Method of Determination of type and amount of a filler masterbatch to reduce cost of a polymeric products while saving its required standard properties

1- Ahmadreza Shafieizadegan-Esfahani A.R
2- Mahmoud Tafvizi Zavareh M.
3- Ehsan Sabbag-Harandi E

Abstract:
An algorithm for finding the type and amount of a filler masterbatch which are most effective in reduction of cost of polymeric product provided that it pass the required mechanical properties, is addressed by optimization calculations based on logical assumptions. These calculations indicate this optimum amount can be achieved by plotting two functions simultaneously. One is the “cost function” which relates the product cost with the weight fractions and weight of the product and the others the “property function” which relates mechanical properties of the product with the amount of the used filler masterbatch. The proposed model shows that addition of filler masterbatch can reduce the cost of the standard product only if the mechanical properties of the product are not adversely affected by the masterbatch.

For example, this product can be a Polyethylene (PE) bagging which consists of PE and calcium carbonate masterbatch.
The cost of one product specimen is showed by g which is a function of polymer cost, masterbatch cost, and production cost.

\[ g = mc + h = \rho V c + h \] (1)
Where m(kg) is the specimen mass, $C\left(\frac{T}{kg}\right)$ is the cost of unit mass of consisting material, h(T) is production cost, $\rho \left(\frac{kg}{m^3}\right)$ is the specimen density and V($m^3$) is the specie volume. Assume that the productions cost is independent from specimen mass and mass fractions.

The specimen density can be calculated from

$$\rho = \frac{m}{V} = \frac{m_p + m_f}{V} = \frac{\rho_p V_p + \rho_f V_f}{V} = \rho_p \phi_p + \rho_f \phi_f$$

(2)

Where $\rho_p \left(\frac{kg}{m^3}\right)$ and $\phi_p$ are the polymer density and weight fraction, and $\rho_f \left(\frac{kg}{m^3}\right)$ and $\phi_f$ are the filler masterbatch density and weight fraction respectively. It can be showed that

$$\rho = \frac{\rho_p \rho_f}{\rho_f - W_f (\rho_f \rho_p)}$$

(3)

Where $W_f$ is the weight fraction of the filler masterbatch.

We neglected small volume changes of mixing. Moreover we have:

$$C\left(\frac{T}{kg}\right) = W_p C_p \left(\frac{T}{kg}\right) + W_f C_f \left(\frac{T}{kg}\right)$$

Or

$$C = W_f C_f + (1 - W_f) C_p$$

(4)

Where $C_p \left(\frac{T}{kg}\right)$ is the unit mass cost of the polymer and $C_f \left(\frac{T}{kg}\right)$ is the unit mass cost of the filler masterbatch.

$W_p$ and $W_f$ are the weight fractions of filler masterbatch and the polymer respectively. Therefore, we have from (1-4):

$$g = \frac{\rho_p \rho_f}{\rho_f - W_f (\rho_f \rho_p)} \times abt \left[ W_f (C_f - C_p) + C_p \right] + h_1$$

This function relates the specimen cost g, to the geometry, composition, unit mass cost of materials and production costs of the specimen.

The following examples illustrate the relations.
Example 1 – Consider a polyethylene bagging
With length \( a = 30 \text{cm} \), width \( b = 10 \text{cm} \) is made from LLDPE
\( (\rho_p = 1000 \frac{\text{kg}}{\text{m}^3}, C_p = 1.43 \frac{T}{\text{kg}}) \) and ordinary calcium carbonate
masterbatch \( (\rho_f = 1200 \frac{\text{kg}}{\text{m}^3}, C_f = 0.57 \frac{T}{\text{kg}}) \) which its
production cost is \( 0.14 \frac{T}{\text{kg}} \) and has two layer thickness of
t(\text{mm}). As a result the cost function is:
\[
g(t, W_f) = \frac{36t}{2.2 - 0.2W_f}(5 - 3W_f) + 5 \quad (T) \quad (6)
\]
This function is plotted in Fig. 2 in which thickness \( t \), changes
from 0 to 1\text{mm} and masterbatch fraction changes from 0 to 100\%.

Fig. 2 (b) shows cost contours on \( W_f - t \) plan.

As it can be seen from the figure the price \( g \) increases when the
thickness \( t \) increases, however, the higher \( W_f \) the lower
increase of cost.

But it is evident that I is impossible for a baggage to stand the
force \( F \) by all of these thickness and weight fractions; therefore,
it is necessary to have another equation that accounts for the
force \( F \).

Fig1. Leads to two important results:
1- The more the cost difference between the Polyethylene and
the masterbatch, the more reduction in product cost by
increasing \( W_f \). Therefore, if the product has an special form (\( t \)
should be constant) and mechanical properties are not
important, the cheapest masterbatch and the highest \( W_f \)
should be employed, (regarding processing emciderations).
2- If the production cost \( h \) is high relative to raw materials, the
type and amount of masterbatch have not significant effects
on the product cost.

We continue with mechanical properties suppose that the
product standard required that the product stands Force \( F \).
If the strength of consisting material of the product is
\( \sigma(\text{pa}) \) and security coefficient is \( K \) we have:
\[
k F \leq \sigma b t \quad (7)
\]
Now we need a Formula that relates $\sigma$ to $W_f$ inorder to relate $t$, $W_f$ and $F_i$.

This is the position that the important of the masterbatch properties is recognized. This formula is obtained by laboratory tests. By examining specimens that have deferent amounts of each masterbatch we obtain $\sigma = \sigma(W_f)$ for each masterbatch. Three following examples illustrate this point.

