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Nonconvex Separable Programming Problem for Optimal Raw Material Mix in Flexible Polyurethane Foam Production

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Abstract

Nonconvex Separable Programming (NSP) for selecting optimal raw material mix for flexible polyurethane foam production (FPFP) was developd. With unit cost function (ψ) as objective function;,Density(P_1); compression set (P_2); elongation(P_3); hardness-index(P_4) and tensile strength *(P_5)* and other boundary conditions as constraints, an NSP foam raw material mix problem was defined and solved. Twelve existing formulation were used for validation .The cost and physical properties were determined and compared to the existing products using t-test. The optimal raw material mix 1.00, 0.4366, 0.0398, 0.0066, 0.0115, 0.0026, 0.0046 kg of polyol, toluene-di-isocynate, water, amine, silicone-oil, stannous-octoate and methylene-chloride respectively, were significantly different from the existing formulations. The validated values of P_1, P_2, P_3, P_4, P_5 from optimally formulated foams were 23.83kgm^{-3}, 8.6%, 159.35%, 143.19N, and 117.33kNm^{-2}, respectively and conformed to standard. The associated costs per metric tonne of the optimal mixes were lower than that of existing mixes.

Keywords: Polyurethane foam, Optimal-mix, Separable programming , nonconvex, elongation.

1.0 Introduction

Flexible polyurethane foams are produced by the controlled expansion of gas during the polymerization process and its uses include applications such as seating, cushioning, carpet underlayment, fabric backing, insulation, and packaging (Demir *et al,* 2008). The formation of flexible polyurethane foams relies on a complex interaction between physical and chemical phenomena in which there are no independent chemical or process variables (Mills, 2007) to give foam its physical properties.

Manufacturing cost savings is a challenge to foam manufacturers all over the world due to the economic dynamics of the sector exibited in the continued pressure on their profitability from high raw materials costs and volatile energy prices, making price increases essential for margin recovery (Taylor, 2004). Several foam companies in the growing economies apart from skyrocketing raw materials cost that is typical of challenges that polyurethane foam firms are addressing around the world, they also often face restrictive financial controls and punitive tax system in their countries, as well as competition from foreign firms (Moore, 2001).

Other related reports on foam production reveal that more than 80% of cost of production of foam is associated to the cost of raw materials used especially for the third world nations (Makanjuola, 1999, IAL, 2005; Zhang, *et al*, 2007). Thus, a non optimal raw materials mix results in arbitrarily high prices of foam products. It thus becomes more pertinent to analyse the raw material mix that will minimize the cost inorder to improve the profit margin of the producers and the burden of the buyers. Therefore, process operations optimisation otherwise called operations research is essential for any manufacturer involved in this type of process if he wants to stay competitive in the industry.

Most mathematical efforts on foam production have centred on effect of the state of the foam on the final properties of the foam (Sims & Bennet, 1998; Widdle Jr, *et al*, 2008) while much attention has not been given quantitatively to what leads to these states. For instance, the cell openness determines the density of the foam and much work have been done to relate the cell diameter to the density of the foam but more importantly, it is very necessary to relate the amount of raw materials used to the foam density since it directly influences the cell openness.

This present approach employed the concept of response surface methodology (RSM) to formulate a separable programming problem for minimising raw materials cost by finding the optimal raw material mix that satisfies the quality constraints. Separable programmes are nonlinear mathematical programmes in which the objective functions and constraints can be expressed as sum of all functions, each nonlinear term involving only one variable (Li & Yu,1999; Niederhoff, 2007; Patriksson, 2008). According to Stefanov (2001a), a function $f: X \rightarrow \Re, X \subset \Re^n$ is said to be separable if

$$f(x) = \sum_{j=1}^{n} f_j(x_j), \qquad (1)$$

that is, if $f(x_1,...,x_n)$ can be expressed as the sum of n single-variable functions $f_1(x_1),...., f_n(x_n)$. When the objective function and the constraints are separable, the nonlinear programme is called a separable programme that can either be convex or nonconvex (Li & Yu, 1999; Stefanov, 2004). Suppose that *j=1,. . .,n,* the function $f_j(x): \Re \rightarrow \Re$ and $g_{ij}(x): \Re \rightarrow \Re$ are differentiable and that $-\infty \leq L_j < U_j \leq +\infty$ holds. Also, if $b_i \in \Re$, then a separable programming problem has the following general statement:

$$Minimize \quad f(x) = \sum_{j=1}^{n} f_j(x_j) \qquad (2)$$

Subject to:

