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A Gauss-Newton Approach for Nonlinear Optimal Control Problem with Model-Reality Differences

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Abstract

Output measurement for nonlinear optimal control problems is an interesting issue. Because the structure of the real plant is complex, the output channel could give a significant response corresponding to the real plant. In this paper, a least squares scheme, which is based on the Gauss-Newton algorithm, is proposed. The aim is to approximate the output that is measured from the real plant. In doing so, an appropriate output measurement from the model used is suggested. During the computation procedure, the control trajectory is updated iteratively by using the Gauss-Newton recursion scheme. Consequently, the output residual between the original output and the suggested output is minimized. Here, the linear model-based optimal control model is considered, so as the optimal control law is constructed. By feed backing the updated control trajectory into the dynamic system, the iterative solution of the model used could approximate to the correct optimal solution of the original optimal control problem, in spite of model-reality differences. For illustration, current converted and isothermal reaction rector problems are studied and the results are demonstrated. In conclusion, the efficiency of the approach proposed is highly presented.

Keywords

Nonlinear Optimal Control, Gauss-Newton Approach, Iterative Procedure, Output Error, Model-Reality Differences

1. Introduction

Many real processes are not linear in natural, so the actual model would not be necessary known. In addition to this, modeling the real process into a dynamical system could be an alternative solution plan. Since dynamical system has evolved over time, efficient computational approaches are highly demanded, and their development towards to optimize and control dynamical system is properly required. This situation imposes on obtaining the optimal solution of the real process enthusiastically. However, the difficulty level of solving the optimal control problems is increased with respect to the nonlinearity structure of dynamical systems. Simultaneously, the use of output measurement, especially from the industrial control applications [1], becomes importance in constructing the corresponding dynamical system, which covers model predictive control [2] [3] [4] [5], system identification [6] [7] [8], and data-driven control [9] [10] [11].

In fact, the solution methods of linear optimal control problem have been well-developed. Particularly, the linear quadratic regulator (LQR) technique is recognized as a standard procedure in solving the linear optimal control problems [12] [13] [14] [15] [16]. Recently, an efficient computational method, which is based on LQR optimal control model, is proposed to solve the nonlinear stochastic optimal control problems in discrete time [17] [18] [19] [20]. This approach is known as the integrated optimal control and parameter estimation (IOCPE) algorithm. It is an extension of the dynamic integrated system optimization and parameter estimation (DISOPE) algorithm [21]. The applications of the DISOPE algorithm have been well-defined in solving the deterministic nonlinear optimal control problem [22] [23]. By virtue of this, the IOCPE is developed, based on the principle of model-reality differences, for solving the discrete time deterministic and stochastic nonlinear optimal control problems.

Indeed, in both of these iterative algorithms, the adjusted parameters are introduced in the model-based optimal control problem. The aim is to calculate the differences between the real plant and the model used. These differences are then taken into account in updating the model used iteratively. Once the convergence is achieved, the iterative solution could approximate to the correct optimal solution of the original optimal control problem, in spite of model-reality differences. On the other hand, the use of the model output is an additional feature in the IOCPE algorithm [20], which does not executed in the DISOPE algorithm.

Definitely, in this paper, the use of the output measurement, rather than adding the adjusted parameters into the model used, is further discussed. In our approach, the LQR optimal control model with the output measurement is simplified from the nonlinear optimal control problem. The differences between the output measurements, which are, respectively, from the model used and the real plant are defined. Follow from this, a least squares scheme is established. The aim is to approximate the output that is measured from the real plant in such a way that the output residual between the output measurements is minimized. In doing so, the linear dynamic system in the model used is reformulated and the control sequence is added into the output channel. Then, the model output is presented as input-output equations.

During the computational procedure, the control trajectory is updated iteratively by using the Gauss-Newton algorithm. As a result, the output residual between the original output and the model output is minimized. Here, the optimal control law is constructed from the model-based optimal control problem, which is not adding the adjusted parameters. By feed backing the updated control trajectory into the dynamic system, the iterative solution of the model used approximates to the correct optimal solution of the original optimal control problem, in spite of model-reality differences. Hence, the efficiency of the approach proposed is highly recommended. On the basis of this, it is highlighted that applying the least-square updating scheme for solving discrete-time nonlinear optimal control problems, both for deterministic and stochastic cases, are well-presented. See [24] for more details on stochastic case.

The rest of the paper is organized as follows. In Section 2, a discrete time nonlinear optimal control problem is described and the corresponding model-based optimal control problem is simplified. In Section 3, the construction of the feedback optimal control law is discussed. The output residual is defined in which a least-squares minimization problem for the model-based optimal control problem is formulated. The iterative algorithm based on the Gauss-Newton method is established, and the computational procedure is summarized. In Section 4, two illustrative examples, which are current converted and isothermal reaction rector problems, are demonstrated, and their results show the efficiency of the approach proposed. Finally, some concluding remarks are made.

2. Problem Statement

Consider a general discrete time nonlinear optimal control problem, given by

$$\begin{aligned} &\min_{u(k)} g_0(u) = \varphi(x(N), N) + \sum_{k=0}^{N-1} L(x(k), u(k), k) \\ &\text{subject to} \quad x(k+1) = f(x(k), u(k), k), \ x(0) = x_0 \\ &\qquad\qquad\quad y_P(k) = h(x(k), k) \end{aligned} \tag{1}$$

where $u(k) \in \Re^m, k = 0,1,\cdots,N-1$, $x(k) \in \Re^n, k = 0,1,\cdots,N$ and $y_P(k) \in \Re^p$, $k = 0,1,\cdots,N$ are, respectively, control sequence, state sequence and output sequence, $f : \Re^n \times \Re^m \times \Re \to \Re^n$ represents the real plant and $h : \Re^n \times \Re \to \Re^p$ is the output measurement, whereas $\varphi : \Re^n \times \Re \to \Re$ is the terminal cost and $L : \Re^n \times \Re^m \times \Re \to \Re$ is the cost under summation. Here, g_0 is the scalar cost function and x_0 is the initial state. It is assumed that all functions in Equation (1) are continuously differentiable with respect to their respective arguments.

