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THE DESIGNING OF THE FOUR – COMPONENT COMPOSITION OF THE BLEND OF THE POLYMER FIBRES ON THE BASIS OF THE NUMERICAL SIMULATION

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Preliminary Note – Prethodno priopćenje

In the paper is presented a part of the project for determining basically permissible the four – component coposition of the (4K) mixture of the polymer fibres on the basis of the numerical simulation. The mathematical models of the composition are developed on the basis of the linear equations . The computer solution of some variants of these models is performed by Gaus procedures in combination with the numerical method of Monte Carlo simulation.

Key words: Polymers, Blending Matters Theory, Design, Monte Carlo Simulation

INTRODUCTION

The defining of the composition of the determined substances in: chemistry [1], textile [2], metallurgy [3], food industry, pharmacy, thermodynamics, theoretical physics [4] etc., means finding an optimal percentage-quantative relation of the com-ponents with best satisfying charac-teristics in the mixture in which they take part. During combining of the mixture where participate the fibres of various physical-chemical characteristics, one must take care about the established rule of the proportional limits of the fibres participating in the mixture. Each component taking part in the composition of the mixture, participates in determing its prices, relatively to its participation. If, e.g., the price of one /kg/: of the *A* component *Ca*, of the component *B: Cb*, of the component *C: Cc*, ... of the com-ponent *N: Cn*, and their proportional participations in the mixture with *x, y, z, ... , n,* then the price of the mixture *Cm* has been obtained as the linear combination of the following values in the currency units per piece (Cur, Unit/Piece):

$$\frac{x \cdot Ca}{100} + \frac{y \cdot Cb}{100} + \frac{z \cdot Cc}{100} + \ldots + \frac{n \cdot Cn}{100} = Cm \qquad (1)$$

For the proportional participations of *n*-components is always important the relation:

$$\frac{x}{100} + \frac{y}{100} + \frac{z}{100} + \ldots \frac{n}{100} = 1 \quad (100\%) \qquad (2)$$

And the inequalities: $0 \le \frac{x}{100}, \frac{y}{100}, \frac{z}{100}, \ldots, \frac{n}{100} \le 1.$

The same is with the condition that the price of the mixture is higher than the cheapest one, and lower than the most expensive component, i.e.

$$\min\{Ca, Cb, \ldots, Cn\} \le Cm \le \max\{Ca, Cb, \ldots, Cn\} \qquad (3)$$

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DETERMINIG THE COMPOSITION OF THE MIXTURE WITH FOUR COMPONENTS

The defining problem of the various proportional participation of the components in the mixture was for many years a vexed question [2]. Namely, the calculation method that is still the only one in the majority of our technological systems, is known as "cross reckoning". These calculation procedures give relatively quickly a solution, but only a restricted number of such solutions (2 up to 3). Very often with this calculation groups of two components each ought to participates equally in the blend. The mixture composing in this way doas not giva the capability of the analysis of various combinations and at the same time as well the finding of some hidden savings. By solving two equations with four unknowns, this problem can be simply solved with the combination of the linear programming and simulation [5]. If in the mixture *M* whose price per one /kg/ is known, participate four components with the prices per the weight units *Ca, Cb, Cc* and *Cd* with the supposition that:

$$Ca < Cb < Cc < Cd \text{ and}$$
$$Ca < Cm < Cd \qquad (4)$$

Determine percentage participations of *x, y, z* and *w* of the components *A, B, C* and *D* in the mixture *M*. Using the task conditions, one obtains the system of the two linear equations with the four unknowns values *x, y, z* and *w*. this system has infinitely many solutions if we solve it on the basis two unknowns, e.g. per *x* and *y*:

$$\text{Given } x + y + z + w = 1 \qquad (5)$$
$$Ca \cdot x + Cb \cdot y + Cc \cdot z + Cd \cdot w = Cm$$
$$find(x, y) \rightarrow$$
$$\begin{bmatrix} \frac{-1}{Ca - Cb} \cdot (Cb + Cc \cdot z - z \cdot Cb - Cb \cdot w + Cd \cdot w - Cm) \\ \frac{-(-Cc \cdot z - Cd \cdot w + Cm + Ca \cdot z + w \cdot Ca - Ca)}{Ca - Cb} \end{bmatrix}$$

