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A verification of thermophysical properties of a porous ceramic investment casting mould using commercial computational fluid dynamics software

C A Jones¹, M R Jolly¹, A E W Jarfors², M Irwin³, R Svenningsson⁴, J Steggo² and J Eriksson³

¹ Sustainable Manufacturing System Centre, Cranfield University, Bedfordshire, MK43 0AL, UK

² Jönköping University, School of Engineering, Box 1026, 551 11 Jönköping, Sweden

³ TPC Components AB, Brånstaleden 2, 734 32 Hallstahammar, Sweden

⁴ RISE Research Institute of Sweden, Tullportsgatan 3, 553 22, Jönköping, Sweden

Email: c.a.jones@cranfield.ac.uk

Abstract. Defects in cast metals remain a common problem in many areas of the foundry industry, particularly in the investment casting of large area, thin-walled components for aerospace applications. During previous research, the thermophysical properties, density and porosity of a fibre reinforced ceramic investment casting mould were determined using several experimental techniques. Without verification, these experimental results remain nothing more than educated guesswork. The purpose of this study is to verify previous results and to more fully characterise the ceramic mould material with complementary measurements. A commercially available computational fluid dynamic (CFD) simulation package, Flow-3D[®], was used in conjunction with a full-scale Ni-superalloy (IN718) casting to assess the accuracy of these results. By placing thermocouples strategically across the mould thickness, temperature profiles were determined and compared directly to predicted profiles extracted from the simulation by a custom-written Python script.

1. Introduction

This work continues from results obtained in a previous study [1] where the thermophysical properties of a fibre-reinforced, porous ceramic mould used in aerospace casting were experimentally determined. Techniques including laser flash analysis (LFA), differential scanning calorimetry (DSC) and gas pycnometry were used to obtain the thermal diffusivity, specific heat capacity and material density respectively. This paper reviews these properties in the light of improvements to the experimental methodology, re-presenting data along with a discussion of any differences relative to previously drawn conclusions. Fulfilment of the aim to verify these properties was achieved through comparison with results obtained from a CFD simulation package, Flow-3D[®]. Cast aerospace components have strict microstructural and residual stress limitations to ensure they are fit for service, the control of which requires accurate, substantiated simulations which are often widely overlooked by industrial entities. Simulation configurations are rarely transferable from one foundry situation to another making characterisation work an essential part of all operations.



2. Methodology

2.1. Experimental casting trials

A full-scale casting experiment was conducted at the TPC Components AB foundry in Sweden to provide data points for comparison with simulation results for property verification. A ten layer test mould was produced consisting of eight step structures organised into two groups of four divided into upper and lower groups; a computer generated version of which is shown in figure 1. This test mould had a structural composition comparable to that of the genuine aerospace moulds, the breakdown of which is detailed in table 1. It should be noted that the composition of sample 2 was altered between the sample preparation and the construction of the mould for experimental casting verification. This change was not radical and hence not anticipated to significantly impact the results, but should be noted as a variable.

Two parts in the upper grouping and two parts in the lower grouping (four in total) positioned directly opposite one another were coated with Superwool® Plus insulation. Six K-type thermocouples were positioned in the upper group of test parts in the mould, three in an insulated part and three in an uninsulated part. One S-type thermocouple was placed centrally in the cavity of the 8 mm section of the insulated component. The exposed wires of these thermocouples were sleeved with ceramic tubing for protection and were connected to a data-logger which in turn was placed inside an insulated container. In both parts, the K-type thermocouples were positioned with one on the second mould layer, one on the sixth layer and one on the eighth layer. All of the thermocouples were active and generated data throughout the experiment with the exception of the centrally positioned S-type thermocouple which was damaged as a result of manual handling. A Python script was produced to extract the data from the simulation output and compare it to the thermocouple results obtained in the casting trials.

