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A MATHEMATICAL MODEL AND COMPUTER SIMULATIONS FOR PREDICTING THE RESPONSE OF ALUMINUM CASTING ALLOYS TO HEAT TREATMENT

ChangKai (Lance) Wu[1], Makhlouf M. Makhlouf[1]
[1]Advanced Casting Research Center; Worcester Polytechnic Institute (WPI); 100 Institute Rd. Worcester, MA 01609, USA

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Abstract

In this publication we report on our efforts to develop a mathematical model and the necessary material database that allow predicting physical and material property changes that occur in aluminum casting alloys in response to precipitation-hardening heat treatment. We use the commercially available finite element software ABAQUS and an extensive database that was developed specifically for the aluminum alloy under consideration – namely, A356.2 alloy. The model produces multiple outputs at each node including the thermal history of the component that develop in the component and mechanical properties.

Introduction and Background

The objective of this work is to develop a model and the necessary material database that allow predicting the physical and material property changes that result from precipitation hardening heat treatment. The structure of the model is described in Figure 1. First, a thermal analysis module that makes use of an extensive database which includes the necessary initial conditions, boundary conditions, quenching heat transfer coefficients, and thermal properties calculates the time-temperature changes that the component experiences in response to quenching. A second thermal analysis module calculates the changes that occur in the component in response to the aging step. A third module makes use of the calculated thermal history of the component during the quenching and aging steps to predict the hardness of the component after aging. This calculation is done by combining a Quench Factor Analysis [1] and the well-known Shercliff and Ashby equations [2].

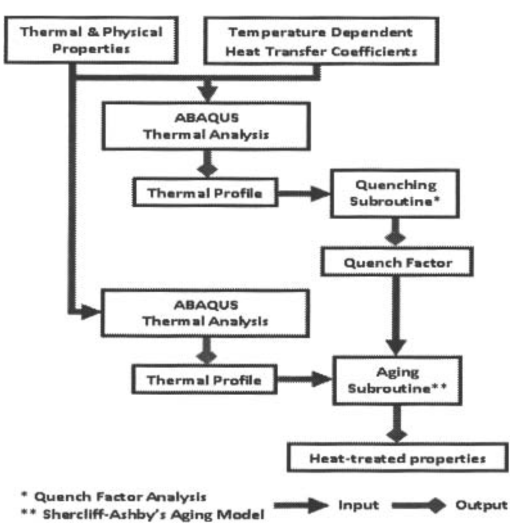


Figure 1. The structure of computer model.

The Quench factor Analysis

The Classical QFA model – The classical QFA model is based on using isothermal precipitation kinetics (i.e., it assumes that the reactions are iso-kinetic) to predict the results of non-isothermal conditions during continuous cooling. It considers the cooling curve to be made up of a series of isothermal transformation steps, and then adds up the amount of material transformed during each one of these isothermal steps in order to simulate the overall degree of supersaturation of the alloy. The classical QFA method also assumes that the vacancies and solute atoms that are lost during quenching[1] do not contribute to strengthening. Scheil [3] was the first to propose the additive nature of the cooling curve to describe nucleation during phase transformation; and Cahn [4, 5] showed that transformations that occur by heterogeneous nucleation often obey the classic Johnson-Mehl-Avarmi-Kolmogorov (JMAK) equation [6], and he also showed that the kinetics of continuous transformations can be successfully predicted from the kinetics of isothermal transformations. For continuous transformations, the isothermal holding time (t) in the JMAK equation may be replaced by the Quench Factor (Q) [1], as shown in Equation (1), where σ is the predicted peak property, σ_{min} and σ_{max} are the minimum and maximum values of the property achievable for the alloy, respectively, K_1 is a constant, and n is the Avrami exponent.

$$\frac{\sigma-\sigma_{min}}{\sigma_{max}-\sigma_{min}} = [exp(-K_1 Q)]^n \quad (1)$$

In obtaining the quench factor (Q), the incremental quench factor (q_f) is calculated for each increment on the cooling curve as the ratio of the time that the material spends at the specific temperature (Δt_i) divided by the critical time that is required in order for a certain amount of transformation to occur at that temperature (ΔC_{ti}). The summation of the incremental quench factors over the entire transformation temperature range is the cumulative Quench Factor (Q) [7] as shown in Equation (2).