$$g_i(x) = \sum_{j=1}^{n} g_{ij}(x_j) \leq b_i \qquad i = 1,2...m \qquad (3)$$

$$x_j \in X_j = [L_j, U_j], j = 1,...n, \qquad (4)$$

where $X \subset \Re^n$ denotes the feasible set of the problem (2) – (4). The problem has a finite optimal solution if, for example, X is bounded or if each of $f_j(x)$ is such that $f_j(x_j) \rightarrow +\infty$ whenever $x_j \rightarrow \pm\infty$. (Glen, 2006 ; Patriksson, 2008). Therefore, the purpose of this paper is thus to formulate and apply separable programming to optimal raw materials mix for flexible polyurethane foam production that minimises raw material cost subject to foam property standard requirements.

2.0 Separable Programming Problem for Optimal Raw Material Mix

The problem addressed in this study is that of developing and minimising a nonconvex separable programming problem of raw material cost function subject to constraints of foam physical properties functions (density, elongation, compression set, hardness and tensile strength) This constitutes a separable mathematical programming model for selecting optimal raw materials mix that minimises the cost of raw materials subject to the quality requirements of the flexible polyurethane foam and bounds on the raw materials quantities in a batch process.

2.1 Notations

P_1 Density of Polyurethane foam in kgm^{-3}

P_2 Compression set of Polyurethane foam in %

P_3 Elongation of Polyurethane foam in %

P_4 Hardness index of Polyurethane foam in kN

P_5. Tensile strength of Polyurethane foam in kNm^{-3}

X_1 Mass of Toluene-di-isocynate (TDI) in kg/ kg of Polyol.

X_2 Mass of Water in kg / kg of Polyol.

X_3 Mass of Amine in kg/kg of Polyol.

X_4 Mass of Silicone Oil in kg/kg of Polyol.

X_5 Mass of Stannous Octoate in kg/kg of Polyol.

X_6 Mass of Methylene Chloride in kg/kg of Polyol

2.2 Raw Materials Minimization Problem

The total cost of raw material (ψ) (in Nigerian Naira) is the sum of the product of each of the unit cost and the quantity x_i of raw material *i*. Ogunleye (2009) reported that six categories of models were identified to be sufficient to describe the process of flexible polyurethane foam production The detail derivation of these models is available in Ogunleye & Oyawale (2011) and will not be presented here but only the resulting formulations. Adopting Taha (2004) and Hillier & Lieberman (2005) principles of separable mathematical programming, the problem statement that minimizes the raw material cost for the material mix in flexible polyurethane foam production subject to the various physical property requirements is thus given below:

Minimize $\psi = 195 + 265\mathbf{X}_1 + 20\mathbf{X}_2 + 535\mathbf{X}_3 + 875\mathbf{X}_4 + 1500\mathbf{X}_5 + 120\mathbf{X}_6$ (5)

Subject to

$$59.15\mathbf{X}_1 + 1.31\mathbf{X}_2^{-1} - 111.45\mathbf{X}_3 + 475.81\exp(-\mathbf{X}_4) + 6632.27\mathbf{X}_5 + 61.60\exp(-\mathbf{X}_6) + 585.62 \geq \mathbf{P}_1 \quad (6)$$

$$-214.42\mathbf{X}_1 + 3247.53\mathbf{X}_2 - 283.37\mathbf{X}_3 + 0.023\mathbf{X}_4^{-1} - 0.077\mathbf{X}_5^{-1} + 103.56\exp(\mathbf{X}_6) - 82.21 \leq \mathbf{P}_2 \quad (7)$$

$$-55.38\mathbf{X}_1^{-1} - 7024.81\mathbf{X}_2 - 602.86\mathbf{X}_3 - 0.05\mathbf{x}_4^{-1} - 0.33\mathbf{X}_5^{-1} - 2812.10\mathbf{X}_6 + 758.66 \geq \mathbf{P}_3 \quad (8)$$

$$-97.07\exp(\mathbf{X}_1) + 1266.55\exp(\mathbf{X}_2) - 1430.64\mathbf{X}_3 + 2707.74\mathbf{X}_4 + 8183.55\exp(\mathbf{X}_5) + 492.12\exp(-\mathbf{X}_6) - 9709.41 \geq \mathbf{P}_4 \quad (9)$$