Table 1. Compositional breakdown of the mould by layer

Sample Identity	Layer	Composition		
		Name	Details	
Sample 1	1	Cobalt Aluminate with 90 mesh Zircon sand	Chilches Microzir Flour 200M IC	ZrSiO ₂ > 63.5% TiO ₂ < 0.2% Fe ₂ O ₃ < 0.15% Al ₂ O ₃ < 1.3% SiO ₂ < 33%
			Cobalt Aluminate Primecote® Plus	CoAl ₂ O ₄ Binder
Sample 2	2	Intermediate with 54 mesh Alumina sand	-	-
Sample 3	3	Backup with 30/80 mesh molochite sand	Ranco-Sil 140F	SiO ₂
			Matrixol 30	Binder
			MXC Excel X2 30/80 Sand	Fibre Reinforcement
Sample 4	4	Backup with 16/30 mesh molochite sand	-	-
	5		Ranco-Sil 140F	SiO ₂
	6		Matrixol 30	Binder
	7			
	8			
	9		MXC Excel X2 16/30 Sand	Fibre Reinforcement
				-

The thermocouples were secured onto the dried surface of the previous mould layer using ceramic slurry, with their position determined using a digital calliper to measure the mould thickness at the thermocouple site. These positions are recorded in figure 1 and the positions of the inner and middle thermocouples were matched to measurement nodes in the simulations. The thermocouples in the insulated and uninsulated have been assumed to be at the same positions as they were attached at the same time, following the same number of slurry dips.

The data logger was set to commence recording as the mould was placed into the preheat furnace. 1050°C was selected as the preheat temperature of the furnace, which the mould remained in overnight

to allow time for a stable temperature to be reached. Immediately prior to casting, the mould was transferred to a vacuum chamber and the vacuum drawn to 3.8×10^{-4} Torr (0.0507 Pa) at which point the Inconel 718 melt at 1468 °C was poured.

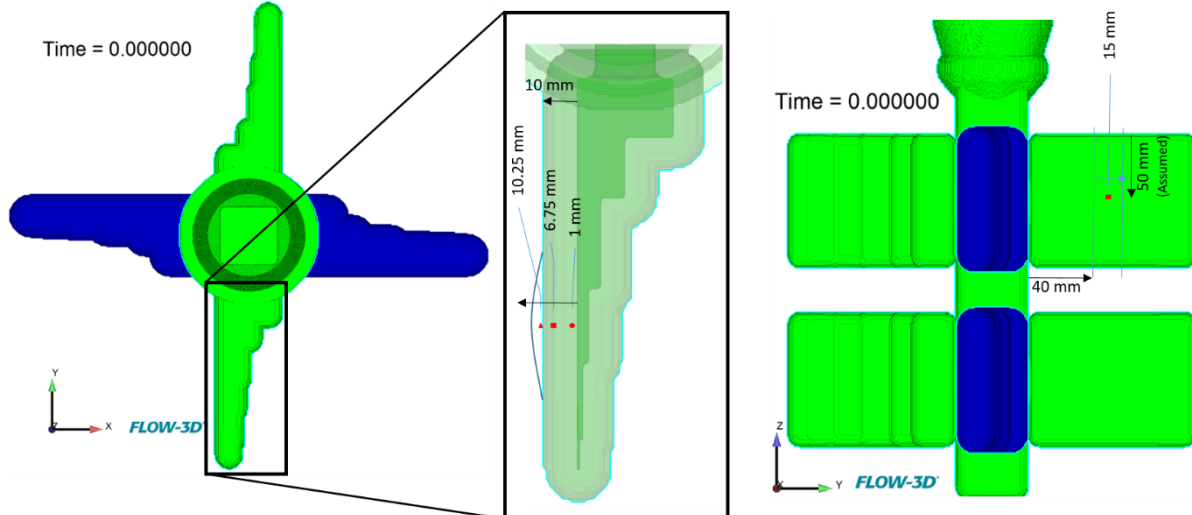


Figure 1. Computer generated representation of the casting geometry taken from Flow-3D® pre-processor. The locations of the three thermocouples are indicated in red with distances marked relative to the interface between mould and cavity. Blue indicates wool insulation.