$$Q = \sum q_f = \sum_{T_i}^{T_j} \frac{\Delta t_i}{C_{ti}} \quad (2)$$

In order to calculate the cumulative Quench Factor (Q), the critical time over the entire transformation temperature range must be known. One way of representing the critical time is by a time-temperature-property (TTP) curve. This curve is often referred to as the 'C' curve of the material. The TTP curve is a graphical representation of the transformation kinetics that influences the material's mechanical properties and defines the time that is required to precipitate sufficient solute to alter the strength of the material by a specified amount. The C curve may be defined mathematically by the critical time function (C_t), which is given

[1] By precipitation as coarse heterogeneously nucleated particles of the equilibrium phase.

by Equation (3), where C_t is the critical time required to form a specific quantity of a new phase, typically 0.5%, and K_1 to K_5 are constants that depend on the mechanical properties of the material [8]. K_1 is equal to the natural logarithm of the fraction of material which is untransformed during quenching, K_2 is related to the reciprocal of the number of nucleation sites, K_3 is related to the energy required to form a nucleus (J/mol K), K_4 is related to the solvus temperature (K), and K_5 is related to the activation energy for diffusion (J/mol), R is the universal gas constant (J/mol K), and T is absolute temperature (K).

$$C_t = -K_1 K_2 exp\left[\frac{K_3 K_4{}^2}{RT(K_4 - T)^2}\right] exp\left[\frac{K_5}{RT}\right] \tag{3}$$

The Rometsch's model – Based on the original QFA model, Rometsch [9] suggested that some of the assumptions in the classical QFA model may be invalid. One of those "invalid" assumptions is the linear relationship between strength and the amount of solute in the matrix which is available for precipitation. Therefore, based on results of experiments [2, 10-14], he proposed that the development of strength in a precipitation hardened metallic component should be proportional to the square root of the volume fraction of precipitate, so that the maximum achievable strength for any given alloy may be described by Equation (4).

$$\frac{\sigma - \sigma_{min}}{\sigma_{max} - \sigma_{min}} = [exp(-K_1 Q)]^{\frac{1}{2}} \tag{4}$$

The Non-isokinetic model – In the classical QFA model, the rate of precipitation is assumed to be a function of temperature and the amount of precipitate that forms. However, Flynn and Robinson [15] proposed that the rate of precipitation is also related to the amount of solute that remains in the matrix, which is temperature dependent. Therefore, they suggested a non-isokinetic QFA model in which the minimum strength is related to the concentration of the solute as given by Equations (5) to (8). In these Equations, $\Delta\sigma_j$ is the loss of an incremental amount of strengthening capability (MPa), Δt_j is the time interval, C_t is the critical time described in Equation (3), $\sigma_{min}(T)$ is the minimum obtainable strength, σ_{int} is the solutionized strength, T_{int} is the minimum solution temperature required, and K_6 and K_7 are new material constants.

$$\sigma = \sigma_{max} - \sum_{j=1}^{j=n} \Delta\sigma_j \tag{5}$$

$$\Delta\sigma_j = \left(\sigma_{j-1} - \sigma_{min}(T_j)\right)\left[1 - \exp\left[-\frac{\Delta t_j}{C_t(T)}\right]\right. \tag{6}$$

$$\sigma_{j-1} = \sigma_{max}(T_j) = \sigma_{max} - \sum_{n=1}^{n=j-1} \Delta\sigma_n \tag{7}$$

$$\sigma_{min}(T) = \sigma_{int} + K_6\left(\exp\left(-\frac{K_7}{T}\right) - \exp\left(-\frac{K_7}{T_{int}}\right)\right) \tag{8}$$