This problem, which is referred to as Problem (P), is complex. Solving Problem (P) would increase the computational burden and the exact solution might not exist due to the nonlinear structure of Problem (P). Nevertheless, in order to obtain the optimal solution of Problem (P), the linear model-based optimal control model, which is referred to as Problem (M), is proposed. This problem is given by

$$\min_{u(k)} g_1(u) = \frac{1}{2}x(N)^{\mathrm{T}} S(N)x(N) + \frac{1}{2}\sum_{k=0}^{N-1}\left(x(k)^{\mathrm{T}} Qx(k) + u(k)^{\mathrm{T}} Ru(k)\right)$$
$$\text{subject to} \quad x(k+1) = Ax(k) + Bu(k),\ x(0) = x_0 \qquad (2)$$
$$y_M(k) = Cx(k)$$

where $y_M(k) \in \Re^p, k = 0,1,\cdots,N$ is model output sequence, $A \in \Re^{n\times n}$ is a state transition matrix, $B \in \Re^{n\times m}$ is a control coefficient matrix, and $C \in \Re^{p\times n}$ is an output coefficient matrix, while $S(N) \in \Re^{n\times n}$ and $Q \in \Re^{n\times n}$ are positive semi-definite matrices and $R \in \Re^{m\times m}$ is a positive definite matrix. Here, g_1 is the scalar cost function.

Notice that only solving Problem (M) would not give the optimal solution of Problem (P). However, by constructing an efficient matching scheme, it is possible to obtain the optimal solution of the original optimal control problem, in spite of model-reality differences.

3. System Optimization with Gauss-Newton Updating Scheme

Now, consider the following solution method on system optimization. Define the Hamiltonian function for Problem (M) as follows:

$$H(k) = \frac{1}{2}\left(x(k)^{\mathrm{T}} Qx(k) + u(k)^{\mathrm{T}} Ru(k)\right) + p(k+1)^{\mathrm{T}}\left(Ax(k) + Bu(k)\right). \qquad (3)$$

Then, the augmented objective function becomes

$$g_1'(u) = \frac{1}{2}x(N)^{\mathrm{T}} S(N)x(N) + p(0)^{\mathrm{T}} x(0) - p(N)^{\mathrm{T}} x(N) + \sum_{k=0}^{N-1}\left(H(k) - p(k)^{\mathrm{T}} x(k)\right) \qquad (4)$$

where $p(k) \in \Re^n$ is the appropriate multiplier to be determined later.

3.1. Necessary Optimality Conditions

Applying the calculus of variation [12] [14] [15] [16] to the augmented cost function in Equation (4), the necessary optimality conditions are obtained, as shown below:

(a) Stationary condition:

$$\frac{\partial H(k)}{\partial u(k)} = Ru(k) + B^{\mathrm{T}} p(k+1) = 0 \qquad (5)$$

(b) Costate equation:

$$\frac{\partial Hk}{\partial x(k)} = Qx(k) + A^{\mathrm{T}} p(k+1) = p(k) \qquad (6)$$

(c) State equation:

$$\frac{\partial H(k)}{\partial p(k+1)} = Ax(k) + Bu(k) = x(k+1) \qquad (7)$$

with the boundary conditions $x(0)=x_0$ and $p(N)=S(N)x(N)$.

3.2. Feedback Optimal Control Law

According to the necessary conditions given in Equations (5) to (7), a feedback optimal control law could be constructed in which the optimal solution of Problem (M) is obtained. For this purpose, the corresponding result is stated in following theorem.

Theorem 1. For the given Problem (M), the optimal control law is the feedback control law defined by

$$u(k)=-K(k)x(k) \tag{8}$$

where

$$K(k)=\left(B^{\mathrm{T}}S(k+1)B+R\right)^{-1}B^{\mathrm{T}}S(k+1)A \tag{9}$$

$$S(k)=A^{\mathrm{T}}S(k+1)\left(A-BK(k)\right)+Q \tag{10}$$

with the boundary condition $S(N)$ given.

Proof: From Equation (5), the stationary condition is rewritten as follows:

$$Ru(k)=-B^{\mathrm{T}}p(k+1). \tag{11}$$

Applying the sweep method [15] [16], that is,

$$p(k)=S(k)x(k), \tag{12}$$

and substitute Equation (12) for $k=k+1$ into Equation (11) to yield

$$Ru(k)=-B^{\mathrm{T}}S(k+1)x(k+1). \tag{13}$$

Taking Equation (7) in Equation (13), and after some algebraic manipulations, the feedback control law (8) is obtained, where Equation (9) is satisfied.

From Equation (6), after substituting Equation (12) for $k=k+1$ into Equation (6), the costate equation is rewritten as follows:

$$p(k)=Qx(k)+A^{\mathrm{T}}S(k+1)x(k+1). \tag{14}$$

Considering the state Equation (7) in Equation (14), we have

$$p(k)=Qx(k)+A^{\mathrm{T}}S(k+1)\left(Ax(k)+Bu(k)\right). \tag{15}$$

Apply the feedback control law (8) in Equation (15), and doing some algebraic manipulations, it is concluded that Equation (10) is satisfied after comparing the manipulation result to Equation (12). This completes the proof. ♦

Taking Equation (8) in Equation (7), the state equation becomes

$$x(k+1)=\left(A-BK(k)\right)x(k) \tag{16}$$

and the model output is measured from

$$y_M(k)=Cx(k). \tag{17}$$

Hence, the solution procedure of solving Problem (M) is summarized below:

Algorithm 1: Feedback control algorithm

Data Given $A, B, C, Q, R, S(N), x_0, N$.

