

ON THE NEWTONIAN THERMAL ANALYSIS OF CASTING: A CRITICAL APPROACH.

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ABSTRACT

One of the primary aims of Newtonian thermal analysis (NTA) is the prediction of latent heat and finding solid fraction. When the prediction is made, Newtonian baseline (NBL) is computed, and the difference to experimental cooling rate curve is analyzed.

In this study, it was seen that NBL calculations had some contradictions and that latent heat calculations gave high errors. After determining these contradictions, a new method, called one-capacitive-system baseline (OCSBL), was developed by gathering the solution advises to each other. Cooling curve of mold-insulated pure Tin was analyzed by both methods to test them. It was seen that OCSBL predicted the latent heat better than NBL when the results were compared with the literal values.

Keywords: *Newtonian thermal analysis, solid fraction, latent heat*

METAL DÖKÜMLERİNİN NEWTON SALISI ANALİZİ ÜZERİNE: ELEŞTİREL BİR YAKLAŞIM

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ÖZET

Döküm için Newtonsal ısı analizinin başlıca amaçları arasında ergime ısı tahmini ve katı kesrinin bulunması gelmektedir. Bu tahmin yapılırken Newton taban eğrisi (NTE) hesaplanıp deneysel soğuma eğrisi arasındaki fark analiz edilmektedir.

Bu çalışmada, Newton taban eğrisi hesaplamasının bazı çelişkileri barındırdığı ve ergime ısı hesaplarının yüksek hatalar verdiği görüldü. Bu çelişkiler tespit edildikten sonra, her birine getirilen çözüm önerileri derlenerek, tekli-kapasitif-sistem taban eğrisi (TKSTE) adında yeni bir yöntem geliştirildi. İki yöntemi test etmek için, kaptan yalıtılmış saf kalayın soğuma eğrisi iki yöntemle de analiz edildi. Sonuçlar literatürdeki termal değerler ile kıyaslandığında, TKSTE nin NTE den daha iyi ergime ısı tahmin ettiği görüldü.

Anahtar Kelimeler: *Termal Analiz, Ergime Isısı, Katı Kesri*

1. INTRODUCTION

Newtonian thermal analysis (NTA) for casting aims to compute latent heat and solid fraction evolution of a solidifying metal by analyzing cooling data. For this purpose, a hot melt is poured into a mold, and temperature is recorded by a thermocouple at every second while the sample is cooling and solidifying [1]. One of the techniques that has been frequently used is computer aided cooling curve analysis (CA-CCA). It requires complicated mathematical tools and sophisticated computer software to analyze the temperature data [2]. The main equation for defining thermal characteristics of the sample is Newton's Law of Cooling (NLC). NLC simply states that the rate of heat loss is proportional to the temperature difference between the sample and ambient.

$$\frac{dQ_{loss}}{dt} = -hA(T - T_a) \quad (1)$$

where dQ_{loss}/dt is the rate of heat loss of the sample, A is effective surface area of the sample, h is heat transfer coefficient between the hot sample and ambient, and T_a is the ambient temperature [3]. NLC (1) describes simple cooling without any source terms that may be caused by thermal reactions such as phase transformation. However, the main point in NTA procedure is to analyze solidification. Therefore, mathematical description of the phase transformational heat rate must be included to the equation. For this purpose, solid fraction is used to represent this source term by the help of latent heat. The rate of heat in a solidification process is given by

$$\frac{dQ_L}{dt} = mL_f \frac{df_s}{dt} \quad (2)$$

where Q_L is the heat arising from latent heat release, m is the mass of sample, L_f is latent heat of fusion, and f_s is solid fraction [4]. As a result, Equation 1 and 2 may be combined in the definition of net heat rate of the sample.

$$\frac{dQ_{net}}{dt} = \frac{dQ_{loss}}{dt} + \frac{dQ_L}{dt} \quad (3)$$

By the definition of net heat change in terms of specific heat, Equations 1, 2, and 3 yield

$$mc_p \frac{dT}{dt} = -hA(T - T_a) + mL_f \frac{df_s}{dt} \quad (4)$$

$$\frac{dT}{dt} = -\frac{hA}{mc_p}(T - T_a) + \frac{L_f}{c_p} \frac{df_s}{dt} \quad (5)$$

where c_p is the specific heat of the sample.