2.2. Computer simulations

The computer simulation in Flow-3D® was configured to replicate these conditions where a mould geometry of a uniform 10 mm thickness, see figure 1, was placed within a time-varying pressure boundary condition to reflect the transitioning environment from atmospheric pressure to vacuum and back. Void pointers were used to define the difference in initial air conditions between the mould cavity, 1050°C, and the surrounding environment, 30°C, as it would have been the instant the mould was removed from the furnace. The complete geometry was meshed using two mesh regions; a coarser mesh of 5 mm cubes covering the complete environment and a finer mesh of 2.5 mm cubes surrounding the insulated and uninsulated parts of interest. This configuration of meshes ensures an improvement in simulation time when compared to a uniform fine mesh situation although when using multiple meshes, it must be ensured that the mesh planes intersect and there is no more than a factor of 2 between the sizes of overlapping mesh regions.

Due to the presence of the thermocouples in the real mould, a local thickening of the mould was seen, as indicated in figure 1, which was not reflected in the simulations because of the method by which the mould was formed. As a result, the outer thermocouple was not actually measurable from the simulation as it lay beyond the outer wall of the simulation mould. The heat transfer coefficients (HTC) between the fluid and mould was defined in a temperature varying manner in an attempt to account for the air gap that forms as the metal solidifies ranging from $3500 \text{ Wm}^{-2}\text{K}^{-1}$ at 2273K to $300 \text{ Wm}^{-2}\text{K}^{-1}$ at 273 K. The HTC between the mould and insulation was set at a constant value $1000 \text{ Wm}^{-2}\text{K}^{-1}$ based on literature values [2]. The emissivity value for the surface of the mould was defined as 0.79 to reflect the fact the dominant material at the surface is Silica and 0.56 for the insulation, determined by proportionally taking the emissivity of the constituent components (Silica, MgO & CaO) relative their percentage abundance in the material. Based on the compositional makeup of the IN718 alloy, the TCFE7: Steels/Fe-Alloys v7.0 database in Thermo-Calc® software version 2019.1.36671-604 was used to determine the latent heat of fusion and solid fraction as a function of temperature to improve the accuracy of the values available in the Flow-3D® materials database.

2.3. Thermophysical properties

Differential scanning calorimetry (DSC) analysis was conducted on various layers of the mould to determine the effective specific heat capacity of the complete mould. When this assessment was conducted in [1] the samples considered were produced by taking scrapings which could result in the inclusion of material from different layers of the mould. In this work, samples of each mould layer – confirmed to contain no contaminants from other regions of the mould - have been investigated. The mould was divided into four samples, defined in table 1, each uniform in composition which together in the correct proportions form the complete mould. Sample masses of 20.4 mg, 20.0 mg, 20.5 mg and 20.7 mg for samples one, two, three and four respectively were selected for DSC analysis, values selected to allow calculations to be made relative to a 20 mg Sapphire reference sample. All samples were tested using the sample heating cycle of 25 °C to 1400 °C at a rate of 10 K per minute before returning to room temperature at the same rate, sampling data continuously.

The linear coefficient of thermal expansion (CTE) of the ceramic mould was measured using dilatometry. In this work, two measurements were taken along orthogonal axes: one in the direction parallel to the heat flux (radially through the mould) and the second in the direction perpendicular to the heat flux (in the plane of the layers). Two cylindrical samples of the complete ceramic mould with an approximate diameter of 6 mm and a length of 12.8 mm and 8.4 mm. Ideally, these samples would both be approximately 12 mm in length to allow comparison to the reference standard. However, as the mould was no thicker than 10 mm in the parallel direction an alternative reference was required in this case. The first sample was evaluated against a 12 mm polycrystalline aluminium oxide whereas the shorter second samples were evaluated against an 8 mm Alumina reference standard. It is important to note that the use of different reference standards does not impact the final results of CTE, it merely ensures the instrument was correctly calibrated to the sample length. Both experiments were run using the same heating cycle; 25 °C to 1400 °C increasing at a rate of 10 K per minute, continuously sampling data.