$$14.63\mathbf{X}_1 + 1.23\mathbf{X}_2 - 49.51\mathbf{X}_3 + 1172.90\exp(\mathbf{X}_4) - 7594.09\exp(\mathbf{X}_5) + 142.91\exp(-\mathbf{X}_6) + 6364.03 \geq \mathbf{P}_5 \quad (10)$$

$$\mathbf{X}_1 - 1.44\mathbf{X}_2 + \mathbf{X}_3 + \mathbf{X}_4 + \mathbf{X}_5 \geq \mathbf{m} \quad (11)$$

$$\mathbf{X}_1 \geq 13.5\mathbf{X}_2 \quad (12)$$

$$0.25 \leq \mathbf{X}_1 \leq 0.85 \quad (13)$$

$$0.015 \leq \mathbf{X}_2 \leq 0.075 \quad (14)$$

$$0.001 \leq \mathbf{X}_3 \leq 0.01 \quad (15)$$

$$0.007 \leq \mathbf{X}_4 \leq 0.025 \quad (16)$$

$$0.001 \leq \mathbf{X}_5 \leq 0.005 \quad (17)$$

$$0 \leq \mathbf{X}_6 \leq 0.35 \quad (18)$$

2.3 Solution Strategy

With respect to equation (2) –(4) , Stefanov(2001b), Lu & Ito (2003),Taha (2004), Gao *et al (*2005), Hillier & Lieberman (2005), Glen (2006) , Yu *et al* ,2007; Patriksson (2008) however, stated that when *f(x)* and the $g_i(x)$ satisfy the assumptions of separable programming, an approximate piecewise linear functions can be written. In doing this, let *K* be the number of line of segments (grid points) in the $f_j(x_j)$ so that

$$x_j = \sum_{k=1}^{K} x_{jk} \tag{19}$$

And, if the function $f_j(x_j)$ can be represented by the figure 1 with the *kth* breaking point of the function given by $x_j = y_{kj}$ Considering Figure 1, if ρ_{kj} represent the gradients of the function $f_j(x_j)$ at break point *k* and if function $g_{ij}(x_j)$ behaves essentially the same way with gradients ρ_{kij} ,

$$\rho_{kj} = \frac{f_j(y_{kj}) - f_j(y_{k-1,j})}{y_{kj} - y_{k-1,j}} \tag{20}$$

$$\rho_{kij} = \frac{g_{ij}(y_{kj}) - g_{ij}(y_{k-1,j})}{y_{kj} - y_{k-1,j}} \tag{21}$$

Let x_{kj} be the increment of variable x_j in the range $(y_{k-1,j}, y_{kj})$,$k=1,2.....K_i$

Then

$$x_j = \sum_{k=1}^{Kj} x_{kj} \tag{22}$$

$$f_j(x_j) \cong \sum_{k=1}^{Kj} (\rho_{kj} x_{kj}) + f_j(y_{0j}) \tag{23}$$

$$g_{ij}(x_j) \cong \sum_{k=1}^{Kj} (\rho_{kij} x_{kj}) + g_{ij}(y_{0j}) \quad j=1..,n \quad i=1...,m \tag{24}$$

Equations (22) - (24) will hold if and only if

$$0 \le x_{kj} \le y_{kj} - y_{k-1,j} \qquad k = 1, 2...,K_i \tag{25}$$

Based on the linearization principle discussed above, equations (22) and (23) are essentially linear in nature and an equivalent linear programme problem to that of equations (2) –(4) is given as:

$$Minimize \quad f(x) = \sum_{j=1}^{n} \left(\sum_{k=1}^{Kj} (\rho_{kj} x_{kj}) + f_j(y_{0j}) \right) \tag{26}$$

Subject to:

$$\sum_{j=1}^{n} \left(\sum_{k=1}^{Kj} (\rho_{kij} x_{kj}) + g_{ij}(y_{0j}) \right) \le b_i \qquad i = 1, 2...,m \tag{27}$$

$$0 \le x_{kj} \le y_{kj} - y_{k-1,j} \qquad k = 1, 2...,K_j, j=1, 2...,n \tag{28}$$

Equations (26)-(28) therefore constitute a linear programme problem that is well suited for any Linear Prpgramming solution approach depending on the number of variables involved and ease of solution. This new problem can be solved by simplex method with upper bound variable.

However, Hillier & Lieberman (2005) approach on interior point algorithm was adopted for the solution of the linear equivalence of the problem. The concept of the interior point algorithm is as follows:

The four basic concepts of the interior point method are as follows:

1. Obtain an Initial feasible solution (using Gaussian elimination)
2. Shoot through the interior of the feasible region towards an optimal solution.
3. Move in a direction that improves the objective function value at the fastest rate.
4. Transform the feasible region to place the current trial solution near the centre, thereby enabling a large improvement when concept 2 is implemented.

