



Curing Properties of Furotec 132 Resin-Bonded Foundry Sand

M.M. Mashingaidze

University of Namibia

Private Bag 13301 Windhoek, Namibia

Corresponding author. E-mail address: mmashingaidze@unam.na

Received 19.07.2019; accepted in revised form 01.10.2019

Abstract

The study evaluated the curing properties of natural silica sand moulded with 1% by weight Furotec 132 resin binder catalysed by Furocure CH Fast acid and Furocure CH Slow acid. Physical properties of this sand included an AFS number of 47.35, 4.40 % clay, 0 % magnetic components, 0.13 % moisture, and 64.5 % of the size distribution spread over three consecutive sieves (150 – 600 μm). The sand was washed repeatedly to remove all the clay and oven dried. 2 kg washed sand samples were mulled with pre-determined weights of either catalyst to give 30 %, 50 % and 70 % by weight of 20 g Furotec 132 resin which was added last. Furotec 132 resin + Furocure CH Slow acid catalyst system gives longer bench lives and strip times but the maximum compressive strength in excess of 5000 N/cm² is attained after more than 8.5 hours curing time irrespective of the weight % of catalyst added relative to the resin. On that basis, exceeding 30 weight % Furocure CH Slow acid catalyst when sand moulding with Furotec 132 resin has neither technical nor economic justification. In comparison, the Furotec 132 resin + Furocure CH Fast acid catalyst system was only capable of producing mould specimens with maximum compressive strength above 5000 N/cm² at 30 weight % catalyst addition rate. At 50 and 70 weight % catalyst addition rates, the mulled sand rapidly turned dark green then bluish with a significant spike in temperature to about 40 °C, far exceeding the optimum curing temperature of Furotec 132. This high temperature accelerates the curing rate but with a very low degree of resin curing which explains the low compressive strength. In fact the sand grains fail to bond and have a dry, crumbly texture implying dehydration. Thus, not more than 30 weight % Furocure CH Fast acid catalyst should be used in sand moulding.

Keywords: Curing properties, Foundry sand, Furotec 132 resin, Furocure CH acid catalyst, Curing temperature

1. Introduction

Sand is used in foundries as a moulding material and for core making. Sand particles lack the inherent ability to stick to each other necessitating addition of binding agents when moulding for metal casting [1-10]. Binders enable consolidation of loose sand into integral, solid moulds capable of withstanding metallostatic pressure of molten metal during casting [3]. Foundry sand properties are affected by several factors inclusive of sand chemistry and particle morphology [2-6, 8-11]. Undesirable impurities in foundry sand include alkaline earth metal and iron

oxides on account of their tendency to reduce the sand refractoriness. Highly refractory sands like silica, magnesite, zircon, silimanite, and olivine are preferred for foundry applications with silica sand used the most [3-7]. Foundry sand quality and the binder are critical to the production of sound castings apart from the other various sand casting parameters [8].

Moulding sand can be naturally bonded or synthetically bonded. Modern foundries are increasingly using synthetically bonded sands. Selection of binding agents is affected by technical standards, environmental friendliness and recyclability of the used foundry sand with synthetic organic binders gaining widespread usage [7]. Due to increasingly stringent environmental regulations

and drives to lower foundry costs, foundry sand reclaiming has become the norm but is affected by binder type [9]. Thus, foundries now also base binder selection on how it will affect moulding sand reuse. Several kinds of chemical binders abound, organic and inorganic. According to Holtzer and Dańko [10], there are three general categories of resin binder processes:

1. *Cold-setting processes (no-bake systems)* - include furan-acid catalysed.
2. *Gas-hardened processes (cold-box system)* - require injection of a gaseous catalyst.
3. *Hot curing processes* – utilise amino resins which are essentially thermosetting polymers. Shell moulding is an important casting process where such binders are used.