**Example 2** : Suppose for filling the polyethylene of example 2 We have used conventional CaCO$_3$ masterbatch that costs $57 \frac{T}{kg}$ and suppose the property function that is obtained in laboratory by using this masterbatch for filling PE films has the form:

$$\sigma = \sigma_p (1 - W_f)$$

Where $\sigma$ and $\sigma_p$ are the produced film and neat PE film strengths. This means that strength of the film is linearly reduced bu increasing masterbatch contant. If as in example 1, the masterbatch density is $1200 \frac{kg}{m^3}$, $F_i$ is $600N$, K is considerd 2 and the strength of the neat LLDPE is $20 MPa$ from (7) we have:

$$2 \times 600N \leq 20 \times 10^6 (1 - W_f) \times 0.10 \times t$$

$$t \geq \frac{6 \times 10^{-4}}{(1 - W_f)} (m) = \frac{0.6}{1 - W_f} (mm)$$

$$w_f \leq 1 - \frac{0.6}{t(mm)}$$

FIG. 1
If we plot this inequality (7) in Fig. 2’s contour cost plans we can find the point that shows minimum cost of product in $W_f - t$ plane. This point shows the minimum price of a polyethylene baggage which can stand force $F$ by security coefficient 2. Fig. 3 shows this plot and the minimum cost point. $(W_f, t)$ couples above this curve pass the condition (9).

As Fig. 2 shows the minimum cost that is obtained by using this cheap masterbatch is obtained in $W_f=0$.

This is because the deterioration of properties caused by this cheap masterbatch, leads to higher thickness $t$ and higher cost of material In $W_f=0$ the thickness at least is 0.6mm and one baggage costs 1.546.

**Example 2:** Suppose in example 2 we have used high quality CaCO$_3$ masterbatch that costs $63 \frac{t}{kg}$ and the same density of 1200 $\frac{kg}{m^3}$.

Suppose regration calculations, determine the property function (obtained from mixing this masterbatch with LLDPE in different weight fractions as

$$\sigma = \frac{\sigma_p}{1 + 3 W_f^4}$$

As Fig. 4 shows, by using this type of masterbatch the mechanical properties remain unchanged up $W_f \approx 0.4$.

From (7) we have:

$$2 \times 600 = \frac{20 \times 10^6}{1 + 3 W_f^2} \times 0.10 \times t$$

$$t = 0.6(1 + 3 W_f^4) \text{ (mm)}$$

$$W_f \leq \sqrt[4]{\frac{t(mm)}{1.8} - \frac{1}{3}} \quad (10)$$

If we plot this curve in $W_f - t$ contour plane (Fig. 4), the lowest cost of the baggage is seen to be at $W_f = 0.4$. Also it is seen that the cost contours are not so different from example 1.

In this example 2 the cost function is:
\[(5-2.8 \, \text{wt}) + 5 \, g(t, \text{wt}) = \frac{36t}{2.2-0.2\text{wt}}\]

The minimum cost that is obtained in \( W_f = 0.4 \), \( t=0.64 \) is 1.34 for a baggage.

Comparing Fig. 3 and Fig. 4 shows that:
1- Whenever the slope of \( W_f = W_f(t) \) in \( W_f - t \) plane is not more than cost contour slopes the filler masterbatch cannot reduce the product cost; i.e., it is important that filler masterbatch must not deteriorate the properties.
2- If suitable processing procedures employed that do not deteriorate the product properties up to high weight fraction of filler masterbatch and the masterbatch cost still is lower than PE cost, significant economical benefits is made.
(Example 3 shows 13% reduction in one baggage cost compared with example 2).

Example 4: suppose the consumer of masterbatch is going to produce a baggage which has a deferent thickness to and can stand tensile force \( F \).
If the tensile force is higher than the force limit of neat PE, this production is impossible, but if the force is not higher than the neat PE limit (for example a baggage with 0.8mm thickness for 600N tensile load and security coefficient of 2), then a horizontal line \( t_0 \) should be plotted in \( W_f - t \) plane for each type of the masterbatch.
The intersection of this line with the property function is the minimum cost of the product.
In Fig.3 and Fig.4 intersections of the \( t=0.8 \)mm line demonstrate that although the reinforcing masterbatch is more expensive than conventional masterbatch, it results in cheaper baggage product even in the same thickness.

Conclusion
The procedure of selection of type and amount of filler masterbatch – regarding the presented discussion the following algorithm can be applied for the selection of the optimum type and optimum amount of filler masterbatch for the production of a special specimen that passes required standard properties:

a- Firstly the consumer of masterbatch must determine the cost functions \( g = g(t, W_f) \) based on costs of intended masterbatches.

b- The \( \sigma = \sigma(W_f) \) function for each type of intended masterbatches is determined based on experiments on each type of masterbatches.

c- The cost function contours and the property function are plotted simultaneously in \((W_f, t)\) couple. This point is the optimum for this type of masterbatch. By comparing the cost and selecting the minimum cost, the optimum type and amount of masterbatch is determined.

It should be mentioned that the presented procedure is applied for filler master batch and in the case of color master batch like carbon black, titan and the like, which are used in low weight fractions, the cast variations are not significant.

In these cases it is recommended that the master batch dose not deteriorate required mechanical properties.

Finally it is noted that the specific character of Nano size filler is that if they are compounded in correct way, they not only do not deteriorate mechanical properties but also can improve the properties. In this case the calculation can be conducted in the same way.
FIG. 2
Price function in example 1
FIG. 3
The curve of properties and price cont. in example 2

FIG. 4
The curve of properties and price cont. in example 3