Equation 5 roughly explains a typical cooling process of a solidifying metal from pouring temperature to cold solid phase. From the temperature data recorded in the NTA experiment, the coefficients of the equation are computed by the curve fitting for zero curve (or baseline). Baseline is the hypothetical curve under the assumption of no-phase transformation [5]. In the case of no-phase transformation, Equation 1 is assumed valid, and the solution for cooling rate as a function of time defines a zero curve. This solution, which is in the form of exponential decay, is given by

$$\left(\frac{dT}{dt} \right)_{NBL} = ae^{-bt} \quad (6)$$

where a and b are the parameters that may be calculated experimentally, and the subscript denotes Newtonian baseline (zero curve). They are defined as:

$$b = \frac{hA}{mc_p}, \quad a = -(T_0 - T_a) \frac{hA}{mc_p} \quad (7)$$

Newtonian baseline (NBL), in Equation 6, has exponential form so its coefficient can be computed by curve fitting tools of any mathematical software by excluding the solidification region of dT/dt curve. After obtaining the coefficients, latent heat and solid fraction are computed by the difference between NBL and the experimental cooling curve. Since the values of solid fraction at the start and end times of solidification (t_s and t_e) are zero and unity respectively, this difference can be found by integrating both sides between t_s and t_e .

$$L_f = c_p \int_{t_s}^{t_e} \left[\left(\frac{dT}{dt} \right)_{\text{exp}} - \left(\frac{dT}{dt} \right)_{NBL} \right] dt \quad (8)$$

$$f_s = \frac{c_p}{L_f} \int_{t_s}^t \left[\left(\frac{dT}{dt} \right)_{\text{exp}} - \left(\frac{dT}{dt} \right)_{\text{NBL}} \right] dt \quad (9)$$

where t_s and t_e are the start and end times of solidification [6]. Graphical expression of Equations 8 and 9 are shown in Figure 1. Latent heat per specific heat (L_f/c_p) is the area between two curves in the interval $t_s < t < t_e$ while f_s is the cumulative area between t_s and t .

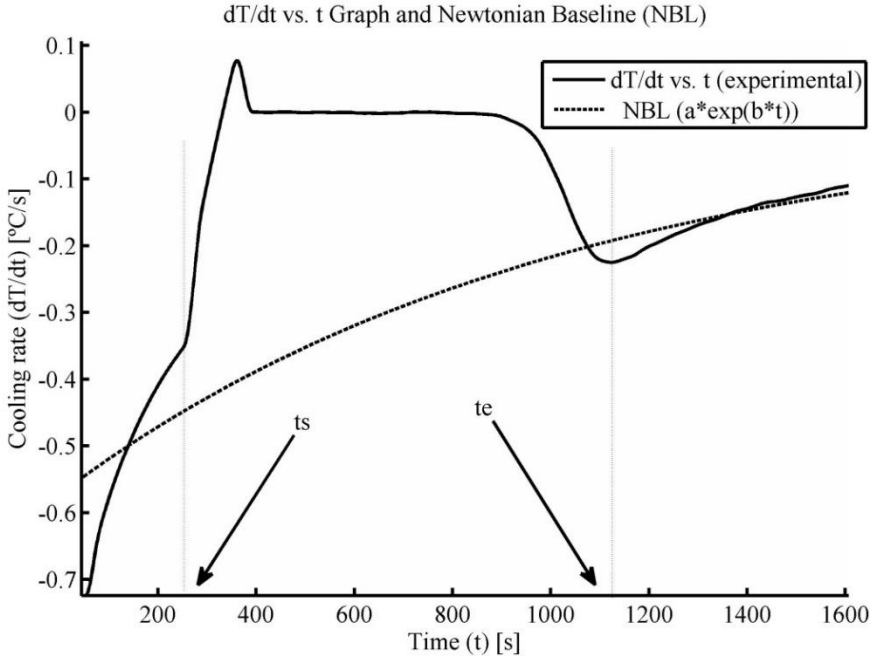


Figure 1. Cooling rate curve and Newtonian baseline (NBL). Start and end time of solidifications are denoted by t_s and t_e respectively.

