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NUMERICAL PREDICTING OF RECYCLING FRIENDLY WROUGHT ALUMINIUM ALLOY COMPOSITIONS

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Abstract

The model presented in this work enables the design of optimal (standard and non-standard "recycling-friendly") compositions and properties of wrought aluminium alloys with significantly increased amounts of post-consumed scrap. The following two routes were modelled in detail: (i) the blending of standard and non-standard compositions of wrought aluminium alloys starting from post-consumed aluminium scrap sorted to various degrees simulated by the model; and (ii) changing the initial standard composition of wrought aluminium alloys to non-standard "recycling friendly" ones - with broader concentration tolerance limits of alloying elements, without influencing the selected alloy properties, specified in advance.

Introduction

The sustainability of wrought aluminium alloys for demanding structural applications (e.g. in transportation) is still relatively low. The prevailing raw materials for their production are primary aluminium and pure alloying elements, in combination with internal and new scrap. For this reason, a significant part of world production of primary aluminium is actually consumed for the production of wrought aluminium alloys. The technological reason for that is in the fact that standard wrought aluminium alloy compositions prescribed by international standards [1] are difficult to formulate by recycling post-consumed aluminium scrap, while the economic reason lies in the generally higher average cost of wrought in comparison with cast aluminium end-products.

Post-consumed aluminium scrap exists in waste with changeable, non-exact chemical composition and definitely not as a raw material fabricated with respect with customer's demands. Hence, it is clear that the share of post-consumed scrap in wrought aluminium alloys could be increased either by sorting to fractions with the required chemical composition and/or by broadening the standard compositional tolerance limits of alloying elements. The first solution requires hand or automatic sorting of post-consumed scrap as alloys or groups of alloys to the degree of separation sufficient to enable the blending of standard compositions of wrought alloys [2, 3]; the second solution is much more radical, predicting changes in the existing standards for wrought aluminium alloys toward non-standard alloys but yet having properties acceptable for customers [4]. In this case, the degree of separation of incoming post-consumed scrap required is much less demanding.

Nevertheless, to be of interest for customers, broadening the compositional tolerance limits of wrought aluminium alloys should result in alloy properties still of value for end users. In order to tailor the required (combination and individual values of) properties in wrought aluminium alloys with alternative composition, it is necessary to develop the ability to predict the properties from a given chemical composition and vice versa – starting from alloy properties, to predict the necessarily chemical composition of post-consumed scrap streams or, in other words, the necessary level of scrap sorting. Such predictable algorithms for wrought aluminium alloys have been reported by several authors-for a review see Ref. [5], but are not focused on the recycling of wrought aluminium alloys from post-consumed scrap.

Thus, the purpose of this paper is to present the possibilities for numerical modelling of both technological options for increasing the amount of post-consumed aluminium scrap in wrought aluminium alloys. Based on the model developed, the optimal solution was suggested as the starting point for further development and implementation of the appropriate technology of wrought aluminium alloy recycling.

Modelling of wrought aluminium alloy properties as a function of their chemical composition

Generally, the selected properties of a wrought aluminium alloy (e.g. yield strength-YS, ultimate strength – US, elongation-L and hardness, H) can be all expressed as different functions of the alloy composition:

$$YS = F\,(X_1, X_2, X_3, \dots, X_n) \tag{1}$$

$$US = G(X_1, X_2, X_3, \dots, X_n) \tag{2}$$

$$L = L(X_1, X_2, X_3, \dots, X_n) \tag{3}$$

$$H=H(X_1, X_2, X_3, \dots, X_n) \tag{4}$$

Here, X_1, X_2, X_3, … , X_n represent the concentrations of particular alloying elements.

On the other hand, the concentrations of alloying elements in wrought aluminium alloys, especially in recycled ones, are most often designed for achieving maximal strength. To achieve the proper combination of properties (not only mechanical but also electrical, thermal, corrosion resistant etc.), the concentrations of alloying elements should be inside the standard tolerance limits.

However, in wrought compositions containing an increased amount of scrap, usually it is not easy and certainly not cost-effective to assure such narrow compositions. Therefore, producers of recycled wrought alloys try to develop so-called “recycling friendly” compositions with broader tolerance limits, which at the same time do not significantly influence the selected (usually some of the mechanical) properties of the alloys.