The scale of production in a particular foundry operation is decisive in choosing a resin binder [10]. Kumaravadev and Natarajan [8] have demonstrated that the process window approach (PWA) readily lends itself to the optimisation of the sand casting process at this process development phase. Whereas the present study did not adopt the Taguchi method and response surface methodology used by Kumaravadev and Natarajan [8] due to the nature of the investigation, it is a case study in judicious selection of a synthetic binder system.

The objective of this study was to evaluate and compare the curing properties of silica sand mulled with Furotec 132 resin binder catalysed by Furocure CH Fast acid and Furocure CH Slow acid. The evaluation of the curing properties was on the basis of bench life, strip time and maximum compressive strength. The study hypothesis was:

H₀: The maximum compressive strength of the Furotec 132 resin bonded sand with Furocure CH Fast acid catalysis is equal to that for Furocure CH Slow acid catalysis, at a 5% level of significance.

H₁: The maximum compressive strength of the Furotec 132 resin bonded sand with Furocure CH Fast acid catalysis is not equal to that for Furocure CH Slow acid catalysis.

2. Experimental methods

The study was quantitative with a series of completely randomized experiments conducted on foundry sand sourced from a riverbed. Chemical analysis of the sand with a Bruker S1 500 Titan XRF hand-held X-Ray analyser preceded all the other experiments. The moisture content, clay content, acid demand value, particle size distribution, and average grain fineness of the sand were also experimentally determined. Magnetic separation was employed to remove iron oxide particles from the bulk sand sample in preparation for moulding. Clay was removed by washing the bulk sand in a weak basic solution, pH 8.5, of sodium hydroxide and distilled water, followed by three stages of washing in distilled water only and oven drying at 110 °C.

Tests were carried out according to Indian Standard (IS) 1918 (1966) [11], the guidelines in [5] and with due regard to the safety and materials handling aspects prescribed in [12-13]. An acid-catalysed, furane sand binder called Furotec 132 resin was used. This free flowing, yellow-brown liquid cold-setting binder is constituted of urea formaldehyde resins dissolved in monomeric furfuryl alcohol [12], such that it gives off the odour of that alcohol. Two types of acid catalysts, Furocure CH Fast acid and Furocure CH Slow acid were used to activate the sand binder. Detailed information about these catalysts is available in [13]. Materials used apart from the sand samples included:

1. Reagents for titration (acid demand value test) - 0.1 M HCl and 0.1 M NaOH.
2. Reagents for moulding tests - Furotec 132 resin binder, Furocure CH Fast acid and Furocure CH slow acid.
3. Equipment and apparatus - pH meter, Bruker S1 500 Titan XRF hand-held X-Ray analyser, analytical balance, sieve shaker + nest of sieves, Uniaxial Compressive Test machine, beakers, pipettes, burretes, stands, stop watch, thermometer, sand mixer, and assorted foundry tools.

Curing properties were determined after mulling 2 kg sand samples with the acid catalysts and the Furotec 132 resin in a sand mixer, and in an air-conditioned room where the temperature was kept constant at 25 °C. The average atmospheric relative humidity for the duration of the testwork was 16 %. The mulling parameters are specified in Table 1.

Table 1.
Sand, acid catalyst and resin binder mulling parameters

Resin density g/cm ³	Resin volume, cm ³	Weight of resin, g	Weight of sand, g	Sand weight % Resin	Catalyst %	Catalyst weight, g	Catalyst volume, cm ³
1.2	16.7	20.0	2000.0	1.0	30	6.0	5.0
1.2	16.7	20.0	2000.0	1.0	50	10.0	8.3
1.2	16.7	20.0	2000.0	1.0	70	14.0	11.7