The Aging Database

An alloy-specific database is necessary for accurately modeling the heat-treated strength after aging. Generating such an extensive database can be very time-consuming and labor-intensive. However, Shercliff and Ashby [2] developed an efficient method for populating the database and since its introduction in 1990, the Shercliff-Ashby method has been employed successfully to obtain the as-aged properties (e.g., hardness, strength, etc.) of many aluminum alloys. The Shercliff-Ashby method calls for the use of dimensionless variables to significantly reduce the number of measurements that is required for constructing the complete aging behavior of an alloy. As shown in Figure 2, the Shercliff-Ashby method uses few data points (measurements) from different aging temperatures as input and it "calibrates" some material-dependent unknown parameters that can be used to construct the complete aging behavior of the alloy. The method assumes that the as-aged alloy properties (e.g., strength or hardness) is a sum of the intrinsic property of the material (σ_i), hardening due to formation of a solid solution ($\Delta\sigma_{ss}$), and hardening due to second phase precipitates ($\Delta\sigma_{ppt}$). This is represented mathematically by Equation (9).

$$\sigma(t, T) = \sigma_i + \Delta\sigma_{ss} + \Delta\sigma_{ppt} \tag{9}$$

In this work, a new approach was adopted to facilitate coupling the Quench Factor Analysis with the Shercliff-Ashby aging model. In this approach, instead of measuring the maximum achievable strength (i.e., σ_{max}) for each one of the aging conditions under consideration, the as-aged strength as given by the Shercliff-Ashby model is used. This is accomplished by re-defining (σ_{max}) in Equations (1, 4 and 5) so that it becomes available to the Quench Factor Analysis.

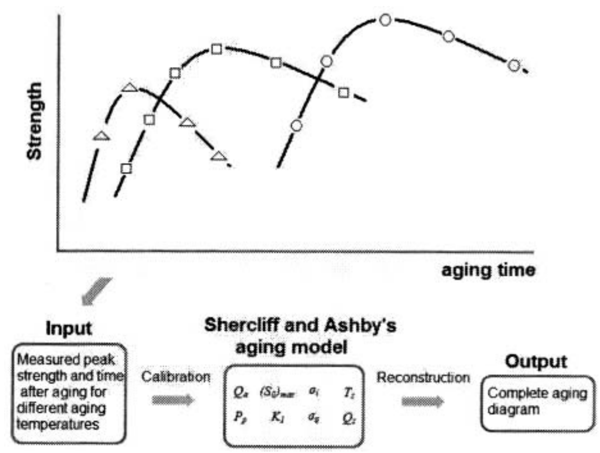


Figure 2. The Shercliff-Ashby method.

Materials and Procedures

Materials

Aluminum casting alloy A356.2 is used to demonstrate the procedure for obtaining the necessary database and modeling the response of aluminum alloy cast components to heat treatments. The data includes mechanical properties, thermal conductivity and heat transfer coefficients for the various steps of precipitation strengthening heat treatment as functions of temperature. Other required thermal and physical properties, such as density, specific heat and thermal expansion coefficients, were obtained from JMatPro Software[2].

[2] Developed and marketed by Sente Software Ltd., Surrey Technology Centre, 40 Occam Road, GU2 7YG, United Kingdom.

Procedures

Measurement of thermal conductivity and quenching heat transfer coefficients – Measurement of the alloy's thermal conductivity is described in detail elsewhere [16].

Determination of the kinetic parameters – The required kinetics parameters K_1, K_2, K_3, K_4, and K_5 that appear in the C_t function described in Equation (3), are measured and calibrated. For determining the K constants, the maximum and minimum aged-hardness was needed. Therefore, the aging curve was obtained by measuring the Rockwell Hardness F scale (HRF)[3] of the alloy. The measured results are shown in Figure 3. Error bars indicate standard deviations. The smoothed curve was averaged by adjacent averaging method of 10 points. In order to obtain this data, small identical samples of A356.2 alloy were solutionized at 538°C (1000°F) for 12 hours and then quenched into ice water. These samples represent the maximum possible quenching rate. Subsequently, the samples were aged at 155°C (311°F) for different periods of time and their hardness was measured. The HRF hardness values were averaged from 20 to 40 measurements and the maximum value was found to be 93.3. It was achieved after 19 hours of aging. This number represents the maximum hardness value in Equation (1), (4) and (5); i.e., σ_{max}. The value for the minimum hardness in Equation (1), (4) and (5); i.e., σ_{min}, was obtained by furnace cooling the samples after solutionizing. The cooling rate in the furnace was found to be less than 0.2°C/s, and σ_{min} was found to be 20.7 HRF.