where z and w take arbitrary values. Taking into consideration these solutions and conditions, this applies for every single variable: $0<x<1$, $0<y<1$, $0<z<1$ and $0<w<1$, equivalent as well to the found values x and y:

$$0 \le \frac{-Cb - Cc \cdot z - Cd \cdot w + Cm + z \cdot Cb + w \cdot Cb}{-Cb + Ca} \le 1$$
$$0 \le \frac{-(Ca - Cc \cdot z + Ca \cdot z + Ca \cdot w - Cd \cdot w + Cm)}{(-Cb + Ca)} \le 1 \qquad (6)$$

Solving these in equations, one gets for w, for:

$$x = 0 \quad find\ (w) \rightarrow \frac{Cb - Cm - Cb \cdot z + Cc \cdot z}{Cb - Cd}$$
$$x = 1 \quad find\ (w) \rightarrow \frac{Ca - Cm - Cb \cdot z + Cc \cdot z}{Cb - Cd}$$
$$y = 0 \quad find\ (w) \rightarrow \frac{Ca - Cm - Ca \cdot z + Cc \cdot z}{Ca - Cd} \qquad (7)$$
$$y = 1 \quad find\ (w) \rightarrow \frac{Cb - Cm - Ca \cdot z + Cc \cdot z}{Ca - Cd}$$

The system of the linear in equations can be solved as well by graphical method [6]. The group of the limitations in the field of the permissible solutions is presented by the equations of the straight lines. Using general obtained forms, it is possible to present several characteristic cases of the graphic and table results of the composition of 4K mixture with the components: *x, y, z* and *w*.

THE FIRST CASE: *Ca<Cm<Cb*

For the chosen (selected) vector the price of the components and the mixture /CU/kg/ follows:

$$[Ca\ Cb\ Cc\ Cd\ Cm] = [15\ \ 27\ \ 25\ \ 31\ \ 24] \qquad (8)$$

and the function domain of the component z in the interval: z=0, 0,1…1, taking into consideration the solved system of the linear equations, follows the graphical and table interpretation in the Figure 1 and Figure 2.

Determing of the marginal point *Zmax* of the *z* function.

$$\text{Given}\ \frac{-(Ca + Cc \cdot z - Ca \cdot z - Cm)}{(-Ca + Cd)} = 0 \qquad (9)$$
$$Z\max := find\ (z) \quad \therefore \quad Z\max = 0{,}9$$

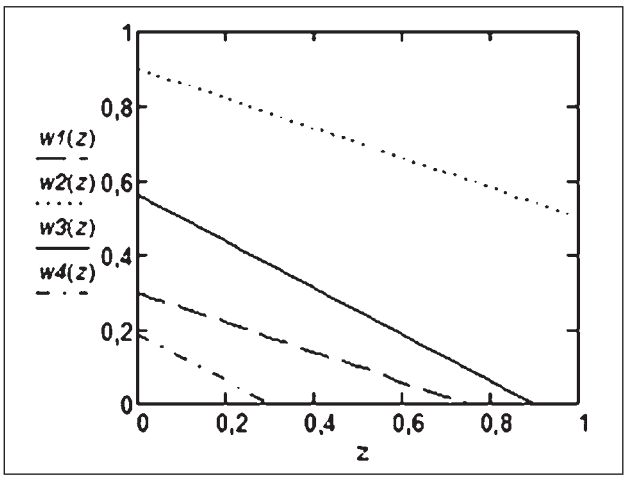

Figure 1 The graphic(al) interpretation of the solution in the domain of the independent variable *z*

z =	w1(z) =	w2(z) =	w3(z) =	w4(z) =
0	0,3	0,9	0,56	0,19
0,05	0,28	0,88	0,53	0,16
0,1	0,26	0,86	0,5	0,13
0,15	0,24	0,84	0,47	0,09
0,2	0,22	0,82	0,44	0,06
0,25	0,2	0,8	0,41	0,03
0,3	0,18	0,78	0,38	0
0,35	0,16	0,76	0,34	-0,03
...	...	...	...	...