2. EVALUATION OF NTA

Newtonian zero curve method has some theoretical contradictions and limitations. It does not consider the thermal capacity of the mold, and therefore, the temperature of mold. It could be neglected if the mold's capacity were very smaller than metal's capacity. Emadi et.al. reported that they used a crucible whose thermal mass was less than 0.5% of the total thermal mass of the system [7]. Yet, the thermal capacity of resin-coated sand molds used in this study were measured 117 J/K, while that of pure

tin is 83 J/K. Therefore, it is voluntary to eliminate the effects of thermal capacity of the mold in the experiments.

The lack of standards on the choice of temperature interval and curve fitting methodology is another restriction of NTA. Different choice of the temperature intervals around solidification affects the outputs of curve fitting, and certainly, the results of latent heats. It is observed that different trials of latent heat calculations by several data inclusions gave inconsistent results. Narrower intervals may be somewhat reliable, but they did not work at every attempt [1].

Moreover, NBL requires data smoothing in case time derivative of cooling curve could be plotted. Whereas, smoothing of the temperature data and its limits are variable for the choice of researchers. More smoothed data results in a smooth but deviated derivative. It deforms the original data, so it gives incidental outputs at every different trial of smooth parameters.

NBL uses exponential decay as a choice of zero-curve. Equation 6 is tried to fit the cooling rate curve in the non-solidification part. However, the integration constant “a” in (6) should be particular to solid and liquid region because it comes from the initial conditions of (5). In fact, the correct solution of the differential equation in (5) should be (10) or (11).

$$\left(\frac{dT}{dt}\right)_{z_c} = (a_s \theta(t - t_e) + a_L \theta(t_s - t)) e^{-bt} \quad (10)$$

$$\left(\frac{dT}{dt}\right)_{z_c} = \begin{cases} a_s e^{-bt} & \text{solid phase} \\ a_L e^{-bt} & \text{liquid phase} \end{cases} \quad (11)$$

where a_S and a_L are the integration constants for solid and liquid phases, θ is Heaviside step function, and z_c denotes zero curve (or baseline). Alternatively, this contradiction can be expressed graphically. In figure 2, experimental dT/dt graph and expected no-solidification theoretical curve are shown. If there were no solidification, the cooling rate curve would continue on a different path in the solid region.

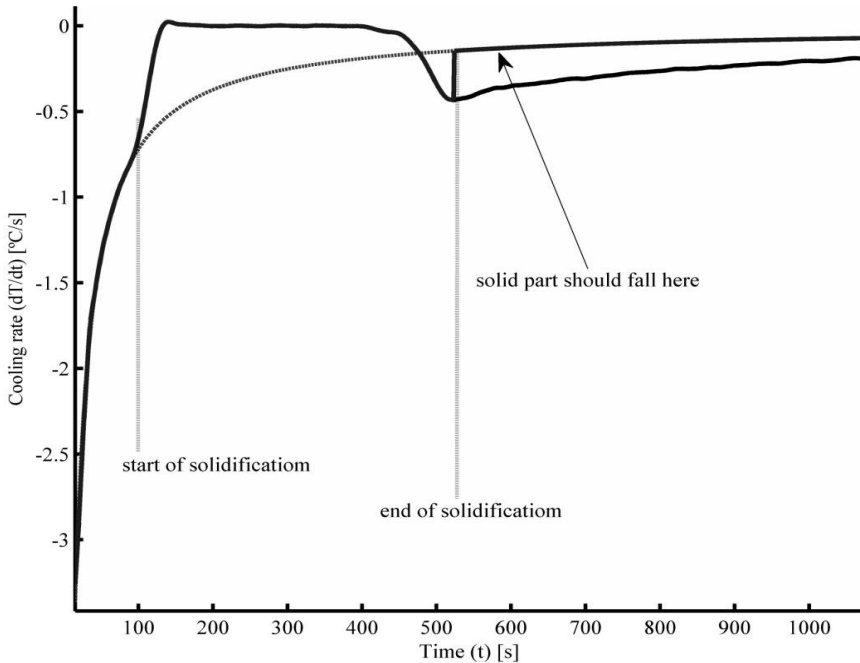


Figure 2. Cooling rate (dT/dt) with respect to time and the virtual curve if solidification did not occur.