The mulled sand for each of the three combinations of resin and % catalyst for either catalyst type were moulded into six standard uniaxial compressive strength test pieces of 50 mm diameter and 50 mm height within 12 minutes of mixing. A timer was set the moment mulling ended, while the mulled sand was immediately transferred into a plastic bucket which was sealed with a lid. Sand temperature was obtained by inserting a thermometer into the

bucket, and recording the maximum temperature of the sand. Subsequently, scoops of the mulled sand were placed in the moulds, and gently compacted by hand with a sand rammer until each specimen was level with the top surfaces of the moulds. The specimens were covered with plastic cups to prevent drying out. In order to evaluate the maximum compressive strength of the mulled sands, one specimen at a time was mounted in the

Uniaxial Compressive Test machine at 1 hour intervals for 6 hours, taking into account the time after mixing. Tests to determine the compressive were replicated twice for each treatment resulting in 54 specimens for each resin and catalyst combination. For bench life and strip time determination of Furotec 132 resin binder + Furocure CH Slow acid system, compressive strength measurements of the test specimens were measured at 5 minute intervals for 20 minutes, taking into account the time after mixing. For Furotec 132 resin binder + Furocure CH Fast acid system, the interval was reduced to 2 minutes for 20 minutes with test samples prepared one at a time but the same number (2) of replications was observed.

Table 2.

Chemical composition of moulding sand

Oxide/Element	% SiO ₂	% CaO	% K ₂ O	% Al ₂ O ₃	% P ₂ O ₅	% Fe ₂ O ₃	ppm TiO ₂	% MgO	% Cl	ppm ZrO ₂	ppm MnO
Composition	90	0.20	0.10	2.00	<LOD	0.14	458	<LOD	<LOD	30	52

3.2. Physical properties of loose moulding sand

The sieve analysis results are presented in Table 3 and were used to calculate the sand AFS number. From the AFS number of 47.35 the average grain size of the sand was estimated at 0.280 mm - 0.300 mm, implying the fineness sand is close to the range specified in [5]. Table 3 illustrates that the moulding sand had a size distribution spread over three consecutive sieves (150 – 600 µm), which is favourable for moulding [5, 11]. It enhances tight packing of the sand particles after ramming or jolting during

Table 3.

Sieve analysis for a 100g foundry sand sample

Sieve Aperture size (µm)	Mass Retained (g)	% Retained (A)	Cumulative % Retained	% Passing	Multiplier (B)	Product (A*B)
2360	0.1	0.1	0.1	99.99	4.2	0.42
1180	8.4	8.5	8.6	91.4	9.1	77.4
600	23.7	23.9	32.5	67.5	20	478
300	31.8	32.0	64.5	35.5	40	1280
150	30.3	30.5	95	5	70	2135
75	4.6	4.6	99.6	0.4	140	644
Pan	0.4	0.4	100	-	300	120
TOTAL	99.3	100				4734.82

3.3. Acid demand value

The Acid Demand Value (ADV) test diagnoses acid soluble content of moulding sand, e.g. CaO and K₂O, and is critical for furan no-bake (FNB) systems which are acid catalysed. Any such material in the sand would end up being hydrolysed by the catalyst, increasing overall catalyst consumption and escalating process costs [5, 16]. Obviously, the ADV of moulding sand should ideally be low with <6 ml desirable when using no-bake resin binder systems [5]. Fig. 2 portrays that the maximum acid demand value was 2.73 ml which is quite low indicating that this

3. Results and discussion

3.1. Chemical analysis of moulding sand

Table 2 summarises the X-ray fluorescence results. The moulding sand contained 90 % silica (SiO₂) with favourably low alkali oxides (CaO and K₂O), iron oxide (Fe₂O₃) and titania (TiO₂) concentrations. Excessive lime is not good in moulding sands as it raises the acid demand value which poses problems when moulding with acid catalysed binders like Furotec 132 resin.

mould making. Size-frequency and cumulative distribution curves are presented in Fig. 1. Sand morphology is known to affect the quality of castings and as such, is an important parameter in a sand casting foundry [14, 15]. The sand grains shape could best be described as rounded with medium sphericity which is desired for high flowability and permeability. This sand is best classified as bank sand suitable for cores and as base for synthetic moulding sand [6].

sand was suitable for the Furotec 132 resin binder + Furocure CH Fast acid/Furocure CH Slow acid system.