Step 0 Calculate $K(k), k = 0,1,\cdots, N-1$ and $S(k), k = 0,1,\cdots, N$ from Equations (9) and (10), respectively.

Step 1 Solve Problem (M) that is defined by Equation (2) to obtain $u(k), k = 0,1,\cdots, N-1$ and $x(k), y_M(k), k = 0,1,\cdots, N$, respectively, from Equations (8), (16) and (17).

Step 2 Evaluate the cost function g_1 from Equation (2).

Remarks:

a) The data A, B, C are obtained by the linearization of the real plant f and the output measurement h from Problem (P).

b) In Step 0, the offline calculation is done for $K(k), k = 0,1,\cdots, N-1$ and $S(k), k = 0,1,\cdots, N$.

3.3. Gauss-Newton Updating Scheme

Now, let us define the output residual by

$$r(u) = y_P(k) - y_M(k), \tag{18}$$

where the model output (17) is reformulated as

$$y_M(k) = Cx(k) + Du(k). \tag{19}$$

Rewrite Equation (19) as the following input-output equations [25]:

$$\begin{bmatrix} y_M(0) \\ y_M(1) \\ y_M(2) \\ \vdots \\ y_M(N) \end{bmatrix} = \begin{bmatrix} C \\ CA \\ CA^2 \\ \vdots \\ CA^N \end{bmatrix} x_0 + \begin{bmatrix} D & 0 & 0 & \cdots & 0 \\ CB & D & 0 & \cdots & 0 \\ CAB & CB & D & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ CA^{N-1}B & CA^{N-2}B & CA^{N-3}B & \cdots & D \end{bmatrix} \begin{bmatrix} u(0) \\ u(1) \\ u(2) \\ \vdots \\ u(N-1) \end{bmatrix} \tag{20a}$$

for convenience,

$$y_M = Ex_0 + Fu \tag{20b}$$

where

$$E = \begin{bmatrix} C \\ CA \\ CA^2 \\ \vdots \\ CA^N \end{bmatrix} \text{ and } F = \begin{bmatrix} D & 0 & 0 & \cdots & 0 \\ CB & D & 0 & \cdots & 0 \\ CAB & CB & D & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ CA^{N-1}B & CA^{N-2}B & CA^{N-3}B & \cdots & D \end{bmatrix}.$$

Notice that the matrix $E \in \Re^{(N+1)p \times n}$ is the extended observability matrix, and the matrix $F \in \Re^{(N+1)p \times (N+1)m}$ is one type of block Hankel matrix [25].

Hence, consider the objective function, which represents the sum squares of error (SSE), given by

$$g_2(u) = r(u)^{\mathrm{T}} r(u). \tag{21}$$

Then, an optimization problem, which is referred to as Problem (O), is defined as follows:

Problem (O):

Find a set of the control sequence $u(k), k = 0,1,\cdots,N-1$, such that the objective function g_2 is minimized.

To solve Problem (O), consider the second-order Taylor expansion [26] [27] about the current $u^{(i)}$ at iteration i:

$$g_2\left(u^{(i+1)}\right) \approx g_2\left(u^{(i)}\right) + \left(u^{(i+1)} - u^{(i)}\right)^{\mathrm{T}} \nabla g_2\left(u^{(i)}\right) + \frac{1}{2}\left(u^{(i+1)} - u^{(i)}\right)^{\mathrm{T}} \left(\nabla^2 g_2\left(u^{(i)}\right)\right)\left(u^{(i+1)} - u^{(i)}\right). \tag{22}$$

The first-order condition for Equation (22) with respect to $u^{(i+1)}$ is expressed by

$$0 \approx \nabla g_2\left(u^{(i)}\right) + \left(\nabla^2 g_2\left(u^{(i)}\right)\right)\left(u^{(i+1)} - u^{(i)}\right). \tag{23}$$

Rearrange Equation (23) to yield the normal equation,

$$\left(\nabla^2 g_2\left(u^{(i)}\right)\right)\left(u^{(i+1)} - u^{(i)}\right) = -\nabla g_2\left(u^{(i)}\right). \tag{24}$$

Notice that the gradient of g_2 is calculated from

$$\nabla g_2\left(u^{(i)}\right) = 2\nabla r\left(u^{(i)}\right)^{\mathrm{T}} r\left(u^{(i)}\right) \tag{25}$$

and the Hessian matrix of g_2 is computed from

$$\nabla^2 g_2\left(u^{(i)}\right) = 2\left(\nabla^2 r\left(u^{(i)}\right)^{\mathrm{T}} r\left(u^{(i)}\right) + \nabla r\left(u^{(i)}\right)^{\mathrm{T}} \nabla r\left(u^{(i)}\right)\right) \tag{26}$$

where $\nabla r\left(u^{(i)}\right)$ is the Jacobian matrix of $r\left(u^{(i)}\right)$, and its entries are denoted by

$$\left(\nabla r\left(u^{(i)}\right)\right)_{ij} = \frac{\partial r_i}{\partial u_j}\left(u^{(i)}\right) = F,\ i = 1,2,\cdots,N-1;\ j = 1,2,\cdots,N-1. \tag{27}$$