In order to determine the thermal conductivity of the ceramic mould, it was necessary to combine the heat capacity and the material density (ρ) with the thermal diffusivity (α), see equation (1), which was measured using Netzsch laser flash analysis (LFA). The CTE was supplied to the LFA software to allow compensation for changes in sample dimensions during the temperature cycle. Thin cylindrical wafers of the sample materials were prepared with an approximate diameter of 10 mm and a thickness

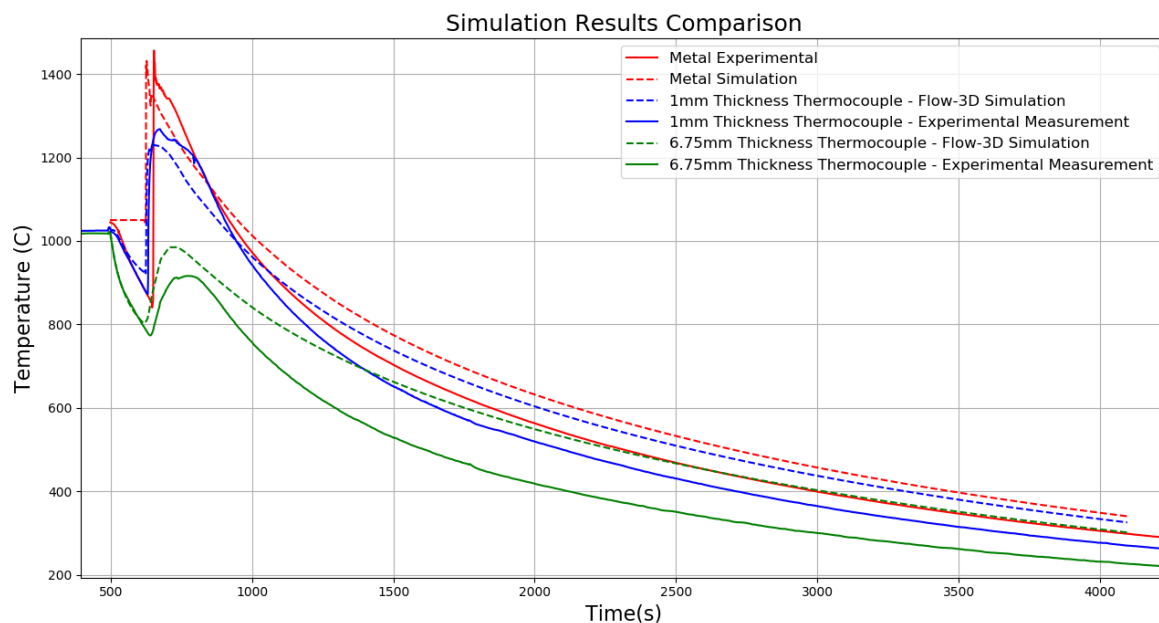


Figure 2. Experimental results obtained from the thermocouple contrasted against predictions from computer simulations

of 1.94 mm, 2.10 mm, 1.99 mm and 3.8 mm for samples 1, 2, 3 and 4 respectively. Difficulties were experienced during the determination of the thermal diffusivity in [1], largely as a result of the laser flash analysis setup where the suspected transparency of the mould to the laser wavelength (1064 nm) prevented the acquisition of data by obscuring the sample response, particularly at elevated temperatures. With the aim of obtaining improved data, the LFA analysis was repeated with the samples placed into a sealed crucible fitted with a Sapphire window in the lid and into the bottom to restrict the area upon which the laser was incident. The system was configured to increase the temperature from ambient to 1400 K at a rate of 50 K per minute with five measurements taken at each 200 K temperature increment.

$$\lambda = \rho \alpha C_p \quad (1)$$

3. Results

3.1. Casting trials and simulations

Figure 2 shows the comparison between casting experiment and simulation of the uninsulated part indicating a good agreement between the experimentally measured thermal gradients and those predicted by the simulation in both the metal and mould, hence validating the accuracy of the specific heat capacity, thermal expansion and thermal conductivity of the mould determined via the discussed methodologies. At this stage, only the uninsulated part has been considered in order to isolate the mould thermophysical properties in the comparison by removing the uncertainty associated with the properties of the insulation material. The properties of the insulation will require further specification before inclusion in the future. Spikes in the data profiles obtained by experiment were caused by exposed sections of the thermocouple wires making contact with one another and have been largely removed from the plot as outliers, with a linear interpolation conducted between the remaining data points to ensure continuity.