3.4. Curing properties of the Furotec 132 resin bonded sand

The bench life, strip time and maximum compression strength were inferred from the relevant compression strength vs. time curves.

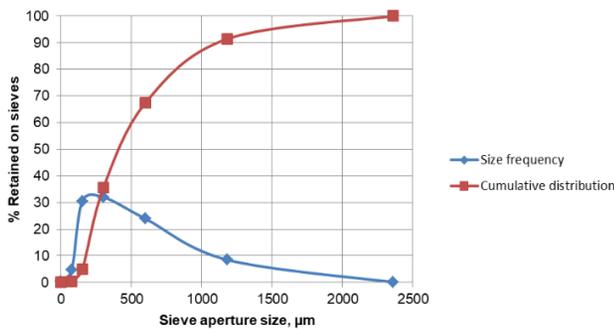


Fig. 1. Curves constructed from the sieve analysis of the moulding sand comparing size-frequency and cumulative distribution curves

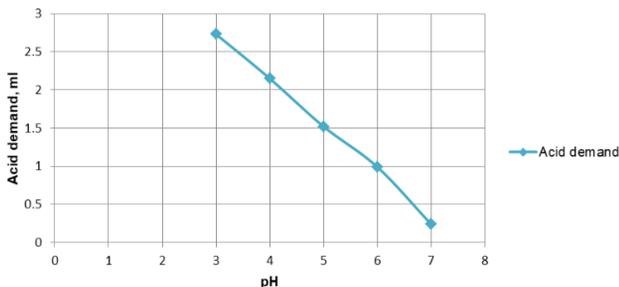


Fig. 2. Acid demand curve

3.4.1. Bench life and strip time

The bench life curve of the Furotec 132 resin bonded sand at 30% Furocure CH Fast acid catalyst addition is depicted in Fig. 3. The curve is aptly described ($R^2 = 0.9916$) by the polynomial trendline equation 1:

$$UCS = 7.3599t^2 + 91.344t - 0.0904 \quad (1)$$

Where UCS is the uniaxial compressive strength in N/cm^2 , and t is the curing time in minutes.

This equation was solved in MS Excel Solver to determine the bench life and strip time of the chemically bonded sand. These parameters are presented in Table 4.

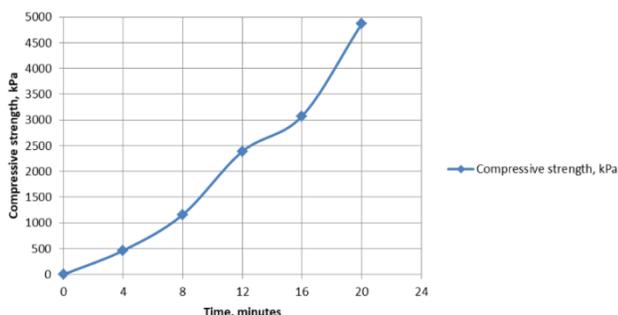


Fig. 3. Bench life curve for Furotec 132 resin bonded sand at 30% Furocure CH Fast acid catalyst addition rate

Table 4.

Furotec 132 resin binder + 30 % Furocure CH Fast acid catalyst system curing properties