Subsequently, the Jominy End Quench test described in ASTM-A255 was used to determine the kinetics parameters. The experimental conditions are described in detail elsewhere [16]. HRF measurements were performed around the perimeter of each Jominy bar and therefore each measured hardness value was matched to a unique cooling condition. Because the measured Rockwell Hardness (HRF) is an arbitrary number with no physical meaning, the HRF values were converted into Meyer hardness [17] for the purpose of calculation and then they were converted back to HRF for the result presentation.

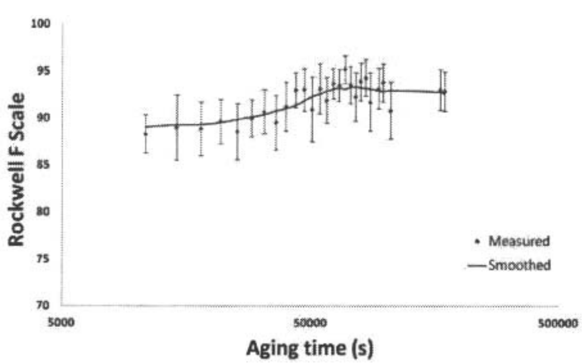


Figure 3. Measured HRF vs. aging time.

[3] The HRF measurements were performed with a steel ball indenter that is 1/16 inch (1.59 mm) in diameter and a minor and major load that are 98N and 491N, respectively.

The Classic QFA Model – For the classical QFA model, Equation (1) may be re-written as follows,

$$Q = \exp\left[\frac{\ln\ln\left(\frac{\sigma-\sigma_{min}}{\sigma_{max}-\sigma_{min}}\right)}{n} - \ln(-K_1)\right] \tag{10}$$

According to Equation (10), the Quench Factor (Q) can be determined from the measured hardness values (σ) provided that the σ_{max}, σ_{min}, Avarmi exponent (n) and the constant K_1 are known. Similarly, the Quench Factor (Q) also can be determined from the local cooling data and the C_t function. The C_t function is given by Equation (3), which can be re-written as follows,

$$Q = \sum_{T_i}^{T_j}\left[\frac{\Delta t_i}{-K_1K_2\exp\left[\frac{K_3K_4{}^2}{RT(K_4-T)^2}\right]\exp\left[\frac{K_5}{RT}\right]}\right] \tag{11}$$

Using matched data (hardness with cooling curve) from the Jominy End Quench test, the kinetic parameters K_1 to K_5 that appear in Equation (11) may be determined. Three out of the five unknown kinetics parameters; namely, K_1, K_4, and K_5, were fixed, and only K_2 and K_3 were made to vary [16] .

Various magnitudes for the Avarmi exponent, n, were used in Equation (10). These are: n = 1.5, 2.5 and 4.0; and in each case, the calculated Quench Factor in the Equation (10) was plotted against the Quench Factor calculated from Equation (11). Then the remaining unknown kinetics parameters; i.e., K_2 and K_3, in Equation (11) were continuously adjusted until the scatter best fitted a line that passes through the origin and makes a slope that equals to 1. This procedure allowed obtaining all kinetics parameters (K_1 through K_5) and the results are shown in Table I.

The Rometsch's QFA Model – Similarly, for the Rometsch's QFA model Equation (4) may be re-written as follows,

$$Q = 2\ln\left(\frac{\sigma-\sigma_{min}}{\sigma_{max}-\sigma_{min}}\right)\frac{-1}{K_1} \tag{12}$$

Using the same matched data from the Jominy End Quench test, followed the same fashion described above, a different set of kinetic parameters were also determined for the Rometsch's QFA model, and results are also shown in Table I.

The Non-isokinetic QFA Model – The non-isokinetic model requires some extra material constants, namely, σ_{int}, T_{int}, K_6 and K_7. Flynn and Robinson [15] assume that K_6 is a material constant related to the solute content of the alloy and K_7 is a material constant related to the standard enthalpy of the alloy, σ_{int} is the annealed strength and T_{int} is a minimum temperature limit; below this temperature, the driving force is insufficient for precipitation to happen.