The mathematical condition for “recycling friendly” alloy compositions under which the selected alloy properties will all remain the same is expressed by Eqs. (5-8):

$$dYS = (\partial YS/\partial X_1)dX_1 + (\partial YS /\partial X_2)dX_2 + \ldots\ldots + (\partial YS /\partial Xn)dXn = 0 \quad (5)$$

$$dUS = (\partial US/\partial X_1)dX_1 + (\partial US/\partial X_2)dX_2 ++ \ldots\ldots + (\partial US/\partial Xn)dXn = 0 \quad (6)$$

$$dL = (\partial L/\partial X_1)dX_1 + (\partial L/\partial X_2)dX_2 + \ldots\ldots + (\partial L/\partial Xn)dXn = 0 \quad (7)$$

$$dH = (\partial H/\partial X_1)dX_1 + (\partial H/\partial X_2)dX_2 + \ldots\ldots + (\partial H/\partial Xn)dXn = 0 \quad (8)$$

where $(\partial YS/\partial X_1)dX_1$, $(\partial YS /\partial X_2)dX_2$, …. $(\partial YS /\partial Xn)dXn$, $(\partial US/\partial X_1)dX_1$, $(\partial US /\partial X_2)dX_2$, … $(\partial US /\partial Xn)dXn$, $(\partial L/\partial X_1)dX_1$, $(\partial L /\partial X_2)dX_2$, …. $(\partial L/\partial Xn)dXn$ and $(\partial H/\partial X_1)dX_1$, $(\partial H /\partial X_2)dX_2$, …. $(\partial H/\partial Xn)dXn$ are the partial differentials of the functions YS, US, A and H where $\pm dX_1$, $\pm dX_2$, $\pm dX_3$, …… , $\pm dX_n$ correspond to the infinitesimal tolerance limits. Here and in what follows, the symbols presented in bold correspond to the values inside standard tolerance limits, whereas the symbols in non-bold represent values outside the tolerance limits.

Proposing that the selected alloy properties (e.g. yield strength- YS, ultimate strength-US, elongation-L and hardness-H) are polynomial functions of the alloy composition one can write:

$$YS = YS(X_1, X_2, X_3, \ldots ,X_n) = A_1X_1^{p1} + A_2X_2^{p2} + A_3X_3^{p3} + \ldots + A_nX_n^{pn} \quad (9)$$

$$US = US(X_1, X_2, X_3, \ldots ,X_n) = B_1X_1^{q1} + B_2X_2^{q2} + B_3X_3^{q3} + \ldots + B_nX_n^{qn} \quad (10)$$

$$L = L(X_1, X_2, X_3, \ldots ,X_n) = C_1X_1^{r1} + C_2X_2^{r2} + C_3X_3^{r3} + \ldots + C_nX_n^{rn} \quad (11)$$

$$H = H(X_1, X_2, X_3, \ldots ,X_n) = D_1X_1^{s1} + D_2X_2^{s2} + D_3X_3^{s3} + \ldots + D_nX_n^{sn} \quad (12)$$

For the experimentally determined functions (14)-(17), we can finally calculate the total differentials dYS, dUS, dL and dH, and formulate the mathematical conditions for constant tensile strength, ultimate strength, elongation and hardness:

$$dYS = A_1p_1X_1^{p1-1}dX_1 + A_2p_2X_2^{\ p2-1}dX_2 + A_3p_3X_3^{\ p3-1}dX_3 + \ldots.. + A_np_nX_n^{\ pn-1}dX_n = 0$$
$$dUS = B_1p_1X_1^{q1-1}dX_1 + B_2p_2X_2^{\ q2-1}dX_2 + B_3p_3X_3^{\ q3-1}dX_3 + \ldots.. + B_np_nX_n^{\ qn-1}dX_n = 0$$
$$dL = C_1p_1X_1^{r1-1}dX_1 + C_2p_2X_2^{\ r2-1}dX_2 + C_3p_3X_3^{\ r3-1}dX_3 + \ldots.. + C_np_nX_n^{\ rn-1}dX_n = 0$$
$$dH = D_1p_1X_1^{s1-1}dX_1 + D_2p_2X_2^{\ s2-1}dX_2 + D_3p_3X_3^{\ s3-1}dX_3 + \ldots.. + D_np_nX_n^{\ sn-1}dX_n = 0 \quad (13)$$