Initially in the mould, all thermocouples were constant at their maximum temperatures attained whilst in the preheat furnace which was approximately 1027.5 °C for the uninsulated at the inner thermocouple site and 1044.5 °C for the insulated at the inner thermocouple site. It was noted that despite the mould remaining in the preheat furnace overnight, none of the six thermocouples in the mould ever attained the targeted 1050 °C and there was a notable difference between those in insulated and those in uninsulated regions. Literature offers a possible justification for this observation. In [3], thermocouples were strategically positioned around a steam autoclave to investigate the temperature distribution which was found to be decidedly non-uniform. Of particular note was that the temperature recorded in the vicinity of the door was consistently lower than that recorded deeper in the autoclave. Although this was conducted in a steam autoclave, it can be conjectured that the same principle applies to the preheat furnace. Given that the mould was positioned near the door of the preheat furnace to accommodate the thermocouple wires emanating out along the shortest possible route, this would explain the lower mould temperature. Even though the S-type thermocouple was not serviceable for this case, an identical casting was conducted the previous day with approximately comparable environmental and preheat conditions with the thermocouple placed in the uninsulated part which did successfully record information about the melt temperature profile with time. By placing a measurement point in the cavity of the simulation it was possible to make a comparison; the exact positioning of the node is not so important in this case due to the very high conductivity of the metal. In the simulated metal case, the melt arrived at the measurement location slightly earlier than in the real case, most likely because of the currently poor understanding of the true mass flow rate of the metal into the mould cavity. Despite this, the profile was a reasonable match although the simulation does over predict the temperature of the metal following approximately 750 seconds.

From the moment the furnace door was opened the mould began cooling, a trend predicted well by the simulations, particularly at the 6 mm thermocouple position, until after approximately 2 minutes and 18 seconds where the temperature increases dramatically as melt fills the cavity. The agreement during this stage, particularly at the inner thermocouple's location (1 mm from the cavity) is very good. As

would be expected, the gradient measured in response to the melt introduction shallows as one measures at positions further from the cavity. For example, the response of the innermost thermocouple is virtually instantaneous whereas the second displays a more gradual increase. This difference emerges as a result of the finite time required for thermal energy to diffuse through materials which increases with thickness. The cooling of the air within the mould cavity was not modelled in this instance resulting in simulated metal temperature appearing as constant with time prior to mould filling. As metal fills the cavity at approximately 2 minutes 18 seconds the temperature profile of the metal began to display the expected trend in agreement with the experimental measurements. The agreement between the simulation and experimental measurements begins to deviate during the final cooling as time progresses with the temperature consistently overpredicted by the simulation. This deviation could be attributed to the fact that the simulated mould was not an exact match to reality, in terms of wall thickness/surface roughness or to poorly captured heat transfer mechanisms. A less obvious source of variation may arise from the simulation mesh size of 2.5 mm in the area of interest, large compared to mould thickness, leading to a potential inprecision in the determination of the temperature profiles. Despite this deviation, the trend remains good with the gradients of the simulated and experimental results beginning to match as time progresses. This agreement suggests the heat transfer mechanism at this time was correctly captured by the simulation using the measured data. The initial discrepancy will require further investigation.