In order to determine these constants, small identical A356.2 alloy samples were solutionized and then furnace-cooled to various isothermal holding temperatures that ranged from ambient temperature to the solutionizing temperature. This was followed by holding the samples at the solutionizing temperature for up to 48 hours in order for them to equilibrate at temperature, and then they were quenched in ice water. Subsequently, the samples were aged at 155°C (311°F) for 19 hours. This process temperature profile is shown in Figure 4. The measured hardness values of the aged samples are shown in Figure 5 where the error bars indicate standard deviations. The annealed strength in Equation (8), σ_{int}, is assumed to be equal to the minimum measured Meyer hardness value and it is 456.9 MPa. The minimum temperature limit, T_{int}, is found from the measured data, and it is 380°C (717°F).

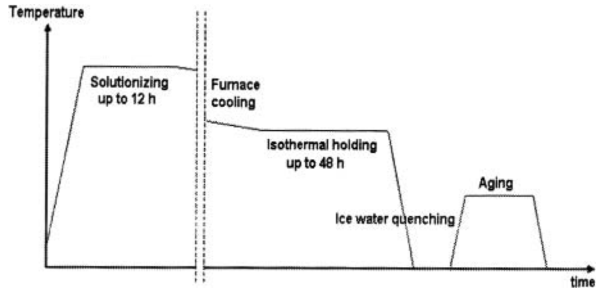


Figure 4. Temperature profile for isothermal holding experiments.

In order to determine the material constants K_6 and K_7, Equation (8) is re-arranged in the form of Equation (13). The additional constants for this model were calibrated by means of measured points and are shown in Table II. The reconstructed curve according to Equation (8) is shown in Figure 5. Subsequently, the kinetic parameters K_1 to K_5 were determined for the non-isokinetic model following the procedure described previously for the other QFA models. For the non-isokinetic model, the K_1 was removed from calculations as the curve represents the accumulated values [15].

$$K_6 = \frac{\sigma_{min} - \sigma_{int}}{\exp\left(-\frac{K_7}{T}\right) - \exp\left(-\frac{K_7}{T_{int}}\right)} \quad (13)$$

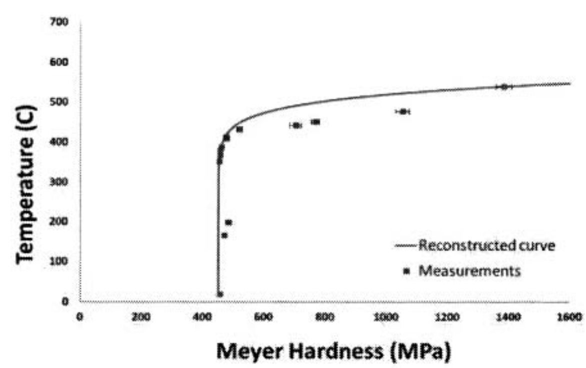


Figure 5. Measured hardness from isothermal holding experiments and curve reconstructed by means of Equation (8).

Table I. The kinetics parameters for A356.2 alloy.

	$-K_1$ $\times 10^3$	K_2	K_3 (J/mol)	K_4 (K)	K_5 (kJ/mol)
n = 1.5	5	4.5×10^{-21}	16307	890.3	130*
n = 2.5	5	8.0×10^{-26}	25227	890.3	130
n = 4	5	6.6×10^{-30}	33575	890.3	130
Rometsch	5	2.8×10^{-17}	9575	890.3	130
Non-isokinetic	-	4.8×10^{-17}	9355	890.3	130

* From reference [18].

Table II. Extra constants for the non-isokinetic QFA model.

σ_{int} (MPa)	T_{int} (°C)	K_6	K_7
456.92	380	9.385×10^{11}	16853.815

The TTP curves obtained from the different QFA models for A356.2 alloy were generated using Equation (3) and the calibrated values shown in Table I are shown in Figure 6. The TTP curve obtained by the classic QFA model with Avrami exponent equal n equal 4 shows the nose at the lowest temperature - approximately 170°C (338°F). The TTP curves obtained by the Rometch's model and the non-isokinetic model show the nose at a much higher temperature - approximately 270°C (518°F).