From Equations (25) and (26), Equation (24) can be rewritten as

$$\left(\nabla^2 r\left(u^{(i)}\right)^{\mathrm{T}} r\left(u^{(i)}\right) + \nabla r\left(u^{(i)}\right)^{\mathrm{T}} \nabla r\left(u^{(i)}\right)\right)\left(u^{(i+1)} - u^{(i)}\right) = -\nabla r\left(u^{(i)}\right)^{\mathrm{T}} r\left(u^{(i)}\right). \tag{28}$$

By ignoring the second-order derivative term, that is, the first term at the left-hand side of Equation (28), we obtain the following recurrence relation:

$$u^{(i+1)} = u^{(i)} - \left(\nabla r\left(u^{(i)}\right)^{\mathrm{T}} \nabla r\left(u^{(i)}\right)\right)^{-1} \nabla r\left(u^{(i)}\right)^{\mathrm{T}} r\left(u^{(i)}\right) \tag{29}$$

with the initial $u^{(0)}$ given. Hence, Equation (29) is known as the Gauss-Newton recursive equation [26] [27].

From the discussion above, the updating scheme based on Gauss-Newton recursive approach for the control sequence is summarized below:

Algorithm 2: Gauss-Newton updating scheme

Step 0 Given an initial $u^{(0)}$ and tolerance ε. Set $i = 0$.

Step 1 Evaluate the output error $r\left(u^{(i)}\right)$ and the Jacobian matrix $\nabla r\left(u^{(i)}\right)$ from Equations (18) and (27), respectively.

Step 2 Solve the normal equation $\nabla r\left(u^{(i)}\right)^{\mathrm{T}} \nabla r\left(u^{(i)}\right) \Delta u^{(i)} = -\nabla r\left(u^{(i)}\right)^{\mathrm{T}} r\left(u^{(i)}\right)$.

Step 3 Update the control sequence by $u^{(i+1)} = u^{(i)} + \Delta u^{(i)}$. If $u^{(i+1)} = u^{(i)}$, within a given tolerance ε, stop; else set $i = i + 1$ and repeat from Step 1 to Step 3.

Remarks:

a) In Step 1, the calculation of the output error $r\left(u^{(i)}\right)$ is done online, while the Jacobian matrix $\nabla r\left(u^{(i)}\right)$ might be done offline.

b) In Step 2, the inverse of $\nabla r\left(u^{(i)}\right)^{\mathrm{T}} \nabla r\left(u^{(i)}\right)$ must be exist. The value of $\Delta u^{(i)}$ represents the step-size for the control set-point.

c) In Step 3, the initial $u^{(0)}$ is taken from Equation (8). The condition $u^{(i+1)} = u^{(i)}$ is required to be satisfied for the converged optimal control sequence. The following 2-norm is computed and it is compared with a given tolerance to verify the convergence of $u(k)$:

$$\left\| u^{(i+1)} - u^{(i)} \right\| = \left(\sum_{k=0}^{N-1} \left\| u(k)^{(i+1)} - u(k)^{(i)} \right\| \right)^{1/2}. \tag{30}$$

d) In order to provide a convergence mechanism for the state sequence, a simple relaxation method is employed:

$$x^{(i+1)} = x^{(i)} + k_x \left(x_p - x^{(i)} \right) \tag{31}$$

where $k_x \in [0,1]$, x_p is the state sequence of the real plant and $x^{(i)}$ is updated from (16).

4. Illustrative Examples

In this section, two examples are illustrated. The first example shows a direct current and alternating current (DC/AC) converter model [28] [29], while the second example gives a model of an isothermal series/parallel Van de Vussue reaction in a continuous stirred-tank reactor [30] [31]. In these models, the real plants are in nonlinear structure and the single output is measured. Since these models are in continuous time, the simple discretization scheme with the respective sampling time is applied. The optimal solution would be obtained by using the approach proposed and the solution procedure is implemented in the MATLAB environment.

To be convenient, the quadratic criterion cost function, for both Problem (P) and Problem (M), is employed, that is,

$$\frac{1}{2} x(N)^{\mathrm{T}} S(N) x(N) + \frac{1}{2} \sum_{k=0}^{N-1} \left(x(k)^{\mathrm{T}} Q x(k) + u(k)^{\mathrm{T}} R u(k) \right)$$

where $S(N) = I_{2\times2}$, $Q = I_{2\times2}$ and $R = 1$.

4.1. Example 1

Consider the state space representation of a direct current/alternating current (DC/AC) converter model [28] [29] given by

$$\dot{x}_1(t) = \frac{\left(x_2(t)\right)^2}{x_1(t)} - 5x_1(t) + 5u(t)$$

$$\dot{x}_2(t) = \frac{(x_2(t))^3}{(x_1(t))^2} - 7x_2(t) + \left(5\frac{x_2(t)}{x_1(t)} + 2x_1(t)\right)u(t)$$

$$y(t) = x_2(t)$$

with the initial $x_0 = (0.1, 0)^{\mathrm{T}}$, where x_1 and x_2 represent the current (in unit of ampere) and the voltage (in unit of volt) flow in the circuit, and u is the control signal. This problem is referred to as Problem (P).

The discrete time model of Problem (M) is formulated by

$$\begin{pmatrix} x_1(k+1) \\ x_2(k+1) \end{pmatrix} = \begin{pmatrix} 1-5\cdot T & 0 \\ 0 & 1-7\cdot T \end{pmatrix}\begin{pmatrix} x_1(k) \\ x_2(k) \end{pmatrix} + \begin{pmatrix} 5\cdot T \\ 0.2\cdot T \end{pmatrix} u(k)$$

$$y(k) = x_2(k)$$

for $k = 0, 1, \cdots, 80$, with the sampling time $T = 0.01$ minute.