or, for sufficiently low variations of ΔX:

$$\Delta YS = \pm A_1p_1X_1^{\ p1-1}\Delta X_1 \pm A_2p_2X_2^{\ p2-1}\Delta X_2 \pm A_3p_3X_3^{\ p3-1}\Delta X_3 \pm \ldots.. \pm$$
$$\pm A_np_nX_n^{\ pn-1}\Delta X_n = 0$$
$$\Delta US = \pm B_1p_1X_1^{\ q1-1}\Delta X_1 \pm B_2p_2X_2^{\ q2-1}\Delta X_2 \pm B_3p_3X_3^{\ q3-1}\Delta X_3 \pm \ldots.. \pm B_np_nX_n^{\ qn-1}\Delta X_n = 0$$
$$\Delta L= \pm C_1p_1X_1^{\ r1-1}\Delta X_1 \pm C_2p_2X_2^{\ r2-1}\Delta X_2 \pm C_3p_3X_3^{\ r3-1}\Delta X_3 \pm \ldots.. \pm C_np_nX_n^{\ rn-1}\Delta X_n = 0$$
$$\Delta H = \pm D_1p_1X_1^{\ s1-1}\Delta X_1 \pm D_2p_2X_2^{\ s2-1}\Delta X_2 \pm D_3p_3X_3^{\ s3-1}\Delta X_3 \pm \ldots.. \pm D_np_nX_n^{\ sn-1}\Delta X_n = 0$$
$$(14)$$

In practice, the system of equations (14) is used for calculating the proper combination of tolerance limits, ΔX_i (i = 1, 2, 3, … , n) of alloying elements under which: (i) the selected mechanical properties of the alloy remain the same as in the standard one, and (ii) the chemical composition of the recycling-friendly alloy is corresponding to the pre-melt chemical composition of the incoming scrap mixture (formulated with the minimal addition of primary aluminium and alloying elements).

The main priorities in formulation of the recycling-friendly compositions are: (1) the minimal addition of primary aluminium and alloying elements, (2) the maximal consumption of regular scrap streams, daily available in the scrap yard, and (3) the non-standard alloy composition for which the selected mechanical properties remain the same as in the standard one.

The practical way to do this is by modelling, starting from the chemical composition of the scrap streams. The precondition is that the chemical composition of the recycling-friendly alloy should be the same as the pre-melt composition of the incoming mixture consisting of the combination of various scrap streams with no or minimal addition of primary aluminium and alloying elements. In addition, the deviations of the recycling-friendly from the standard concentrations of alloying elements should be as small as possible.

Modelling of the degree of post-consumed scrap sorting for recycling-friendly wrought compositions

The recycling-friendly compositions of wrought aluminium alloys should be modelled in accordance with the following two criteria: (i) the selected chemical composition and compositional tolerance limits of a recycling-friendly wrought aluminium alloy should fulfil market expectations regarding the alloy properties; and (ii) the prescribed recycling-friendly alloy composition should be routinely achievable by mixing scrap streams fabricated in the scrap yard by scrap separation (with or without minimal addition of primary aluminium and alloying elements).

In order to achieve these two goals, it is necessary to define the industrial levels of wrought aluminium scrap sorting. An example of the practical levels of sorting of post-consumed wrought aluminium scrap is presented in Table 1. Planning the optimal number of scrap streams, as illustrated in Fig. 1, their chemical composition and the compositional tolerance limits of alloying elements for effective blending of the pre-melting mixture, Fig. 2, with minimal (or even without) addition of pure alloying elements and primary aluminium is essential for successful running of the recycling plant and the final business result.