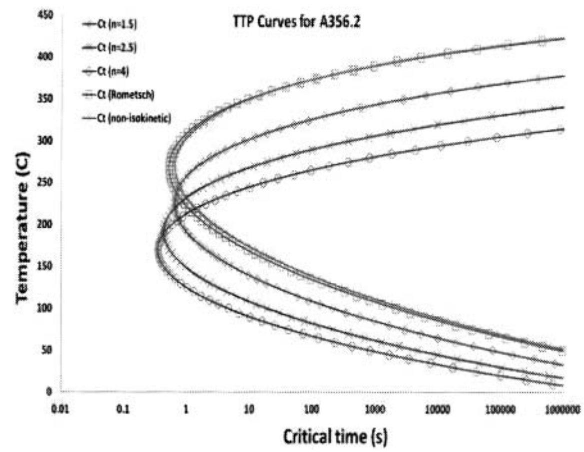


Figure 6. TTP curves of different QFA models for A356.2 alloy.

Simulation Results and Comparison to Measurements

Two quenching processes and two aging conditions were used to verify the computer-predictions. The T6 heat treatment is the most widely used and it is achieved by aging the solutionized and quenched parts at 155°C (311°F) for 4 hours. The T7 treatment is often used for components that are intended for high temperature applications, and it is achieved by aging the parts at 227°C (440°F) for 8 hours.

The component used for validating the model was cast with two thermocouples permanently inserted in it. These are indicated by (1) and (2), in Figure 7(a). The part has thin and thick sections as well as a blind cavity. Three identical parts were used. All three parts were solutionized at 538°C (1000°F) for 12 hours and then two parts were quenched in water that is maintained at 80°C (176°F) and then one aged at 155°C (311°F) for 4 hours, and the other one aged at 227°C (440°F) for 8 hours. The third part was quenched by room temperature forced-air and then aged at 155°C (311°F) for 4 hours.

Computer models of the part were created with both ABAQUS and MAGMA5 HT [4], as shown in Figure 7(b) and (c), respectively. The time-temperature data recorded from both

[4] Developed and marketed by MAGMASOFT, MAGMA Aaschen GmbH.

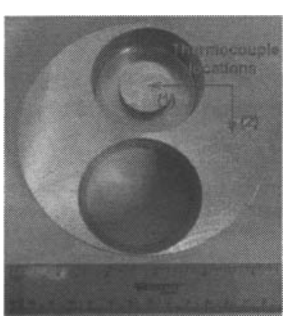
thermocouple locations are reported and compared to the model-predicted data from the same locations. In both thermal analysis calculations, temperature-dependent local quenching heat transfer coefficients were assigned on the casting's surfaces to represent the particular local surface quenching condition [16]. The measured and computer-calculated cooling rate vs. temperature from is shown in Figure 8 (a) and (b), for the hot water quenched part, and in Figure 9 for the forced-air quenched part.

All measured time-temperature data were averaged from 5 adjacent points, in order to eliminate noise. The two commercial softwares (ABAQUS and MAGMA5 HT) yielded similar results. In all cases, the results show excellent agreements between the measured and the computer-calculated cooling rate curves.

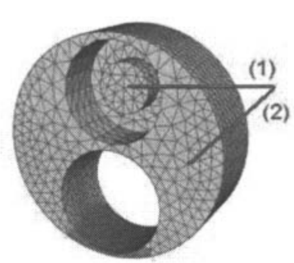
Surface hardness was measured on aged parts. The measured hardness together with computer-predicted hardness values from the different QFA models are shown in Figure 10. Error bars show the standard deviations. Except for Rometch's model, all models give predictions that are significantly lower than the measured values when the models are used to simulate air cooled castings. The reason for this phenomenon is not as yet clear to the authors and it is currently being investigated.