Parameter	Time, minutes
Bench life	0.1
Strip time	3.1

The strip time of the chemically bonded sand when employing the Furotec 132 resin binder + Furocure CH Slow acid catalyst system is of the order of ± 2 hours. Using a *bench life:strip time ratio* of 0.1:3.1 from Table 4, the bench life is ± 3.87 minutes. Thus it gives longer bench lives and strip times than the fast acid catalyst system. Resultant mulled sand mixtures should be readily flowable and compactable. The longer strip times can also be an advantage for manual foundries especially those with small workforces so they can perform dedicated tasks sequentially. According to [5], short strip times call for high speed mixers and can result in sand build-up on the mixer blades which is unfavourable. The fast acid catalyst system did not yield meaningful results at 50% and 70% catalyst addition rates with the mulled sand being crumbly and extremely dry (Fig. 4), which can be explained by the high temperature rise causing rapid evolution of water due to the polycondensation curing reaction [16]. Curing rate of furan resin binders exponentially increases with acid catalyst concentration [17]. And the excessively high curing rate corresponds to a very low degree of resin curing [18], thus there is minimal sand binding. The condensation reaction occurring during the curing of a furan resin binder like Furotec 132 is fully described by [19].



Fig. 4. Picture of crumbly mulled sand obtained for Furotec 132 resin + 70% Furocure CH Fast acid

3.4.2. Maximum compressive strength

Fig. 5 simulates the time-dependent variation of the maximum compressive strength at varying catalyst levels. 30% Furocure CH Fast acid catalyst produced the highest maximum compressive strength. The particular curve starts from a remarkable high of $4513.3 N/cm^2$ at 1 hour, rises sharply to a peak of $7164.73 N/cm^2$ at 2 hours before steadily dropping to $5055.44 N/cm^2$ at the 6 hour

mark. These strength values conform to those described in [5]. Addition of the 20 g of resin to the dry sand and acid catalyst mixture caused the sand to turn dark green, then blue with a significant spike in temperature (38–42 °C). These colour changes are attributable to chromophores formation in the course of the curing reaction and signify fast cure [16]. [20] Offer a comprehensive and well-researched assessment of how these chromophores are formed. Strength curves for 50% and 70 % Furocure CH Fast acid catalyst show a much different trend. In Fig. 5 they are almost flush with the x-axis illustrating little change in maximum compressive strength relative to the dry unbonded sand. The respective test specimens crumbled at the touch of a finger (Fig. 6).

From Fig. 5, slow acid catalyst system strength curves exhibit a slow rise in the initial 2 hours followed by an exponential strength increase capping ~3000 N/cm² after 6 hours. Evidently the moulded sand has not reached its maximum compressive strength at the 6 hour mark meaning the curing reaction is still ongoing. Furotec 132 resin produces water during the acid-catalysed polycondensation reaction, and as a consequence the mulled sand fully cures only after all the water has evaporated [16]. The maximum compressive strength for this binder + catalyst system can surpass the 3000 N/cm² threshold given sufficient curing time of more than 6 hours. This can be demonstrated by fitting the data for the 30% Furocure CH Slow acid catalyst curve to an exponential trendline ($R^2 = 0.946$), Equation 2:

$$UCS = 165.47e^{0.4006t} \quad (2)$$

Where UCS is the uniaxial compressive strength in N/cm², and t is the curing time in minutes.

Solving this equation in MS Excel Solver after setting $UCS = 3000 \text{ N/cm}^2$ returns a curing time of 7.2 hours and 8.5 hours for $UCS = 5000 \text{ N/cm}^2$. These maximum compressive strength values are within the recommended range specified by [5].

Introduction of the Furocure CH Fast acid catalyst to the sand + Furotec 132 resin binder mixture triggered, as expected, an exothermal polymerisation reaction causing curing of the binder. Since the reaction is exothermic, it is very sensitive to sand temperature fluctuations [16], and increases with the temperature. The rate at which the Furotec 132 resin binder cured was much faster than when Furocure CH Slow acid catalyst was used. This supports the assertion by [10] that this rate varies with the acid catalyst and quantity, provided all the other moulding parameters are maintained. Evidently, the Furocure CH Fast acid catalyst is more potent, yielding a faster curing rate and rapid strength increase. But at higher than 30 % acid addition rates, the high temperature rise causes poor polymerisation and low mould compressive strength.