Therefore, adequate organization of the scrap separation streams should provide answers to the following key questions of scrap processing:

- How many scrap streams should be produced by sorting wrought aluminium wastes in the scrap yard;
- How many alloys (just a single one, a mixture of two or more) should be involved in these streams;
- What should the chemical compositions be (qualitatively, regarding alloying elements and also quantitatively, considering their concentrations as well as the compositional tolerance limits) of those streams, and finally;
- For which wrought aluminium alloys and under which production scenarios should the sorted streams used?

Table 1. Possible industrial levels practiced in wrought aluminium scrap sorting

Scrap sorting level	Description
1.	Separation of incoming scrap into cast and wrought aluminium scrap
2.	Scrap of wrought aluminium alloys within the same series
3.	Scrap of wrought aluminium alloys within the same series having the same combination of alloying elements
4.	Scrap of wrought aluminium alloys within the same series consisting of more than 2 compositionally similar/comparable alloys
5.	Scrap of wrought aluminium alloys consisting of 2 alloys within the same series compositionally similar/comparable
6.	Scrap streams of single wrought aluminium alloys

A possible way of providing the answers to the above questions is by calculating the appropriate composition of the pre-melt mixture blended from various scrap streams of different chemical composition:

$$[a_1(x_{1,1}, x_{1,2}, x_{1,3}, \ldots, x_{1,k}) + a_2(x_{2,1}, x_{22}, x_{2,3}, \ldots, x_{2,k}) + a_3(x_{3,1}, x_{3,2}, x_{3,3}, \ldots, x_{3,k}) + \\ + \ldots\ldots + a_{n-1}(x_{n-1,1}, x_{n-1,2}, x_{n-1,3}, \ldots, x_{n-1,k}) + a_n(x_{n,1}, x_{n,2}, x_{n,3}, \ldots, x_{n,k})] + \\ + [b_1L_1, b_2L_2, b_3L_3, \ldots, b_{k-1}L_{k-1}, b_kL_k] = [Y_1, Y_2, Y_3, \ldots, Y_k] \quad (15)$$

The modelling concept is schematically illustrated in Fig. 3.

Generally, the left hand side of Eq. (15) is the sum of the n+ 1 matrix of the same dimensions (1 x k). The sum of the first n-1 matrices defines the composition of the mixture obtained by mixing n different scrap streams, each consisting of k different alloying elements including aluminium, while the last one describes the compositional tuning achieved by addition of pure alloying elements and primary aluminium. The right hand side of Eq. (15) represents the sought for recycling-friendly composition of the alloy, expressed in the matrix form with dimension (1 x k). Also in that case, index k corresponds to the different alloying elements (from 1 to k-1) including aluminium which is indexed by k.

Let us assume having a scrap yard with n different boxes filled with incoming scrap streams of mutually different but always constant chemical composition. The scrap inside the boxes in all cases consists of k different alloying elements (from 1 to k-1; the concentration of some of them could be zero) including aluminium, which is denoted by k.