Due to the rigorous computation involved in the above algorithm, a computer programme to implement this was written in Dephi language that has been proven for high computational efficiency and effectiveness. The user's interphase of the computer programme is given on Figure 2

2.4 Post Optimisation Operations

In validating this optimization framework, twelve (12) randomly selected existing foam formulations (Table 1) were selected and solved for optimal mixes. The foams produced from these optimal mixes were produced and physical properties tested and differences in the existing formulations and the new optimal mix were compared using t-test.

3.0 Results and Discussion

3.1 Optimal Raw Material Mix

The physical properties requirements which constitutes the $P_{i;}$ the right hand side values of the constraints of equations (6) – (9) and the usual raw material mix are given in Table1. The optimisation carried out on these practical problems from the existing practice resulted in the optimal raw material mix and the accompanying physical properties are given in Table 2

The average optimal raw material mix of polyol, toluene-di-isocynate, water, amine, silicone-oil, stannous-octoate and methylene-chloride were 1.00, 0.4366, 0.0398, 0.0066, 0.0115, 0.0026 and 0.0046 kg, respectively while the values of the existing practice were 1.0000, 0.5251, 0.0423, 0.0026, 0.0086, 0.0021 and 0.0073 kg. As shown on Table 3, the t-test statstics for the comparison of the optimal raw material mix with the existing raw material mix that is in practice showed that there are significant differences between the two samples at $p<0.05$.

The result of the physical property test conducted on the twelve foam samples from the validation of the optimal raw material mix is given in Table 2. Similar result on the comparison of the physical properties of the optimal mix foam as compared with the existing ones is presented in Table 4. The density (23.83kgm^{-3}), compression-set (8.6%), elongation (159.35%), hardness-index (143.19N) and tensile strength (117.33kNm^{-2}) of the optimally formulated foam conformed to the ISO5999-2007 quality standards and was not significantly different from the existing ones at $p<0.05$.

This result of the analysis of the physical properties obtained after 24 hours of curing compared favourably with those of existing practice as shown of Table 4. This is an indication that an efficient combination of raw materials can reduce the total amount of material used thus reducing the total cost without losing the desired properties of the foam. The model developed proviides solutions to various problems associated with the production of flexible polyurethane foam. This gives a wholistic approach to the quality assurance of the final products.

The average optimal cost per metric tonne of polyol for TDI, water, amine, silicone oil, stannous octoate and methylene chloride were ₦126387.33, ₦807.00, ₦1382.09, ₦ 10047.92, ₦ 3725.00 and ₦ 960.00 respectively.Similar values for the existing practice were ₦140215.92, ₦ 855.00, ₦ 3513.17, ₦ 7597.92, ₦ 3075.00 and ₦ 963.00. Total average cost of ₦346386.10 per metric tonne of the optimal mix was significantly lower than ₦369827.68 per metric tonne of the existing practice at $p < 0.05$.

3.2 Performance Evaluation of the Optimisation Computer Programme

Several ways are available for evaluating the performance of an algorithm. But Sun *et al* (2008) metrics method was adopted for this work. The performance indices of this method include approximation accuracy, space ratio and CPU time. Space ratio is defined as the ratio of the number of output entries to the number of input entries. Large space ratio means more space and memory consumption. The CPU time spent in computing the output quantifies the computational expense.

The developed strategy was compared with two other algorithms; the simplex method (that is a linear programme method) and a sequential quadratic programme method (a non linear programme method).

By using two case studies as the basis, the result of the evaluation is presented in Table 5. The formulation and costs obtained from the three methods are on the same accuracy level as there are no significant differences between them. SQP has the shortest CPU time, followed by the NSP while the simplex method has the largest computional time. The NSP algorithm is more efficient than the two other algorithms on the basis of space requirement.

Comparing this strategy with an fmincon algorithm that is SQP based in the matlab 6.5 software, SQP has almost the same computational time with the NSP which additionally has the memory requirement advantage. When problems with higher number of variables are encountered, the developed algorithm becomes superior to the SQP and also when the inequality constraints are changed to equality constraints which makes it computationally complex , the SQP algorithm becomes unstable which is not so with NSP.