Figure 2 Some values of the independent variable *z* And dependently variable values *w*(*z*)

The marginal points of the $w(z)$ function are

$$w3(Z\max) = 0 \quad \text{and} \quad w3(0) = 0{,}563 \qquad (10)$$

The field of the permissible solutions (the triangle 0, $w3(z)$, Zmax) for the marginal values of the components z and w is presented in the Figure 2). The preparation for the graphic presentation can be made on the basis of the interval variable Z (with the increment of 0.009) and the function

$$W3(Z) : Z := 0,\ 0{,}09\ ..\ Z\max \text{ and}$$
$$W3(Z) := w3(Z) \qquad (11)$$

The numerical simulation of the values of the Z contents and W components in 4K mixture, is being performed on the basis of the random numbers [7], but only in the isolated field of the acceptable solutions. So, we get:

- The simulated value:

$$Z := rnd(Z\max) \quad \text{i.e.} \quad Z = 0{,}001$$

- The simulated value:

$$W := rnd(W3(0)) \quad \text{i.e.} \quad W = 0{,}109$$

The simulation of the contents X and Y components in the 4K mixture is being performed on the basis of solving the set equations of the mixtures:

$$X + Y = 1 - Z - W \qquad (12)$$
$$Ca \cdot X + Cb \cdot Y = Cm - Cc \cdot Z - Cd \cdot W$$

Where is: *mat* the matrix of the technical coeficients and *vek* limitation vector:

$$mat := \begin{pmatrix} 1 & 1 \\ Ca & Cb \end{pmatrix},\ vek := \begin{pmatrix} 1 - Z - W \\ Cm - Cc \cdot Z - Cd \cdot W \end{pmatrix} \qquad (13)$$

On the basis of the previous, is being set the model for solving:

$$\begin{pmatrix} X \\ Y \end{pmatrix} := lsolve(mat, vek) \qquad (14)$$

So, one gets the remaining two values of the mixture composition:

The simulated value $X \approx 0{,}65$ and $Y \approx 0{,}56$.

THE PROGRAM VERIFICATION OF THE MODEL

The matrix of the interval values of the participation of the components in 4K mixture, has been formed as the control matrix of the values of the least possible, simulated and maximal participations in the mixture composition:

$$M := \begin{bmatrix} 0 & X & 1 \\ 0 & Y & 1 \\ 0 & Z & Z\max \\ 0 & W & W3(0) \end{bmatrix} = \begin{bmatrix} 0 & 0{,}286 & 1 \\ 0 & 0{,}604 & 1 \\ 0 & 0{,}001 & 0{,}9 \\ 0 & 0{,}109 & 0{,}56 \end{bmatrix} \qquad (15)$$

From the matrix can be formed a randon vector of the acceptable values as:

$$M^{<1>} = \begin{bmatrix} X \\ Y \\ Z \\ W \end{bmatrix} = \begin{bmatrix} 28{,}60 \\ 60{,}42 \\ 0{,}110 \\ 10{,}86 \end{bmatrix} /\%/ \qquad (16)$$

The verification of the equation of 4K composition of the mixture on the basis of the second vector of the matrix column can be performed directly in programmed way [5]:

$$\sum M^{<1>} = 100\ \% \text{ or}$$

$$X + Y + Z + W = 1 \qquad (17)$$

The verification of the criterium of the price constancy of the mixture cost price is being performed on the basis of the multiplication produce of the prices vector and the transposed random vector of the premissible 4K composition:

$$\begin{bmatrix} Ca & Cb & Cc & Cd \end{bmatrix} \cdot \begin{bmatrix} X & Y & Z & W \end{bmatrix}^T \qquad (18)$$

It can be stated that both previous equations are satisfied on the basis of the obtained results, and that the vector of the composition is an optimal vector of solution.