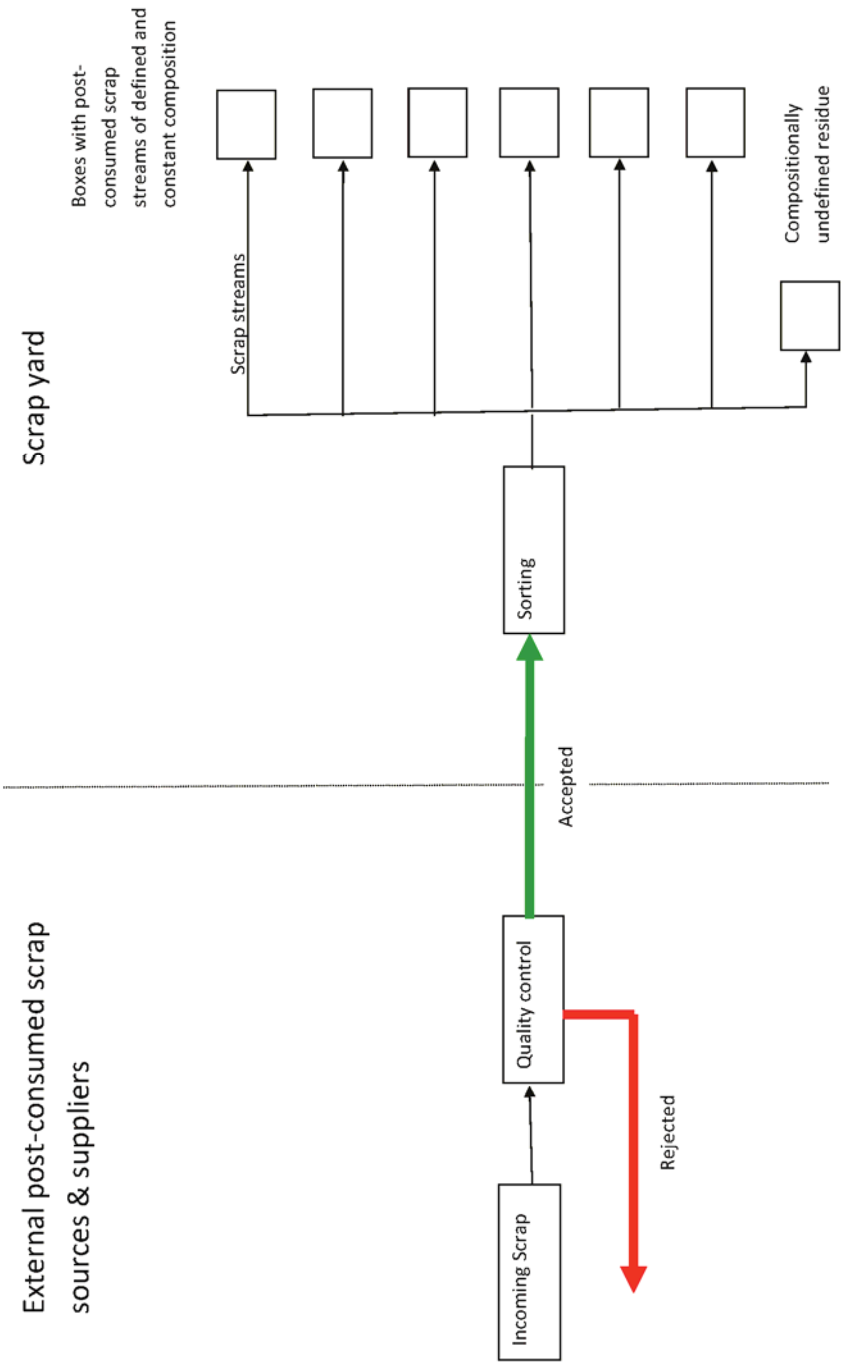

Fig. 1. Organization of scrap yard for recycling of wrought aluminium alloys from post-consumed scrap in accordance with the model.

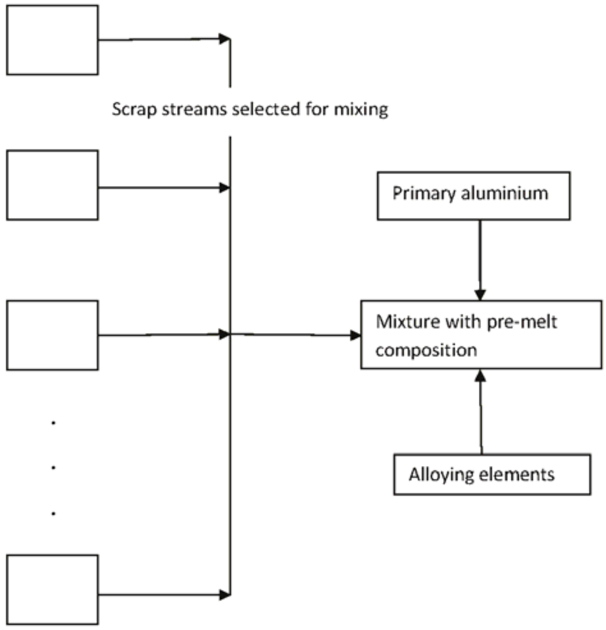

Fig. 2. Providing the pre-melt »recycling-friendly« composition of wrought aluminium alloy by combining different scrap streams of post-consumed scrap.

