison of TG and DTA curves obtained at 10 and 20 K min^{-1}

Fig. 4 Comparison of apparent heat capacities calculated with use of CompuTherm and experimentally obtained values

Fig. 5 Comparison of measured and calculated temperature fields of ingot mould

Table Captions

Table 1 Chemical composition of studied ingot mould, wt. %

Table 2 Apparent heat capacity of studied ingot mould, experimental (Exp.) and calculated (Calc.) values

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Table 1 Chemical composition of studied ingot mould, wt %

Sample	C	Si	Mn	P	S	Cr
Hematite mould	3.6	1.5	0.7	0.02	0.02	0.1

Table 2 Apparent heat capacity of studied ingot mould, experimental (Exp.) and calculated (Calc.) values

T/K	C_p/J K^{-1} g^{-1}		
	Exp.[a]	Calc.	Δ[b]
500	0.57±0.02	0.50	12.7
525	0.56±0.02	0.52	8.7
550	0.57±0.02	0.54	5.6
575	0.57±0.02	0.56	3.2
600	0.58±0.02	0.58	1.5
625	0.60±0.02	0.60	0.0
650	0.61±0.02	0.62	1.2
675	0.62±0.01	0.64	2.4
700	0.63±0.01	0.66	3.5
725	0.65±0.01	0.68	4.7
750	0.66±0.01	0.70	5.8
775	0.67±0.01	0.72	6.9
800	0.68±0.01	0.74	7.9
825	0.70±0.01	0.76	8.6
850	0.71±0.01	0.78	8.8
875	0.73±0.01	0.80	8.5
900	0.76±0.01	0.82	7.4
925	0.79±0.01	0.84	5.4
950	0.84±0.01	0.86	2.4
975	0.89±0.01	0.88	1.6
1000	0.96±0.01	0.90	6.5
1005	0.97±0.02	0.90	7.6
1010	0.99±0.01	1.13	13.9
1015	1.01±0.02	1.50	48.7
1020	1.03±0.01	1.87	82.3
1025	1.04±0.02	2.24	114.5
1030	1.06±0.02	2.21	108.2
1035	1.08±0.02	2.01	85.0
1040	1.05±0.02	1.80	70.4
1045	1.01±0.02	1.59	56.7
1050	0.98±0.02	1.38	40.8
1055	0.95±0.02	1.17	22.8
1060	0.93±0.02	0.96	3.0
1065	0.92±0.08	0.75	18.4
1070	0.91±0.14	0.72	21.7
1075	0.97±0.14	0.72	26.1
1080	1.13±0.14	0.72	36.1
1085	1.26±0.13	0.72	42.6
1090	1.37±0.13	0.72	47.1
1095	1.45±0.14	0.73	50.0
1100	1.51±0.06	0.73	51.9
1125	1.08±0.04	0.74	31.8
1150	0.85±0.02	0.75	12.4
1175	0.78±0.02	0.76	2.7
1200	0.77±0.02	0.77	0.1
1225	0.77±0.03	0.78	1.2
1250	0.76±0.04	0.79	4.1
1275	0.74±0.04	0.80	7.4
1300	0.77±0.03	0.81	4.8

[a]Uncertainties are the standard deviations of three replicates

[b]$\Delta=100(|C_p,\text{Exp.}-C_p,\text{Calc}|/C_p,\text{Exp.})$

Fig. 1 Ingot mould, A-real ingot mould, B-CAD geometry of ingot mould, C-final computational mesh of ingot mould, D-final computational mesh of ingot
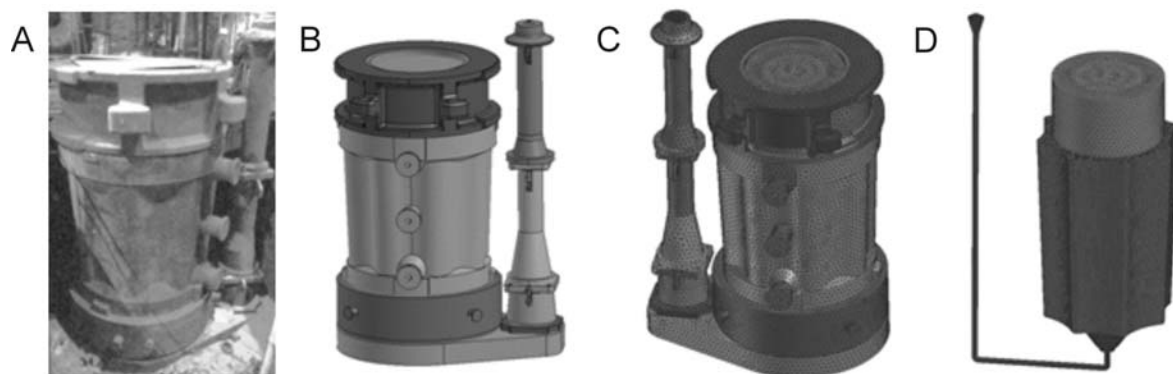