Summary and Conclusions

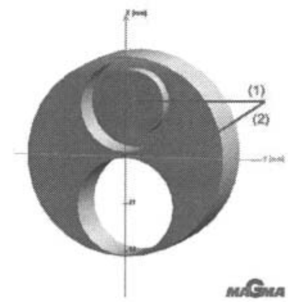
A mathematical model was developed to predict the precipitation-hardened hardness of aluminum casting alloys. The model can use any one of three QFA analysis methods together with the Shercliff-Ashby equations. The method for creating the database necessary for the model was demonstrated for A356.2 alloy. All required kinetic parameters and material constants were measured and calibrated for each of the three QFA analysis methods. The mathematical model was used on a typical cast aluminum alloy component to confirm its validity. The outputs from computer simulations that use the model are: (1) the temperature profile and (2) the as-heat-treated hardness. The model-predicted temperature profiles are in good agreement with measurements. The model-predicted hardness made by the three different QFA methods were in good agreement with measurements made on parts that were quenched in hot water. Only the model-predictions made by the Rometch model were in good agreement with measurements made on parts that were quenched in air. In general, among the three QFA models investigated, Rometch's model gives the most accurate values.



(a)

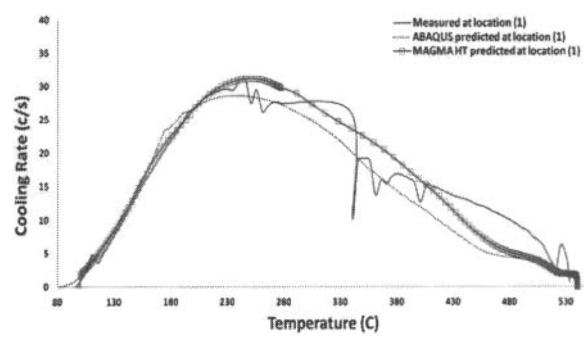


(b)

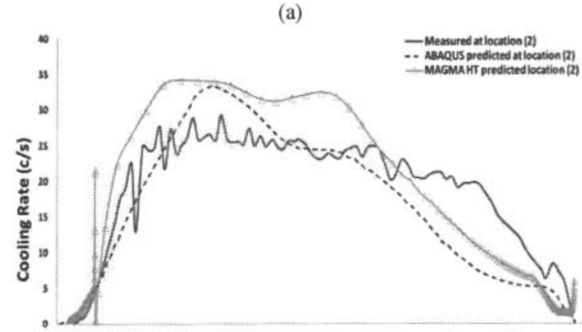


(c)

Figure 7. (a) The part geometry and locations for thermocouple, (b) the computer simulation using ABAQUS, and (a) the computer simulation using MAGMA HT.



(a)



(b)

Figure 8. Measured and computer-calculated cooling rates for a part quenched in hot water (a) at thermocouple location (1), and (b) at thermocouple location (2).

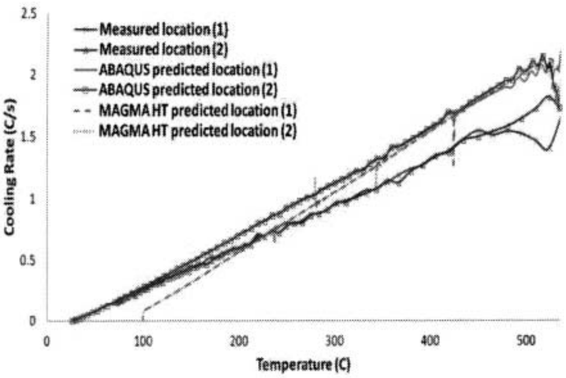


Figure 9. Measured and computer-calculated cooling rates at thermocouple location (1) and (2) for a part quenched by room temperature air.