Another restriction of NBL may be the lack of radiative terms or other temperature dependent effects. Cooling with radiation requires nonlinear temperature terms in Equation 5, and therefore, zero curve definition [8]. Temperature dependent heat transfer coefficients and/or specific heat are other effects having contributions to zero curves [9, 10].

- In summary, the critics of NTA may be listed as follows:
- Effects of thermal capacity of the mold should be eliminated.
- Temperature interval or other variations in the analysis should be standardized.
- Smoothing, therefore differentiating the cooling curve, should be avoided
- Different initial conditions, which are special to solid and liquid phases, should be taken into account.
- Cooling with radiation or other temperature dependent effects such as varying specific heat should be studied.

All of the critics above were considered to propose an alternative model to NTA. This model is named One-capacitive-system baseline (OCSBL) and explained in the next chapter. This model may be applied to small-thermal-mass-crucible experiments or the experiments with thermal insulation between the metal and mold to eliminate mold's effects.

3. ONE-CAPACITIVE-SYSTEM BASELINE

Considering very complicated nonlinear temperature contributions to the differential equation, one can start with to write the cooling rate as a function of temperature (Equation 12). Function F represents the contributions from radiation and other temperature-dependent-parameter effects. Then, Equation 5 becomes:

$$\frac{dT}{dt} = F(T) + \frac{L_f}{c_p} \frac{df_s}{dt} \theta_{PT}(t) \quad (12)$$

$\theta_{PT}(t)$ defines the validation interval of solid fraction. It is given by

$$\theta_{PT}(t) = \begin{cases} 1 & t_s < t < t_e \\ 0 & otherwise \end{cases} \quad (13)$$

This intricate function F can be represented by the first degree Taylor polynomial about melting temperature. Equation 12 can be redefined with new coefficients b and c different from their original meaning: heat transfer coefficients and ambient temperature.

$$\frac{dT}{dt} = -b(T - c) + \frac{L_f}{c_p} \frac{df_s}{dt} \theta_{PT}(t) \quad (14)$$

From now on, one should not expect that the parameters b and c correspond to thermal coefficients and the ambient temperature. Equation 14 is a first order linear differential equation and solved by the help of integration factor [11]. The solution is summarized in Equations 15-18.

$$\left[\frac{dT}{dt} + b(T - T_a) \right] e^{bt} = e^{bt} \frac{L_f}{c_p} \frac{df_s}{dt} \theta_{PT}(t) \quad (15)$$

$$\frac{d}{dt} [e^{bt} (T - T_a)] = e^{bt} \frac{L_f}{c_p} \frac{df_s}{dt} \theta_{PT}(t) \quad (16)$$

$$e^{bt} (T - T_a) - (T_0 - T_a) = \int_0^t e^{bt} \frac{L_f}{c_p} \frac{df_s}{dt} \theta_{PT}(t) dt \quad (17)$$

$$T = T_a + \left[T_0 - T_a + \int_0^t e^{bt} \frac{L_f}{c_p} \frac{df_s}{dt} \theta_{PT}(t) dt \right] e^{-bt} \quad (18)$$

Since $\theta_{PT}(t)$ is zero in the single phase interval, the integral in Equation 18 gives different constants (a_S and a_L) for the expression of single phase temperature (TSP).

$$T_{SP} = (a_S \theta(t - t_e) + a_L \theta(t_s - t)) e^{-bt} + c \quad (19)$$

This single phase definition of temperature can be fitted to experimental temperature data in the no-solidification interval ($t < t_s$ and $t > t_e$). Curve fitting outputs give the required parameters b and c , and a new zero curve, called One-Capacitive-System Baseline (OCSBL), is defined by the help of Equation 14 as follows:

$$\left(\frac{dT}{dt} \right)_{OCSBL} = -b(T_{exp} - c) \quad (20)$$

where T_{exp} is the experimental data recorded from the temperature measurement. The rest of the procedure is the same with Equations 8 and 9.