Let us further agree that the general term $x_{i,j}$ (i = 1,2,3, ..., n; j = 1,2,3, ...,k) appearing in the n-1 matrices on the left side of Eq. (15) represents the weight percentage of the alloying element designated by index j (e.g. silicon) in the particular scrap stream located in the scrap box indexed by index i (e.g. in box 1). Constants a_i (i = 1, 2, 3, ... , n) appearing in the first matrix represent the weight percentage of the scrap stream i contained in the pre-melt mixture.

Symbols L_i (i = 1,2,3,...,k-1,k) appearing in the second matrix on the left hand side of Eq. (15) represent the weight percentage concentrations of alloying elements indexed from 1 to k (k is related to aluminium), while the symbols b_i (i = 1,2,3, ..., k) represent the weight percentage of added elements.

Finally, on the right hand side of Eq. (15), the symbols Y_i (i = 1,2,3, ..., k) represent the concentrations (in wt%) of alloying elements (indexed from 1 to k-1) and aluminium (indexed by k) in the recycling-friendly wrought aluminium alloy obtained by recycling.

In practice, Eq. (15) should be written by applying the appropriate tolerance limit intervals:

$$\begin{aligned}
&[a_1(x_{1,1}\pm\Delta x_{1,1},\ x_{1,2}\pm\Delta x_{1,2},\ x_{1,3}\pm\Delta x_{1,3},\ \ldots,\ x_{1,k}\pm\Delta x_{1,k}) + \\
&+ a_2(x_{2,1}\pm\Delta x_{2,1},\ x_{2,2}\pm\Delta x_{2,2},\ x_{2,3}\pm\Delta x_{2,3},\ \ldots,\ x_{2,k}\pm\Delta x_{2,k}) + \\
&+ a_3(x_{3,1}\pm\Delta x_{3,1},\ x_{3,2}\pm\Delta x_{3,2},\ x_{3,3}\pm\Delta x_{3,3},\ \ldots,\ x_{3,k}\pm\Delta x_{3,k}) + \ldots\ldots + \\
&+ a_{n-1}(x_{n-1,1}\pm\Delta x_{n-1,1},\ x_{n-1,2}\pm\Delta x_{n-1,2},\ x_{n-1,3}\pm\Delta x_{n-1,3},\ \ldots,\ x_{n-1,k}\pm\Delta x_{n-1,k}) + \\
&+ a_n(x_{n,1}\pm\Delta x_{n,1},\ x_{n,2}\pm\Delta x_{n,2},\ x_{n,3}\pm\Delta x_{n,3},\ \ldots,\ x_{n,k}\pm\Delta x_{n,k})] + \\
&+ [b_1(L_1\pm\Delta L_1),\ b_2(L_2\pm\Delta L_2),\ b_3(L_3\pm\Delta L_3),\ \ldots,\ b_{n-1}(L_{n-1}\pm\Delta L_{n-1}),\ \ b_n(L_n\pm\Delta L_n)] = \\
&= [Y_1\pm\Delta Y_1,\ Y_2\pm\Delta Y_2,\ Y_3\pm\Delta Y_3,\ \ldots,\ Y_n\pm\Delta Y_n] \qquad (16)
\end{aligned}$$

Here, $x_{i,j}\pm\Delta x_{i,j}$ (i = 1,2,3, ..., n; j = 1,2,3, ..., k) represents the tolerance limit interval of the alloying element denoted by index j in the scrap stream located in the box designated by index n. $L_i\pm\Delta L_i$ (i = 1,2,3, ..., k) represents the tolerance limit interval of the pure alloying element i, added to the mixture of scrap streams for the final tuning of its chemical composition. Correspondingly, $Y_i\pm\Delta Y_i$ (i = 1,2,3, ..., k) represents the tolerance limit interval of the alloying element i in the recycling-friendly wrought aluminium alloy obtained by recycling.