The simulation result is shown in Table 1. The initial cost of 0.0429 unit, which is the cost function value for Problem (M), is calculated before the iteration. After five iterations, the convergence is achieved. The final cost of 110.8926 units is preferred instead of the original cost of 1.0885×10^3 units. This reduction saves 89.8 percent of the expense. The value of SSE of 7.647011×10^{-12} shows that the model output is very close to the real output. Hence, the approach proposed is efficient to obtain the optimal solution of Problem (P).

Figure 1 shows the final control trajectory, which is used to update the model output, in turn, to approximate the real output trajectory. From Figure 2, it can

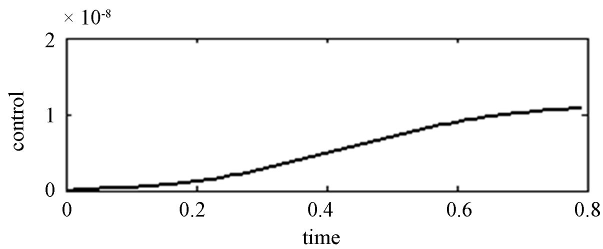

Figure 1. Final control trajectory.

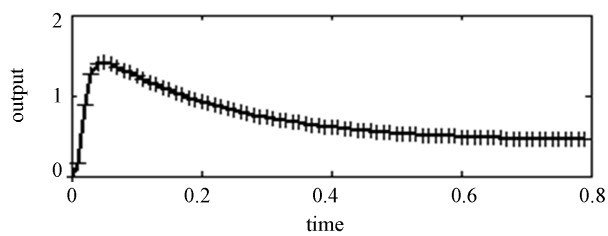

Figure 2. Final output (−) and real output (+) trajectories.

Table 1. Simulation result for Example 1.

Number of Iterations	Initial Cost	Final Cost	Original Cost	SSE
5	0.0429	110.8926	1.0885×10^3	7.647011×10^{-12}

be seen that both of the output trajectories are fitted each other with the smallest value of SSE.

Figure 3 shows the control trajectory, which is applied in the real plant. With the matching scheme that is established in the approach proposed, the final state trajectory tracks the real state trajectory closely, as shown in Figure 4.

Figure 5 and Figure 6 show the initial trajectories of control and state, respectively. They are the optimal solution of Problem (M) before the Gauss-Newton updating is applied.

The differences between the real output and the model output, which are after and before iteration, and are shown in Figure 7 and Figure 8, respectively. These

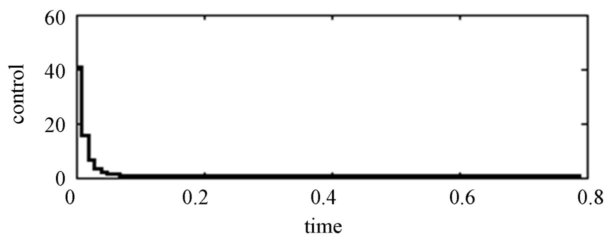

Figure 3. Real control trajectory.

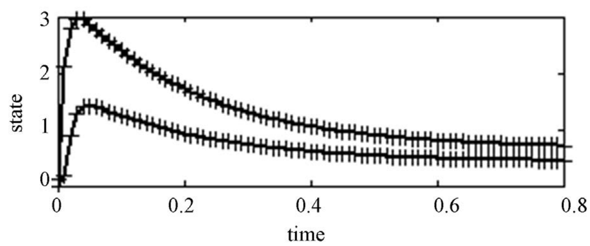

Figure 4. Real state (+) and final state (−) trajectories.

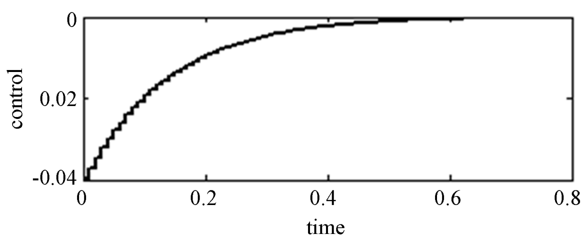

Figure 5. Initial control trajectory.

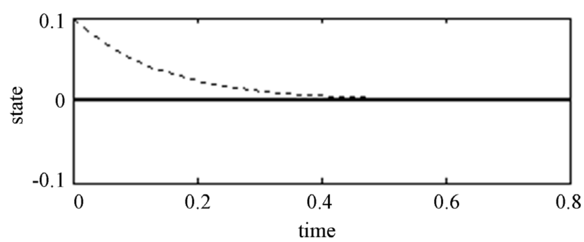

Figure 6. Initial state trajectory.

model-reality differences reveal the applicability and reliability of the approach proposed, where the output error is minimized definitely.

4.2. Example 2

Consider the dynamical system of an isothermal series/parallel Van de Vussue reaction in a continuous stirred-tank reactor [30] [31]:

$$\dot{x}_1(t) = -50x_1(t) - 10(x_1(t))^2 + (10 - x_1(t))u(t)$$

$$\dot{x}_2(t) = 50x_1(t) - 100x_2(t) + x_2(t)u(t)$$

$$y(t) = x_2(t)$$

with the initial $x_0 = (2.5, 1)^{\mathrm{T}}$, where x_1 and x_2 are, respectively, the dimensionless reactant and product concentration in the reactor, and u is the dimensionless dilution rate. Let this problem as Problem (P).

In Problem (M), the model used is presented by

$$\begin{pmatrix} x_1(k+1) \\ x_2(k+1) \end{pmatrix} = \begin{pmatrix} 1-100\cdot T & 0 \\ 50\cdot T & 1-100\cdot T \end{pmatrix}\begin{pmatrix} x_1(k) \\ x_2(k) \end{pmatrix} + \begin{pmatrix} 7.5\cdot T \\ 1\cdot T \end{pmatrix}u(k)$$

$$y(k) = x_2(k)$$

for $k = 0, 1, \cdots, 100$, with the sampling time $T = 0.002$ second.