Main points for this analysis is to select a narrow temperature interval around melting point and to set ambient temperature, represented by c , free because the first order Taylor series approximation requires a narrow region. Terms in Taylor series distort the parameters from their intended meanings. That is, the parameter c may be computed by curve fitting tool different from the ambient temperature.

4. THE EXPERIMENT

This new baseline was tried on an experiment that was made by pure Tin in an insulated mold. The temperature range 50 oC below or above melting temperature was selected as analysis interval. When Equation 19 was tried

to fit temperature data in the interval, the outputs were obtained as in Figure 2 and Table 1.

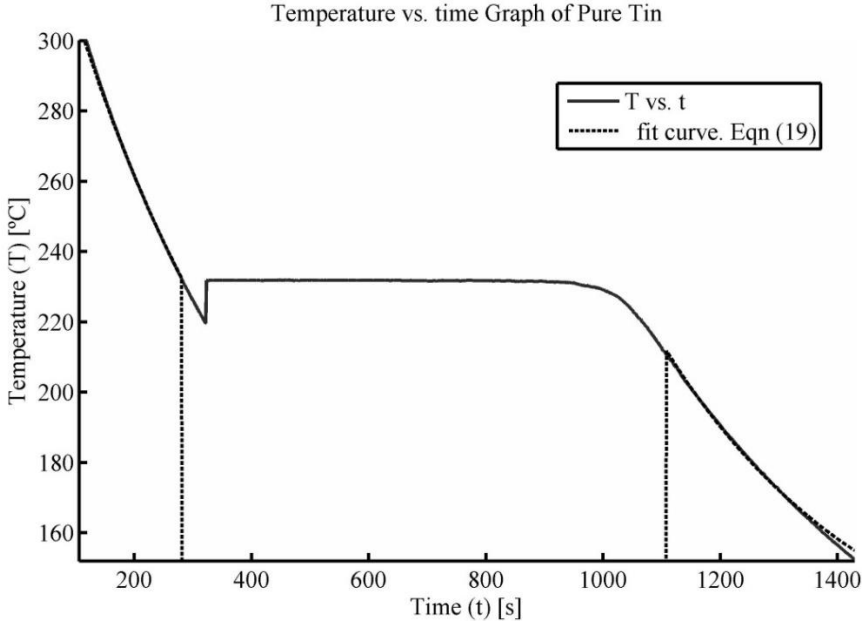


Figure 3. Temperature vs. time graph and OCSBL.

Table 1. Output of curve fitting tool of MATLAB R2010a.

General model	Goodness of fit
$T(t) = (as * \exp(-b * t) + c) * \text{heaviside}(t - 1107) + (al * \exp(-b * t) + c) * \text{heaviside}(282 - t)$	
Coefficients (with 95% confidence bounds):	
al = 253.7 (253.3, 254.2)	SSE : 56.02
as = 2010 (1963, 2056)	R-square : 0.9999
b = 0.002733 (0.002705, 0.002761)	Adjusted R-square : 0.9999
c = 114.5 (113.7, 115.3)	RMSE : 0.3886

5. RESULTS AND DISCUSSION

After obtaining the parameters b and c from Table 1, it was put in Equation 20 to get zero curve. Latent heat per specific heat and solid fraction were calculated by Equation 8 and 9. Latent heat per specific heat value (Lf/cp) for pure Tin (Sn) was calculated 240 K by OCSBL. Solid fraction evolution in time is shown in Figure 4.