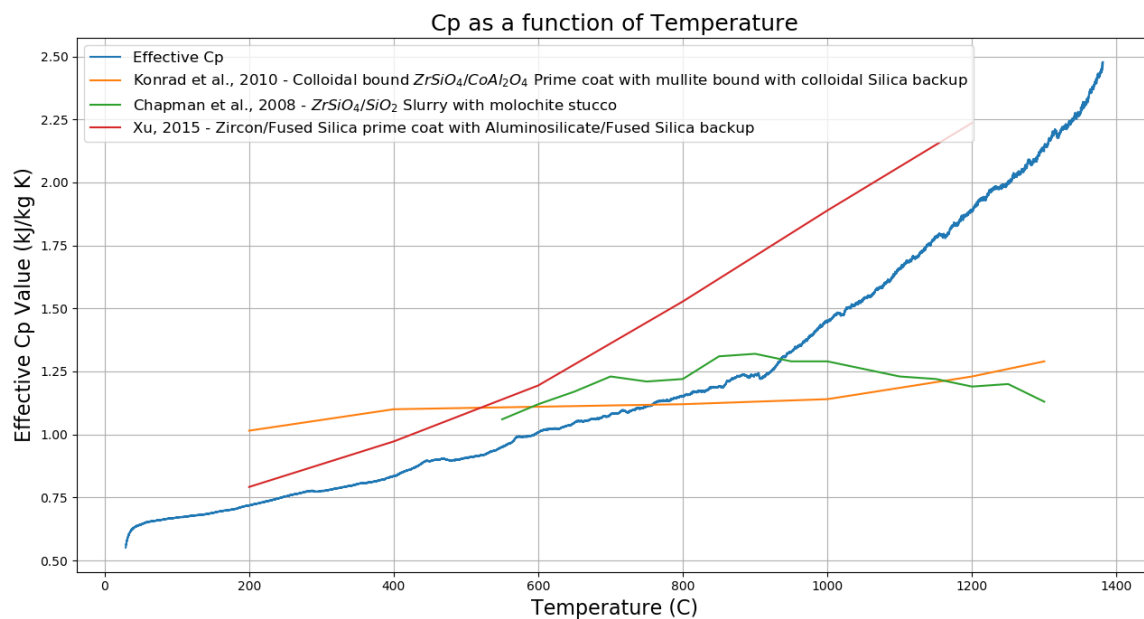


Figure 3. Plot of the effective specific heat capacity alongside other published data ([2, 4-5]).

3.2. Thermophysical properties

3.2.1. Specific heat capacity. The effective specific heat capacity of the ceramic mould shown in figure 3 was determined mathematically using equation 2, where A is a scaling coefficient, M is the sample mass and i is an integer, by combining the individual measured values of each layer based on their contribution to the total mass of the mould through a rule of mixtures approach [6]. The specific heat capacity measurements for samples 3 and 4 showed a significant increase in C_p with temperature, particularly at high temperature, which is not reflected to the same extent in samples 1 and 2 which show a very gradual increase with temperature. The scaling coefficients reflect that samples 1, 2, 3 and 4 contribute in mass percent 7.63%, 15.39%, 15.39% and 61.59% respectively, hence the high increase of sample 4 dominates. When comparing these results to the other published results, below 1000 °C the trend of Konrad *et al.* is in reasonable agreement with experimental data however, conversely exhibits

a decrease at high temperatures. Chapman *et al.* on the other hand does report an increase in C_p at the higher temperatures although not to the same extent as that describes by the experimental data. The mould material investigated by Xu is arguably the most compositionally comparable material to that investigated in this work which, although consistently higher in value, has a strong similarity in trend with temperature. Data that can be found in [6] also made a consideration of the C_p from measuring two compositional elements of their mould; Zircon/Silica prime coat and a 200 mesh molochite. Their results indicated that within a range of 300-800 °C both the Zircon/Silica and molochite have a gradual increase in C_p with temperature from approximately 0.75 to 0.8 kJ kg⁻¹ K⁻¹ and 1 to 1.1 kJ kg⁻¹ K⁻¹ respectively. These results are in good agreement with the measurement of the prime coat conducted in this work (blue line of figure 3) but less so for the molochite backups (red/green lines of figure 3).

$$C_p^{eff} = \sum_i \left(\frac{A_i M_i}{A_1 M_1 + A_2 M_2 + A_3 M_3 + A_4 M_4} \right) C_p^i \quad (2)$$

3.2.2. Coefficient of thermal expansion. It could well be expected that the inhomogeneous nature of the mould material would lead to an inconsistency in the thermal expansion properties depending on the axis one considers. The average results of assessing the thermal expansion in two orthogonal axes, parallel and perpendicular to the direction of heat flux, are shown in table 2. The CTE in the perpendicular direction is consistently lower than that in the parallel direction, although both compare well with similar materials from published sources [5]. It is interesting to note that when comparing the results to the Chapman *et al.* investigation of fused Silica, i.e. comparable to the experimental mould with the exception of Zircon, the results are notably higher indicating the presence of Zircon in a mould increases the CTE. The quoted uncertainty in measurements was determined with reference to previous literature [7], where the same Netzsch instrument reference samples were employed.