Table 2 shows the simulation result, where the number of iteration is 5. The

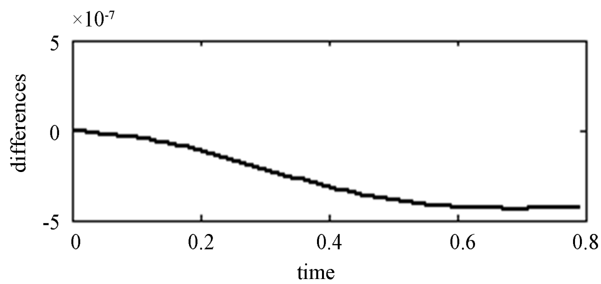

Figure 7. Output error after iteration.

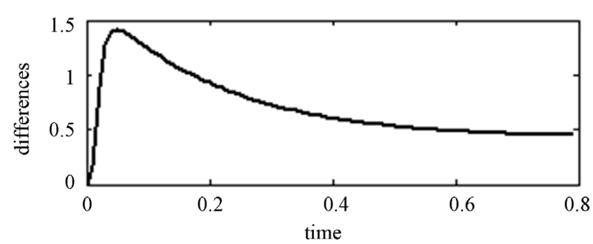

Figure 8. Output error before iteration.

Table 2. Simulation result for Example 2.

Number of Iterations	Initial Cost	Final Cost	Original Cost	SSE
5	12.6916	543.1649	3.0122×10^5	1.587211×10^{-12}

implementation of the approach proposed begins with the initial cost of 12.6916 units. During the iterative procedure, the convergence is achieved with giving the final cost of 543.1649 units. This shows a reduction of 99.8 percent of the saving cost from the original cost of 3.0122×10^5 units. The value of SSE of 1.587211×10^{-12} indicates that the approach proposed is efficient to generate the optimal solution of Problem (P).

The graphical result in Figure 9 and Figure 10 shows, respectively, the trajectories of final control, final output and real output. The final control is stable and this stabilization manner makes the steady state of the final output occurred at 1.2324. Moreover, the final output fits the real output very well.

Figure 11 and Figure 12 show the trajectories of control and state in the real plant. With this control trajectory, the state trajectories are converged to 2.8250 and 1.2324, respectively. In addition, by using the approach proposed, this steady state is tracked closely by the final state trajectory.

The initial trajectories of control and state are shown, respectively, in Figure 13 and Figure 14. They are the optimal solution of Problem (M) before the Gauss-Newton updating scheme is employed.

Figure 15 and Figure 16 show the differences between the real output and the model output, respectively. These differences are the output error, which is minimized apparently.

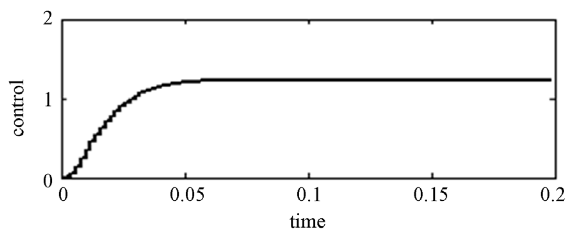

Figure 9. Final control trajectory.

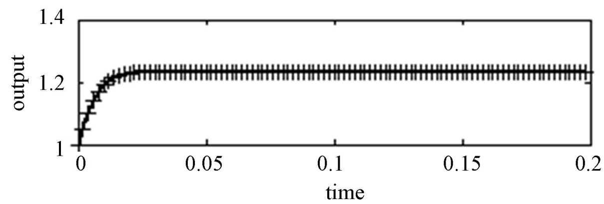

Figure 10. Final output (−) and real output (+) trajectories.

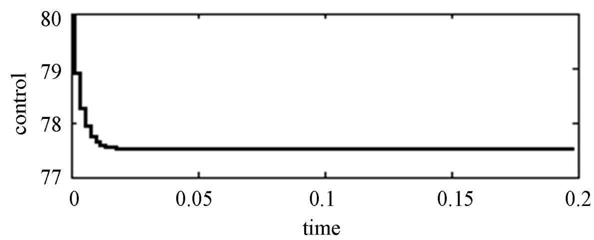

Figure 11. Real control trajectory.

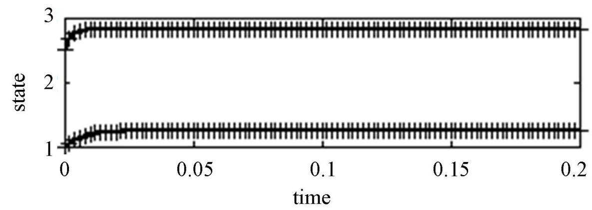

Figure 12. Real state (+) and final state (−) trajectories.

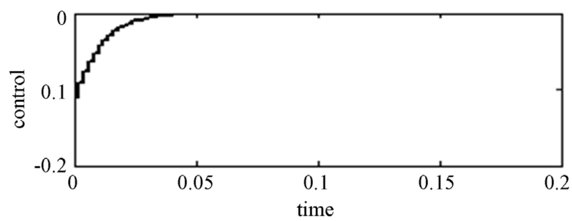

Figure 13. Initial control trajectory.

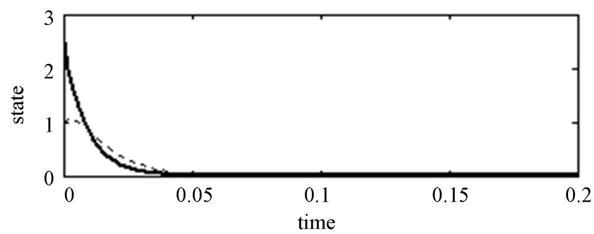

Figure 14. Initial state trajectory.