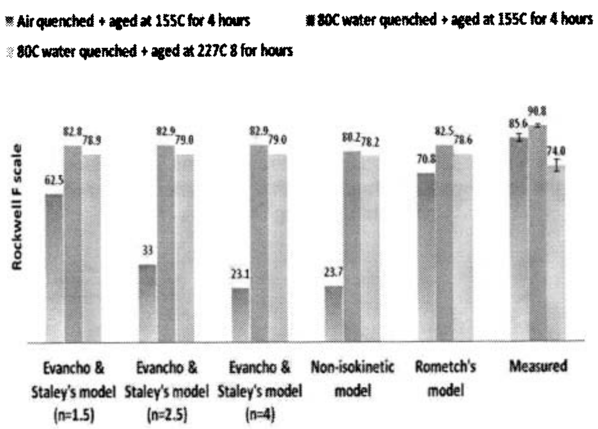


Figure 10. Measured and computer-predicted hardness for hot water quenched and air quenched parts.

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References

1. J.W.Evancho and J.T.Staley, "Kinetics of precipitation in aluminum alloys during continuous cooling," *Metallurgical Transactions*, 5 (1974), 43-47.

2. H.R. Shercliff and M.F. Ashby, "A process model for age hardening of aluminium alloys--I. The model," *Acta Metallurgica et Materialia*, 38 (10) (1990), 1789-1802.

3. E. Scheil, *Arch. Eisenhüttenwes*, 8 (1934) 565.

4. J.W. Cahn, "Transformation kinetics during continuous cooling," *Acta Materialia*, 4 (1956), 572-575.

5. J. W. Christian, *The Theory of Phase Transformations in Metals and Alloys- Part I*, (Oxford, UK: Pergamon Press, 1975).

6. M. Avrami, "Kinetics of Phase Change. I. General Theory," *Journal of Chemical Physics*, 7 (12) (1939), 1103-1112.

7. J.T. Staley, R.D. Doherty, and A.P. Jaworski, "Improved model to predict properties of aluminum alloy products after continuous cooling," *Metall. Trans.* 24 (A) (1993), 2417-2427.

8. J.T. Staley and M. Tiryakioglu, "Use of TTP Curves and Quench Factor Analysis for Property Prediction in Aluminum Alloys," (paper presented in Materials Solutions Conference, ASM International, Indianapolis, IN. 2001).

9. P.A. Rometch, M.J. Starink, and P.J. Gergson, "Improvements in quench factor modelling," *Mater. Sci. Eng*, A339 (2003), 255-264.

10. J.C. Huang and A.J. Ardell, "Addition rules and the contribution of [delta]' precipitates to strengthening of aged Al---Li---Cu alloys," *Acta Metallurgica*, 36 (11) (1988), 2995-3006.

11.P. Gomiero, et al., "Microstructure and mechanical properties of a 2091 AlLi alloy--III. Quantitative analysis of portevin le chatelier instabilities and relation to toughness in Al---Li, Al---Cu---Mg and Al---Li---Cu---Mg (2091) alloys," *Acta Metallurgica et Materialia*, 40 (4) 1992, 863-871.

12. O.R. Myhr, Ø. Grong, and S.J. Andersen, "Modelling of the age hardening behaviour of Al-Mg-Si alloys," *Acta Materialia*, 49 (1) (2001), 65-75.

13. M.J. Starink et al., "Microstrucure and strengthening of Al-Li-Cu-Mg alloys and MMCs: II. Modelling of yield strength," *Acta Materialia*, 47 (14) (1999), 3855-3868.

14. B.C. Lee and J.K. Park, "Effect of the addition of Ag on the strengthening of Al3Li phase in Al-Li single crystals," *Acta Materialia*, 46 (12) (1998), 4181-4187.

15.R.J. Flynn and J.S. Robinson, "The application of advances in quench factor analysis property prediction to the heat treatment of 7010 aluminum alloy," *Journal of Materials Processing Tech.*, (2004), 674-680.

16. C. Wu and M.M. Makhlouf, "Predicting the Response of Aluminum Casting Alloys to Heat Treatment," *Light Metals 2011*, (John Wiley & Sons, Inc. 2011), 835-840.

17.M. Tiryakioglu and J. Campbell, "On macrohardness testing of Al-7wt.% Si-Mg alloys I. Geometrical and mechanical aspects," *Materials Scence and Engineering*, A361 (2003), 232-239.

18. P.A. Rometch and G.B. Schaffer, "An age hardening model for Al-7Si-Mg casting alloys," *Mater. Sci. Eng*, A325 (2002), 424-434.