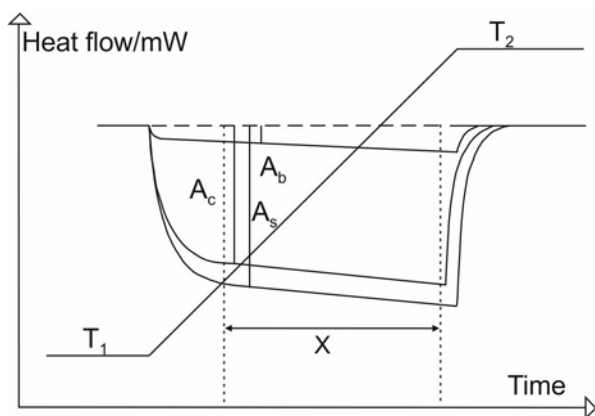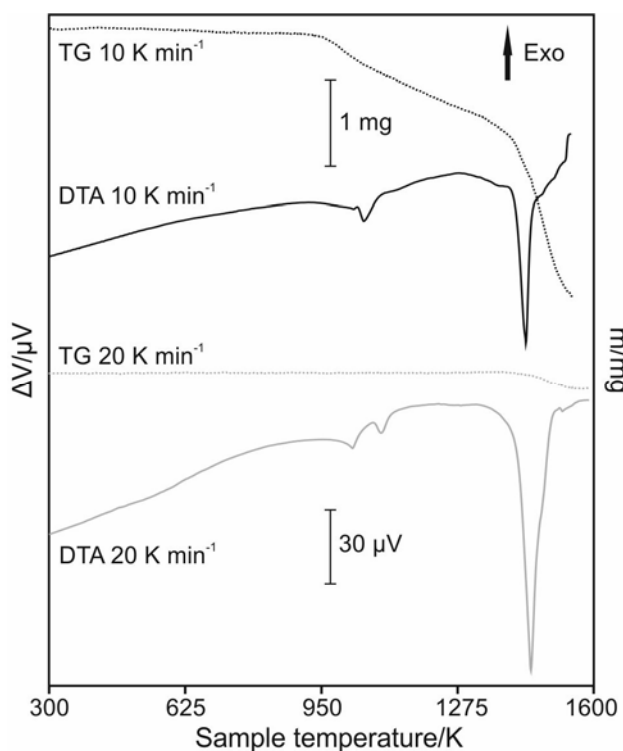**Fig. 2** Scheme of continuous C_p method, X - section of values used for C_p evaluation

Fig. 3 Comparison of TG and DTA curves obtained at 10 and 20 K min^{-1}

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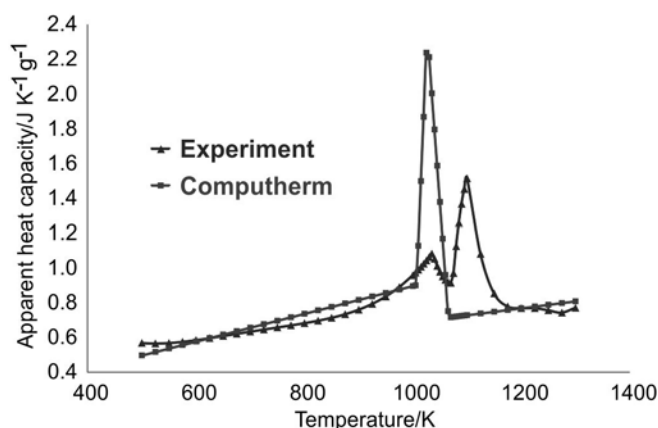

Fig. 5 Comparison of measured and calculated temperature fields of ingot mould