From an economic point of view, it is particularly important to achieve the recycling-friendly composition of the wrought aluminium alloy with no (or at least minimal) addition of pure alloying elements and primary aluminium, which is represented by Eq. (17):

$$\begin{aligned}
&[a_1(x_{1,1}\pm\Delta x_{1,1}, x_{1,2}\pm\Delta x_{1,2}, x_{1,3}\pm\Delta x_{1,3}, \ldots, x_{1,k}\pm\Delta x_{1,k}) + \\
&+ a_2(x_{2,1}\pm\Delta x_{2,1}, x_{2,2}\pm\Delta x_{2,2}, x_{2,3}\pm\Delta x_{2,3}, \ldots, x_{2,k}\pm\Delta x_{2,k}) + \\
&+ a_3(x_{3,1}\pm\Delta x_{3,1}, x_{3,2}\pm\Delta x_{3,2}, x_{3,3}\pm\Delta x_{3,3}, \ldots, x_{3,k}\pm\Delta x_{3,k}) + \ldots\ldots + \\
&+ a_{n-1}(x_{n-1,1}\pm\Delta x_{n-1,1}, x_{n-1,2}\pm\Delta x_{n-1,2}, x_{n-1,3}\pm\Delta x_{n-1,3}, \ldots, x_{n-1,k}\pm\Delta x_{n-1,k}) + \\
&+ a_n(x_{n,1}\pm\Delta x_{n,1}, x_{n,2}\pm\Delta x_{n,2}, x_{n,3}\pm\Delta x_{n,3}, \ldots, x_{n,k}\pm\Delta x_{n,k})] = \\
&= [Y_1\pm\Delta Y_1, Y_2\pm\Delta Y_2, Y_3\pm\Delta Y_3, \ldots, Y_n\pm\Delta Y_n] \qquad (17)
\end{aligned}$$

The same sorting levels should be applied to clean and aluminium scrap contaminated with organics or other impurities.

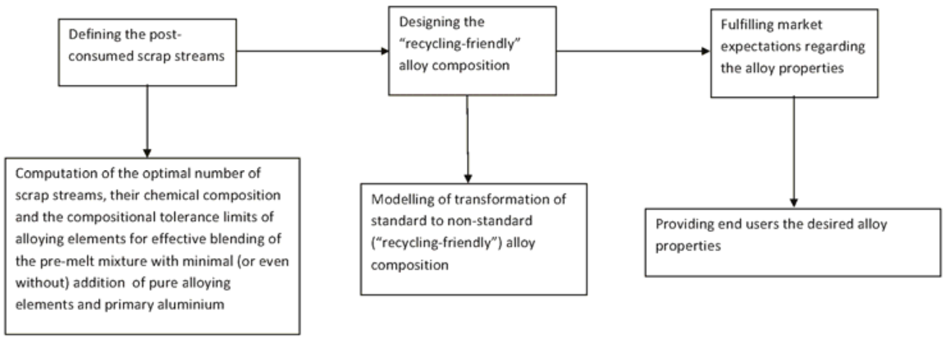

Fig. 3. Processing steps in modelling the »recycling-friendly« composition of wrought aluminium alloy for the desired alloy properties.

Conclusions

The model presented in this work enables the design of optimal (standard and non-standard "recycling-friendly") compositions and properties of wrought aluminium alloys with significantly increased amounts of post-consumed scrap. The following two routes were modelled in detail: (i) the blending of standard and non-standard compositions of wrought aluminium alloys starting from post-consumed aluminium scrap sorted to various degrees simulated by the model; and (ii) changing the initial standard composition of wrought aluminium alloys to non-standard "recycling friendly" ones - with broader concentration tolerance limits of alloying elements, without influencing the selected alloy properties, specified in advance.

The applied algorithms were found to be very useful in the industrial design of both procedures: (i) computation of the required chemical composition of the scrap streams obtained by sorting (or, in other words, the post-consumed scrap sorting level), necessary for achieving the standard wrought alloy composition; and (ii) transformation of standard to non-standard ("recycling-friendly) compositions with the key alloy properties (e.g. tensile strength, elongation) remaining the same.

The most beneficial and particularly promising approach might be the integral (or combined) approach, assuring both possibilities: (i) the standard chemical composition of the alloy achieved by a sufficient level of post-consumed scrap sorting predicted by the model, and (ii) modelling the non-standard alloy composition by less demanding (and more cost-effective) sorting, but yet providing end users with the desired alloy properties.

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