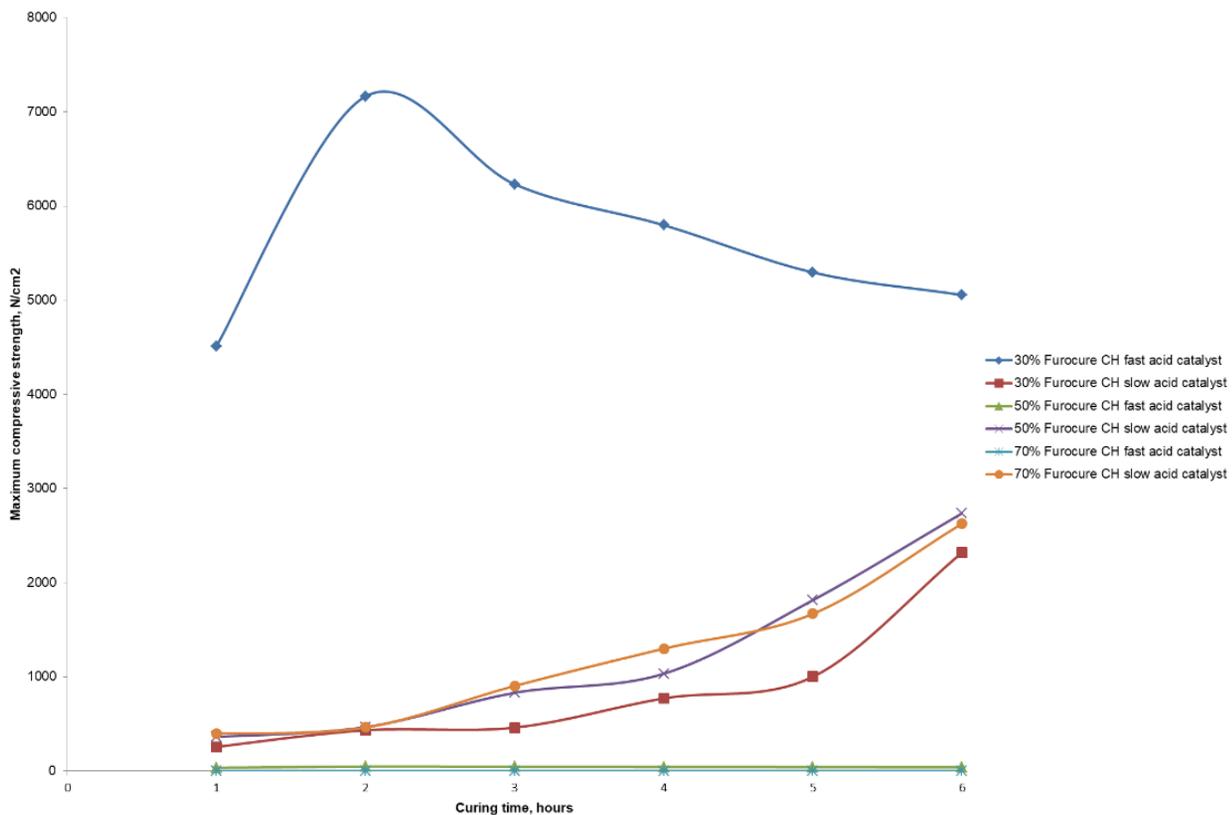


Fig. 5. Time variation of maximum compressive strength of Furotec 132 resin bonded sand catalysed by Furocure CH Fast acid and Furocure CH slow acid



Fig. 6. Picture of test specimen obtained for Furotec 132 resin bonded + 50% Furocure CH Fast acid

3.5. Statistical data analysis

On the basis of Two-Way Analysis of Variance (ANOVA) of the UCS data (Table 5), the null hypothesis is rejected because the F values are greater than the F -critical values and the P -values are less than α (0.05). The alternative hypothesis stating that the maximum compressive strength of the Furotec 132 resin bonded sand with Furocure CH Fast acid catalysis is not equal to that for Furocure CH Slow acid catalysis, thus supports these experimental findings. Fig. 5 and the compressive strength values determined in MS Excel Solver validate this assertion.