Table 2. Average values of the coefficient of thermal expansion

Direction	CTE
Perpendicular	3.53±0.06 x10 ⁻⁶ K ⁻¹
Parallel	4.84±0.06 x10 ⁻⁶ K ⁻¹

3.2.3. Thermal conductivity. Thermal diffusivity measurements were taken for each of the four samples with the intention of determining thermal conductivity by amalgamation with the individual thermal expansion, density and specific heat capacity measurements. Diffusivity measurements taken for sample 4 displayed a periodic, oscillatory behaviour that obscured the expected step response of the profile. It is most likely that as a result of the extended exposure time whilst attempting to determine a stable response the detector did in fact register the periodic temperature fluctuations of the furnace rather than the true response from the sample. As a consequence, the experimental values of thermal diffusivity from a previous investigation [1] were used in combination with the effective specific heat capacity determined in this work to calculate the thermal conductivity, as shown in figure 4. Plotted alongside this data is a set of data from other published sources [2, 4], most interesting of which is that of Xu [2] which shows a remarkably similar trend in conductivity with temperature. Data obtained from Konrad *et al.* [4] shows a much lower variation in thermal conductivity with temperature compared with the experimental data obtained here.

4. Conclusion

The temperature profiles obtained from computer simulations have a good agreement with the experimentally determined temperature profiles, indicating that the measured thermophysical properties of the mould are reasonable. These thermophysical properties are comparable to similar materials presented in the literature. Published literature including [8] illustrating the difference in predictive capabilities of computer simulation packages available on the market, highlighting their sensitivity to the setup of elements including boundary conditions and mesh setting; factors that can have a significant

impact on the results. Care should be taken when configuring simulations for different circumstances. It would be beneficial to investigate the variations in predictions in greater detail, although this is a topic for future research. With thermophysical data available for individual layers of the mould, a more complete model could be constructed by considering each layer individually in the simulation as opposed to combining them into an effective value of the parameter. Questions remain to be answered regarding the specific heat capacity profile of the mould; what is responsible for the increase in C_p observed in samples 3 and 4 at increasing temperatures? This will be investigated in detail in due course.

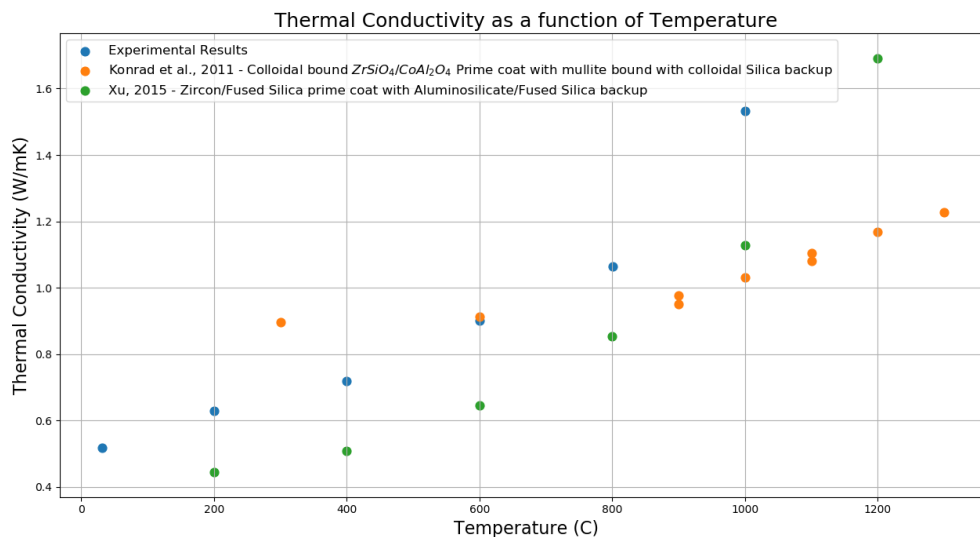


Figure 4. Thermal conductivity as a function of temperature alongside published results.

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