THE SECOND CASE: *Cb<Cm<Cc*

For the chosen vector the prices of the components and the mixture /CU/kg/:

$$\begin{bmatrix} Ca & Cb & Cc & Cd & Cm \end{bmatrix} = \begin{bmatrix} 15 & 20 & 25 & 31 & 24 \end{bmatrix} \qquad (19)$$

And the function domain of the component composition z: z:=0, 0,1…1, the explicit form of the inequation of the mixture composition for the conditions

$(0 \le x,\ y \le 1)$ is being obtained as: (20)

I field: $w1(z) \ge \dfrac{-(Cb + Cc \cdot z - Cm - z \cdot Cb)}{(Cd - Cb)}$

II field: $w2(z) \le \dfrac{-(Cc \cdot z + Cm + z \cdot Cb + Ca)}{(Cd - Cb)}$

III field: $w3(z) \ge \dfrac{-(Ca + Cc \cdot z - Ca \cdot z - Cm)}{(-Ca - Cd)}$

IV field: $w4(z) \le \dfrac{-(-Cc \cdot z + Ca \cdot z + Cm - Cb)}{(Ca - Cd)}$

Note: In the paper are being used as well the syntaxes represented in Mathcad [7], which are similar to the usual mathematical syntaxes which often appear in literature.

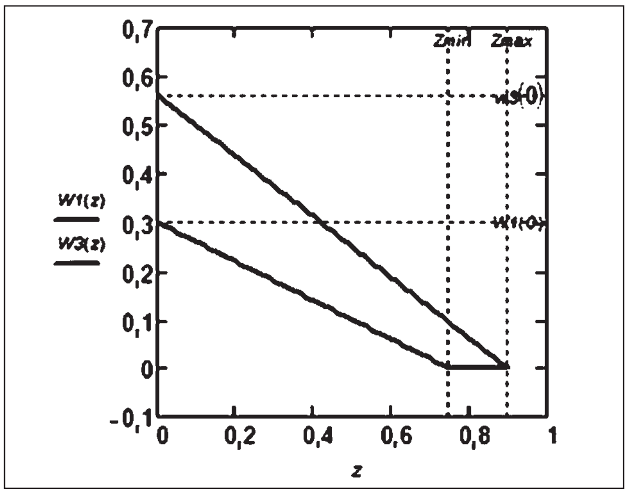

Figure 3 The graphic interpretation of the field of the acceptable solutions

Determing of the marginal point *Zmax* of *Z* function.

Given (21)

$$\frac{-(Ca + Cc \cdot z - Ca \cdot z - Cm)}{(-Ca + Cd)} = 0$$

$$Z\max := find(z) \quad \therefore \quad Z\max = 0{,}9$$

Given

$$\frac{-(Cb + Cc \cdot z - Cm - z \cdot Cb)}{(Cd - Cb)} = 0$$

$$Z\min := find(z) \quad \therefore \quad Z\min = 0{,}8$$

The marginal points of *w(z)* function

$$w3(Z\max) = 0 \quad \text{and} \quad w3(0) = 0{,}563$$

The field of the permissible solutions (the polygon in Figure 3) for the marginal values of *Z* and *W* (Figure 4).

$$Z := 0,\ 0{,}09\ ..\ Z\max \quad \text{and} \quad W3(Z) := w3(Z)$$

$$W1(z) := if\,(z < Z\min,\ w1(z), 0)$$

$$\Delta W(Z) := W3(Z) - W1(Z) \qquad (22)$$

The program solution in Mathcad in the form of the solution vector, is the next:

The numerical simulation of the values of *Z* contents and *W* components in 4K mixture is being performed on the basis of the random numbers of the defined field of the permissible solutions. So, one gets:

Z =	W1(Z) =	W3(Z) =	ΔW(Z) =
0	0,3	0,563	0,263
0,05	0,28	0,531	0,251
0,1	0,26	0,5	0,24
0,15	0,24	0,469	0,229
0,2	0,22	0,438	0,218
0,25	0,2	0,406	0,206
0,3	0,18	0,375	0,195
...	...	...	...