4.0 Conclusions

Based on the development and implemention of a separable mathematical programming model for selecting optimal raw material mix for flexible polyurethane foam production in this study, the following conclusions can be drawn. The optimal raw material mix and the associated cost per metric tonne were significantly lower than that of the existing practice while the physical properties of the optimal foam formulation foam conformed to the quality standards. The optimisation strategy developed has memory advantage over the sequential quadratic programme and simplex method. The separable programming model developed is an effective instrument for optimal formulation of flexible polyurethane foams with desirable quality characteristics.

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Table 2: Optimal Raw Material Mix and its Physical Properties from Validation of the Practical Problems per 1kg Polyol

Raw Materials	Optimal Raw Material Mix for Practical Problems											
	1	2	3	4	5	6	7	8	9	10	11	12
Polyol	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
TDI	0.5557	0.5549	0.5488	0.4940	0 .4829	0.5017	0.5491	0.5133	0 .5113	0.2351	0.3682	0.4082
Water	0.0438	0.0438	0.0440	0.0404	0.0402	0.0402	0.0402	0.0410	0.0416	0.0490	0.0286	0.0314
Amine	0.0026	0.0026	0.0026	0.0026	0.0026	0.0026	0.0026	0.0026	0.0026	0.0020	0.0030	0.0026
Silicone Oil	0.0116	0.0116	0.0116	0.0108	0.0110	0.0114	0.0116	0.0110	0.0120	0.0120	0.0110	0.0122
Stannous Octoate	0.0026	0.0026	0.0026	0.0024	0.0026	0.0026	0.0026	0.0026	0.0026	0.0010	0.0030	0.0026
MC	0.0046	0.0046	0.0046	0.0046	0.0046	0.0046	0.0046	0.0046	0.0046	0.0040	0.0046	0.0460
Physical Properties	**Physical Properties of the Validation Samples**											
Density(kgm^{-3}) :P_1	21.00	20.80	20.60	23.50	23.80	24.20	20.40	22.80	21.90	17.50	32.30	29.80
Compression Set (%):P_2	7.00	7.00	7.00	10.50	12.90	13.30	7.00	7.20	7.00	10.00	4.30	7.80
Elongation at Break(%) : P_3	160.10	160.00	160.00	152.00	147.00	140.00	160.20	190.00	163.00	140.00	276.00	162.00
Hardness Index(KN) : P_4	162.00	162.00	161.00	150.00	144.00	140.00	162.00	161.80	161.90	98.00	170.00	148.00
Tensile-Strength(KNm^{-2}): P_5	120.00	120.00	119.00	116.00	114.00	108.00	120.00	119.00	120.00	113.00	128.00	120.00

Table 1: Physical Properties and Existing Raw Material Mix per 1kg Polyol for Validation Operation

Physical Properties	Practical Problems From Existing Practice											
	1	2	3	4	5	6	7	8	9	10	11	12
Density(kgm^{-3}) :P_1	20.14	20.18	20.35	23.11	23.59	24.03	20.40	22.40	21.80	17.90	32.40	30.8
Compression Set (%):P_2	6.89	6.89	6.89	10.34	13.10	15.52	6.89	7.14	7.10	9.60	4.00	7.8
Elongation at Break(%) : P_3	160.10	160.00	160.00	152.00	147.00	140.00	160.04	189.00	162.00	139.00	274.00	161.5
Hardness Index(KN) : P_4	161.80	161.50	160.00	149.00	143.00	138.00	161.70	161.40	161.80	97.70	168.00	148
Tensile-Strength(KNm^{-2}): P_5	119.44	119.09	118.44	115.28	113.89	106.94	119.10	119.10	119.60	112.50	126.00	119.8
Raw Materials	**Raw Material Mix for Practical Problems From The Existing Practice**											
Polyol	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
TDI	0.5400	0.5400	0.5400	0.5400	0.5400	0.5400	0.5400	0.5300	0.5900	0.6100	0.3700	0.4694
Water	0.0440	0.0440	0.0440	0.0440	0.0440	0.0440	0.0440	0.0420	0.0465	0.0506	0.0280	0.0379
Amine	0.0025	0.0025	0.0025	0.0025	0.0025	0.0025	0.0025	0.0030	0 .0020	0.0518	0.0030	0.0015
Silicone Oil	0.0120	0.0100	0.0080	0.0060	0.0040	0.0020	0.0076	0.0100	0.0115	0.0120	0.0087	0.0124
Stannous Octoate	0.0018	0.0018	0.0025	0.0018	0.0018	0.0018	0.0018	0.0020	0.0019	0.0024	0.0025	0.0025
MC	0.0000	0.0000	0.0482	0.0000	0.0000	0.0000	0.0000	0.0000	0 .0000	0.0000	0.0000	0.0481