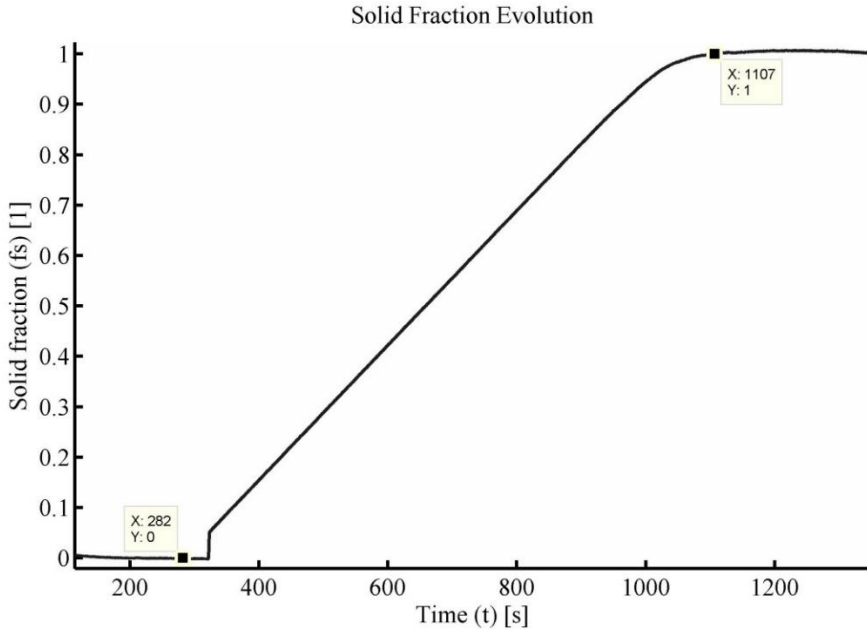


Figure 4. Solid fraction for pure Sn calculated by OCSBL.

For comparison, the literal values of latent heat of pure Sn and the value calculated by NBL were also found. Result of NBL was made by the zero curve method explained in the first Chapter. The literal value was found by Perry’s Chemical Engineering Handbook [12]. These data is listed in Table 2.

	OCSBL	NBL	LITERAL
Specific heat (solid phase) [cal.mol-1.K-1]	-	-	7.24
Specific heat (liquid phase) [cal.mol-1.K-1]	-	-	6.60
Specific heat (average) [cal.mol-1.K-1]	-	-	6.92
Latent heat [cal.mol-1]	-	-	1720
Latent heat per specific heat [K]	240	217	249

Table 2: Thermal properties of pure Sn. Average specific heat was calculated by averaging solid and liquid phase values at melting temperature (504 K). This average value was used in literal latent heat per specific heat.

As seen in Table 2, OCSBL predicted better result than NBL for the estimation of latent heat. Literal average of L_f/c_p value is calculated 240 K about melting point. NBL and OCSBL computed this value 217 and 240 respectively. Their percentage errors are -13% and -3.6% respectively. The temperature ranges of both methods were set to 50 degrees above and below melting point. Changing the range yielded different outputs. For example, NBL and OCSBL gave 229 and 250 K when the range was taken 100 degrees above and below melting point.

One of the advantages of OCSBL is that it does not need deriving temperature data. Differentiating temperature with respect to time requires no standardized choices for the sake of smoothing. More smoothed data does not represent original experiment. Therefore, it should be discussed whether smoothing is ethical or not. Since there is no need to derivative, smoothing is not used in OCSBL.

6. CONCLUSION

NTA for casting was evaluated from different perspectives. After the evaluation, the suggested method, OCSBL, was seen a better predictor for latent heat than NBL.

It was seen that the primary restriction of NBL was not to include different initial conditions for solid and liquid phases. Since the definition of the baseline, in fundamental, is based on no phase transformation case, it can not be represented by single phase region that omits solidification region. Solidification intervenes between solid and liquid phases, therefore initial condition is jumped to a new outset. This failure of NBL is corrected by choosing different integration constants for each phase in the mathematical representation of baseline.

Another failure of NBL originates from taking derivative of temperature with respect to time. Because of noisy temperature data, NBL has to make smoothing. However, smoothing deforms the original data, and deviates the derived curve from its original values. In the new model, there is no need to derivative and smoothing. OCSBL uses the cooling curve itself for analysis.

Determination of temperature range for thermal analysis was detected another restriction. There are no standards for choosing proper temperature interval. Different choices of ranges produce different latent heat results. The range should be so small that differential equation can be explained by the first degree polynomial, but so wide that curve fitting can take enough information about temperature data. In this study, 100 oC above and below melting temperature arose an advisable temperature range.

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