Table 5
Two-way Anova of compressive strengths after curing
Anova: Two-Factor With Replication

SUMMARY	30% catalyst	50% catalyst	70% catalyst	Total		
<i>slow</i>						
Count	6	6	6	18		
Sum	5245.633333	7247.34	7363.17667	19856.15		
Average	874.2722222	1207.89	1227.19611	1103.11944		
Variance	572414.9304	829011.9755	707313.976	648009.532		
<i>fast</i>						
Count	6	6	6	18		
Sum	34001.24	253.51	0.6	34255.35		
Average	5666.873333	42.25166667	0.1	1903.075		
Variance	898643.8618	10610.05602	2.3111E-34	7767482.41		
<i>Total</i>						
Count	12	12	12			
Sum	39246.87333	7500.85	7363.77667			
Average	3270.572778	625.0708333	613.648056			
Variance	6932942.745	752204.3936	732169.498			
ANOVA						
<i>Source of Variation</i>	<i>SS</i>	<i>df</i>	<i>MS</i>	<i>F</i>	<i>P-value</i>	<i>F crit</i>
Sample	5759360.018	1	5759360.02	11.4500396	0.0020073	4.17087679
Columns	56232239.99	2	28116120	55.8969551	7.62E-11	3.3158295
Interaction	71741148.98	2	35870574.5	71.3133922	3.983E-12	3.3158295
Within	15089974	30	502999.133			
Total	148822723	35				

4. Conclusions

The maximum compressive strength obtained with the slow acid catalyst is greater than that with the fast acid catalyst at 50 % and 70 % acid addition rates. While 30 % fast acid catalyst initially yields much higher maximum strengths than the equivalent slow acid catalyst, the strength declines progressively and ultimately after ~ 9 hours the two catalysts yield comparable strength values. Furotec 132 resin binder + 30 % slow acid catalyst will require curing times of ~8.5 hours for dry sand mould strengths of about 5000 N/cm² whereas Furotec 132 resin binder + 30 % fast acid catalyst yield dry sand moulds of comparable strength at 5055.44 N/cm² after a curing time of 6 hours. The slow acid catalyst system gives a longer bench life (± 3.87 minutes) and strip time (± 2 hours) than the fast acid catalyst system (bench life ~ 0.1 minutes and strip time ~3.1 minutes). Considering process economics and the observed moulding sand response to this binder system, 30 % by weight of Furotec 132 or much lower addition rates for both catalysts are recommended. The methodologies adopted for this study can be used with appropriate deviations by foundries utilising two or more binder systems with the goal of overall process optimisation and reduction of sand to-liquid metal ratios; or for evaluation of a new binder system during foundry process development. Future studies on the same binder system can extend the compressive strength measurements to 24 hours to have a better evaluation of the curing behaviour of moulded sand.

Acknowledgements

This work was accomplished with support from our university, local materials testing labs and FOSECO.