Source: Ogunleye (2009)

Table 3: Summary of t-Test for Comparing Optimal and Existing Raw Material Mix for Foam Production

Source of Variation	t-Value Calculated	t-Value Critical	p- value (2 tail)	Remark
Polyol	-	-	-	-
TDI	3.019*	2.201	0.012	Significantly different
Water	3.829*	2.201	0.003	Significantly different
Amine	2.975*	2.201	0.021	Significantly different
Silicone Oil	-3.373*	2.201	0.006	Significantly different
Stannous Octoate	-5.903*	2.201	0.000	Significantly different
MC	2.551*	2.201	0.022	Significantly different

*Significant level at $p < 0.05$

Table 4: Summary of t-Test for Comparing Physical Properties of Foam Samples of the Optimal and Existing Mixes.

Source of Variation	t-Value Calculated	t-Value Critical	p- value (2 tail)	Remark
Density	0.797*	2.201	0.442	No Significant Difference
Compression Set	0.713*	2.201	0.491	No Significant Difference
Elengation	-2.169*	2.201	0.053	No Significant Difference
Hardness Index	-2.192 *	2.201	0.051	No Significant Difference
Tensile Strength	-1.434*	2.201	0.179	No Significant Difference

*Significant level at $p < 0.05$

Table 5: Performance Evaluation of the Optimisation Computer Programme

	Case 1:21kg/m^3 Foam			Case 2:30kg/m^3 Foam		
CRITERIA	**NSP**	**SM**	**SQP**	**NSP**	**SM**	**SQP**
Optimised Values						
Polyol	1	1	1	1	1	1
TDI	0.5133	0.5135	0.4940	0.4082	0.4100	0.4176
Water	0.0410	0.0410	0.0366	0.0314	0.0312	0.0266
Amine	0.0026	0.0025	0.0010	0.0026	0.0025	0.0010
Silicone Oil	0.0110	0.0112	0.0125	0.0122	0.0120	0.0070
Stannous Octoate	0.0026	0.0025	0.0018	0.0026	0.0025	0.0013
Methylene Chloride	0.0046	0.0045	0.0000	0.0460	0.0045	0.0000
Minimized Cost (₦)/kg polyol	347.50	347.54	347.53	320.38	320.42	320.40
Computer Time(secs)	34	42	32	34	45	32
Space Ratio	0.05	1	1	0.05	1	1

*NSP = Separable Mathematical Programme;

SM= simplex method and,

SQP= Sequential quadratic programme

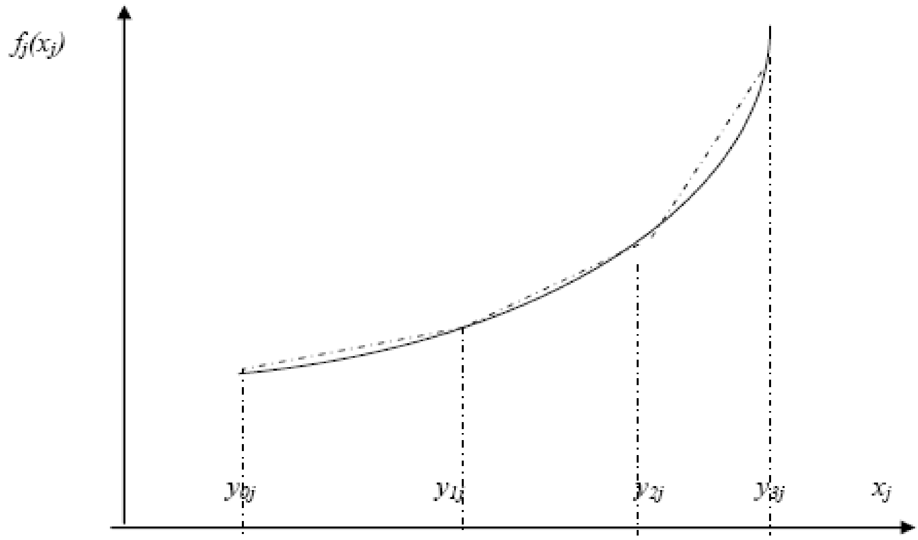

Figure 1: Discretisation point

Figure 2: User's Interface Homepage for the Foam Optimisation Programme