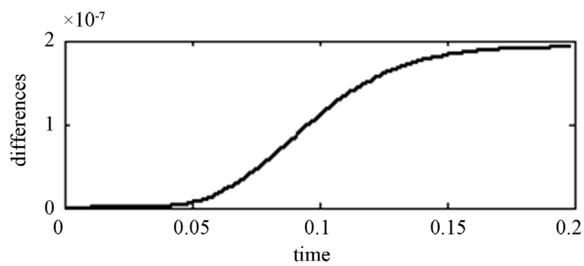

Figure 15. Output error after iteration.

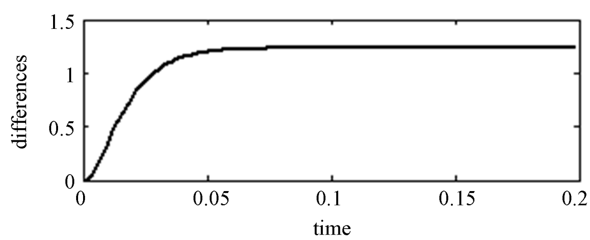

Figure 16. Output error before iteration.

4.3. Discussion

From Examples 1 and 2, the structures of Problem (M) and Problem (P) are clearly different. Solving Problem (M) with taking the Gauss-Newton updating scheme into consideration provides us the iterative solution, which approximates to the correct optimal solution of Problem (P), in spite of the model-reality differences. The results obtained are evidently demonstrated in **Figure 1** and **Figure 16**. Hence, the applicability of the approach proposed is significantly proven.

5. Concluding Remarks

In this paper, an efficient computational approach was proposed, where the least squares scheme is established. In our approach, the model-based optimal control problem is solved in advanced. Consequently, the feedback control law, which is constructed from the model used, is added in the output measurement. Through optimizing the sum squares of error, the Gauss-Newton updating scheme is derived. On this basis, the control trajectory is updated repeatedly during the computational procedure. By feed backing the updated control trajectory into the dynamic system, the iterative solution of the model used approximates to the correct optimal solution of the original optimal control problem, in spite of model-reality differences. For illustration, two examples were studied. Their simulation results and graphical solutions indicated the applicability and reliability of the approach proposed. In conclusion, the efficiency of the approach proposed is proven.

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A Direct Algorithm for the Vertical Generalized Complementarity Problem Associated with *P*-Matrices

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Abstract

We present a direct algorithm for solving the vertical generalized linear complementarity problem, first considered by Cottle and Dantzig, when the associated matrix is a vertical block *P*-matrix. The algorithm converges to a unique solution in a finite number of steps, without an assumption of nondegeneracy on the given problem. The algorithm is simple, efficient, and easy to implement.

Keywords

Complementarity Problems, *P*-Matrix, Direct Algorithms, Linear Programming, Bi-Matrix Game

1. Introduction

The linear complementarity problem for any $n \times n$ matrix M is defined as follows:

For any given $q \in R^n$, find $w, z, \in R^n$ such that

$$w = Mz + q \tag{1}$$

$$w \geq 0, z \geq 0$$

$$w^t z = 0 \quad \left(w_i z_i = 0, i = 1, \cdots, n\right)$$

The study of linear complementarity problems (LCPs) began in the 1960s. Linear programming, quadratic programming, bi-matrix games, as well as certain problems in economics and engineering, can be represented as LCPs.

Murty [1] presented an algorithm that finds a unique solution to (1) in a finite number of steps, if the matrix M associated with the problem is an $n \times n$ P-matrix.

The vertical generalized linear complementarity problem for an $m \times n, m \geq n$, vertical block matrix N of type $(m_1, m_2, \cdots, m_n)$ is:

For any given $q \in R^m$, find $w \in R^m, z \in R^n$ such that

$$w = Nz + q$$

$$w \geq 0, z \geq 0 \tag{2}$$

$$z_j \prod_{i=1}^{m_j} w_i^j = 0 \quad (j = 1, \cdots, n)$$

We will denote this problem by VGLCP(q, N). For a horizontal generalization of the LCP, see the paper by Chakraborty and Ebiefung [2].

In 1970 Cottle and Dantzig published the first paper to describe the VGLCP [3]. They showed that if N is a strictly positive (or copositive plus) vertical block matrix or a P-matrix, the VGLCP(q, N) has a solution, and also introduced a technique for solving the VGLCP(q, N), when N is a copositive plus vertical block matrix. Their technique could be considered as an extension of Lemke's algorithm for the LCP (with covering vector **e**) [4].

The fact that the VGLCP(q, N) has a unique solution when N is a vertical block P-matrix was established by Habetler and Szanc [5], while existence of solutions in terms of representative submatrices was developed by Ebiefung [6]. The set of Q-matrices for the VGLCP(q, N) was characterized by Ebiefung [7], and by Ebiefung and Kostreva [8]. In [8], an algorithm for solving the GLCP for any vector $q \in R^m$, irrespective of the matrix class, is also provided. As expected, the method they provided is complicated and expensive to implement. For this reason, specialized algorithms are needed when properties of the associated matrices can be exploited to have simpler algorithms. One of these specialized algorithms for the VGLCP is given in Ebiefung, Kostreva, and Ramanujam [9], where the associated matrix is a vertical block Z-matrix.

Applications of Vertical Complementarity Problems are becoming more prevalent. One engineering application is that of Mixed Lubrication which was discussed in the paper of Oh [10]. Calculations were made on a journal bearing with elastic support to illustrate the method of solution over a wide range of conditions. Regions of solid-to-solid contact, hydrodynamic lubrication, and cavitation were observed. The solutions were obtained using a version of the direct algorithm presented here. No proof of convergence was given, and the solution of the generalized complementarity problem is contained in one short paragraph.