Figure 4 The part of the limit values in the acceptable field

• The simulated value:

$$Z := rnd(Z\max) \quad \text{i.e.} \quad Z = 0{,}741$$

• The simulated value:

$$W := W1(Z) + rnd\ (\Delta W\ (Z)) \quad \text{i.e.} \quad W = 0{,}040$$

The simulation of the contents of X and Y components in 4K mixture is being performed on the basis of solving the set mixture equations:

$$X + Y = 1 - Z - W \qquad (23)$$
$$Ca \cdot X + Cb \cdot Y = Cm - Cc \cdot Z - Cd \cdot W$$

Where is: *mat* matrix of the technical coefficients and *vek* limitation vector:

$$mat := \begin{pmatrix} 1 & 1 \\ Ca & Cb \end{pmatrix},\ vek := \begin{pmatrix} 1 - Z - W \\ Cm - Cc \cdot Z - Cd \cdot W \end{pmatrix} \qquad (24)$$

On the basis of the previous is set the model for solving:

$$\begin{pmatrix} X \\ Y \end{pmatrix} := lsolve(mat, vek) \qquad (25)$$

So, one gets on the basis of the computer simulation:

The simulated value $X \approx 0{,}03$ and $Y \approx 0{,}19$.

THE PROGRAM VERIFICATION OF THE MODEL

The control matrix of the interval values of the component participation in 4K mixture:

$$M := \begin{bmatrix} 0 & X & 1 \\ 0 & Y & 1 \\ 0 & Z & Z\max \\ 0 & W & W3(0) \end{bmatrix} = \begin{bmatrix} 0 & 0{,}028 & 1 \\ 0 & 0{,}92 & 1 \\ 0 & 0{,}741 & 0{,}9 \\ 0 & 0{,}040 & 0{,}563 \end{bmatrix} \qquad (26)$$

On the basis of this is a random vector of the acceptable values:

$$M^{<1>} = \begin{bmatrix} X \\ Y \\ Z \\ W \end{bmatrix} = \begin{bmatrix} 2{,}78 \\ 19{,}2 \\ 74{,}06 \\ 3{,}97 \end{bmatrix} /\%/ \qquad (27)$$

The verification of the composition equation of 4K mixture on the basis of the second vector of M matrix columin follows:

$$\sum M^{<1>} = 100\ \%\ \text{or}$$
$$X + Y + Z + W = 1 \qquad (28)$$

The verification of the constancy criterium of the cost price of the mixture is being performed, also, on the basis of the multiplacation product of the prices vector and transposed random vector of the permissible 4K mixture:

$$[\,Ca\ Cb\ Cc\ Cd\,] \cdot [\,X\ Y\ Z\ W\,]^{T} = 24\ /\text{CU}/ \qquad (29)$$

Note: CU – Currency Unit.

It can be established that both equations are on the basis of the obtained results satisfied, and that the composition vector is the second optimal solution vector.

CONCLUSION

The solutions that are being perceived in the set of diagrams and tables, present a set of points of the permissible solutions that are among the restricting limiting straight lines: $w1(z)$, $w2(z)$, $w3(z)$ and $w4(z)$ and which present the coordinates within the watched polygon obtained on the basis of the cross – section of the points sets in the looked at fields. These selectional fields are the sole ones which present the basis for the simulation of the two values of the mixture composition. The other two are easily obtained by solving the two equations with the two remained unknown values of the mixture composition. The character of these two calculated values is also random on account of the starting conditions and consequences. Very important componne-nt of this model variants which are many and are not presented here, is the possibility of the program verification of the model. This, as a rule, presents the integral phase in the development of every simulation models. From the practical point of view the importance of the results of this project is great, because it can give certain savings, taking into consideration that the model based on the criterium of the composition optimum at the constant price of the mixture. The application of this model is universal, because it does not refer only to the defining of the composition of the polymer fibres, but as well in the determing of the mixture of new materials for new technologies at the criterium of the constant price. Although in the paper are used the efficient combined methods of the linear progamming and numerical simulation, the ways for more effective solution of the mixture problem would be certainly in the multicriteria optimization. There would be set the conditions that would cover not only the criterion of the constant mixture price, but also very important matter, i.e. which components have the quantative and qualitative limitations in the mixture of different forms of the substance with the example of the polymer mixing in textile.

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Note: The responsible translator of English language is Srđan Šerer, Technical Faculty “M. Pupin”, Zrenjanin, University of Novi Sad, Serbia