References

- [1] American Foundry Society. (2019, January). *Introduction to Foundry Sand*. Retrieved January 07, 2019, from <https://www.afsinc.org/introduction-foundry-sand>.
- [2] Břuska, M., Beňo, J., Cagala, M. & Jasinková, V. (2012). Dilatometric characterization of foundry sands. *Archives of Foundry Engineering*. 12(2), 9-14.
- [3] Grabowska, B., Malinowski, P., Szucki, M. & Byczyński, Ł. (2016). Thermal analysis in foundry technology: Part 1. Study TG–DSC of the new class of polymer binders BioCo. *Journal of Thermal Analysis and Calorimetry*. 126(1), 245-250.
- [4] Mashingaidze, M.M. & Nanyala, S.P.P. (2015). Suitability of sand from Oshanas in Ongwediva for use as mould material in sand casting foundries. In Proceedings of the National Research Symposium 2015, 23-25 September 2015 (pp. 99-101). Windhoek, Namibia: National Commission on Research, Science and Technology.
- [5] Brown, J.R. (Ed.). (2000). *Foseco ferrous foundryman's handbook*. Oxford: Butterworth-Heinemann.
- [6] Ammen, C.W. (1979). *The complete handbook of sand casting*. (1st ed.). New York: McGraw-Hill.
- [7] Grabowska, B. (2008). Biopolimers – structure, properties and applicability in the foundry industry. *Archives of Foundry Engineering*. 8(1), 51-54.
- [8] Kumaravadivel, A. & Natarajan, U. (2013). Optimization of sand-casting process variables – a process window approach. *The International Journal of Advanced Manufacturing Technology*. 66(5-8), 695-709. DOI: 10.1007/s00170-012-4358-y.
- [9] Grabowska, B., Holtzer M., Górný, M., Dańko R., & Grabowski, G. (2011). Microstructure and properties of test castings of cast iron made in moulding sands with the BioCo2 binder. *Archives of Foundry Engineering*. 11(4), 47-50.
- [10] Holtzer, M. & Dańko, R. (2015). Molds and cores systems in foundry. In M. Holtzer, M. Górný & R. Dańko (Eds.), *Microstructure and properties of ductile iron and compacted graphite iron castings* (pp. 27-42), Springer Berlin Heidelberg, Retrieved March 06, 2019, from SpringerLink https://link.springer.com/chapter/10.1007/978-3-319-14583-9_2.
- [11] Bureau of Indian Standards. (1997). *IS 1918: Methods of physical tests for foundry sands*. Indian Standards Institution. Retrieved November 08, 2018, from <https://law.resource.org/pub/in/bis/S10/is.1918.1966.pdf>
- [12] Van Den Berg, K. (2009). *Material Safety Data Sheet - Furotec 132*. Version 02. FOSECO South Africa.
- [13] Van Den Berg, K. (2009). *Material Safety Data Sheet - Furocure CH Fast*. Version 02. FOSECO South Africa.
- [14] Strobl, S. (2014). *The fundamentals of green sand preparation and control*. Simpson Group. Retrieved January 12, 2019, from <https://www.scribd.com/document/340709553/Rpt-sales-Fundamentals-of-Sand-Control>.
- [15] McLaws, I. (1971). *Uses and specifications of silica sand*. Research Council of Alberta. Retrieved March 07, 2019, from http://www.ags.gov.ab.ca/publications/ESR/PDF/ESR_1971_04.pdf.
- [16] Mancuso, G. (2005). *Process overview: chemistry and use of furan binders*. Mancuso Chemicals. Retrieved March 08, 2019, from <http://www.mancusochemicals.com/wp-content/uploads/2013/05/Furan-Binder-Use.pdf>.
- [17] Chanda, M. & Dinesh, S.R. (1978). Monitoring the Curing of Furan Resins through the Exothermic Heat of Reaction. *Die Angewandte Makromolekulare Chemie*. 69(1031), 85-98.
- [18] Zhang, J., Xu, Y. C. & Huang, P. (2009). Effect of cure cycle on curing process and hardness for epoxy resin. *eXPRESS Polymer Letters*. 3(9) 534-541.
- [19] Acharya, S.G., Vadher, J.A. & Kanjariya, P.V. (2016). Identification and Quantification of Gases Releasing from Furan No Bake Binder. *Archives of Foundry Engineering*. 16(3), 5-10.
- [20] Choura, M., Belgacem, N. M. & Gandini, A. (1996). Acid-catalyzed polycondensation of furfuryl alcohol: mechanisms of chromophore formation and cross-linking. *Macromolecules*. 29(11), 3839-3850. DOI: 10.1021/ma951522f.