In the area of economics, the VGLCP has been applied to the generalization of Leontief's production model and the choice of technology by Ebiefung and Kostreva [11]; and to the determination of equilibrium points in multi-unit manufacturing systems, Ebiefung and Kostreva [12]. Other economic applications can be found in Ebiefung, Kostreva, and Majumdar [13], Ebiefung and Isaac [14], Ebiefung [15], and in the references at the end of this paper.

In this paper, we modify Murty's direct algorithm to solve the LCP when the associated matrix *N* is a vertical block *P*-matrix of type $(m_1, m_2, \cdots, m_n)$. We will show that the new algorithm finds a non-negative solution to problem VGLCP(*q*, *N*) in a finite number of steps, where $q \in R^m$ and *N* is a vertical block *P*-matrix of type $(m_1, m_2, \cdots, m_n)$.

The theory needed to prove finite convergence of the direct algorithm is given in detail in [5], and will be covered briefly here. Finite convergence of the algorithm is essential. As we pointed out before, Cottle and Dantzig's algorithm is an extension of Lemke's algorithm which could cycle (or loop) as pointed out by Kostreva [16]. In fact, the example given by Kostreva can be easily modified to show that their algorithm can cycle. Such behavior in a computation would cause a failure in any implementation. Thus, another approach is motivated. It should be noted that the computer routine of Ravindran [17] does cycle when applied to the example of a 3×3 *P*-matrix given in [16].

The rest of the paper is organized as follows. In Section 2, we give notation and definitions that are needed for the rest of the paper. Section 3 is devoted to the description of the new algorithm and proof of convergence. We summarize our results in Section 4.

2. Notation and Definitions

The following notation and definitions are needed for the development of the algorithm.

Definition 1. Let *N* be an $m \times n$ rectangular matrix with $m \geq n$. We call *N* a vertical block matrix of type $(m_1, \cdots, m_n)$ if *N* can be partioned row-wise as

$$N = \begin{bmatrix} N^1 \\ \vdots \\ N^n \end{bmatrix}$$

where the jth block, N^j, is of dimension $m_j \times n$ and $m = \sum_{j=1}^{n} m_j$. The vectors $w \in R^m$ and $q \in R^m$ are also partitioned to conform to the entries in the block, N^j of N:

$$w = \begin{bmatrix} w^1 \\ \vdots \\ w^n \end{bmatrix}, q = \begin{bmatrix} q^1 \\ \vdots \\ q^n \end{bmatrix}$$

where w^j and q^j are $m_j \times 1$ column vectors.

Associated with problem (2) is the related problem: given $q \in R^m$, find $w \in R^m, z \in R^n$ such that

$$w - Nz = q$$

$$z_j \prod_{i=1}^{m_j} w_i^j = 0 \quad (j = 1, \cdots, n) \tag{3}$$

Definition 2. By a $m \times k$ horizontal matrix A of type $(m_1, m_2, \cdots, m_n)$, we shall mean a matrix

$$A = (A^1, \cdots, A^n)$$

where the jth block of A, A^j, is a $(m \times m_j)$ matrix and $\sum_{j=1}^{n} m_j = k$.

The linear system in (3) can be re-written in the form

$$(I, -N)\begin{pmatrix} w \\ z \end{pmatrix} = q$$

where I is the $m \times m$ identity matrix. We shall represent I as a $m \times m$ horizontal block matrix by

$$I = (I^1, \cdots, I^n)$$

where I^j is the jth block of columns associated with the variable $w_i^j, (i = 1, \cdots, m_j)$. Thus I^j is an $m \times m_j$ matrix and $\sum_{j=1}^{n} m_j = m$. The column vector $I_{.i}^j$ is associated with the variable w_i^j and the column vector $-N_{.j}$ is associated with the variable z_j.

Definition 3. Let N be an $m \times n, (m \geq n)$, vertical block matrix of type $(m_1, \cdots, m_n)$. Let I be an $m \times m$ horizontal block identity matrix of type $(m_1, \cdots, m_n)$. Define B as the $m \times m$ horizontal block matrix of type $(m_1, \cdots, m_n)$ given by

$$B = (B^1, \cdots, B^n)$$

such that the ith column of the jth block of columns, $B_{.i}^j$, is either $I_{.i}$ or $-N_{.j}$, and if for any $k \in \{1, \cdots, m_j\}, (j = 1, \cdots, n)$, we have

$$B_{.k}^j = -N_{.j}$$

then for that specific *j*

$$B_{.i}^j = I_{.i}^j$$

for all $i \in \{\{1, \cdots, m_j\} - \{k\}\}$. We call B a basic matrix. The vertical block matrix N of type $(m_1, \cdots, m_n)$ is said to be nondegenerate if and only if for each such basic matrix B, taking all possible combinations, B is nonsingular.

Definition 4. The vector $q \in R^m$ in system (2) is nondegenerate with respect to N if for each $z \in R^n$ at most n of the $(m+n)$ variables (w, z) are zero.

Definition 5. For each *j*, $(j = 1, 2, \cdots, n)$, the variables $(w_1^j, \cdots, w_{m_j}^j, z_j)^t$ constitute the jth ordered related $(m_j + 1)$-tuple. The set of $m_j + 1$ columns $\{I_{.1}, \cdots, I_{.m_j}, -N_{.j}\}$ will be known as the jth ordered related set of column vectors in system (2).

Definition 6. A related basic matrix associated with system (3) is the $m \times m$ horizontal block matrix B of type $(m_1, \cdots, m_n)$ defined in Definition 3. The set of variables corresponding to the jth block of columns of B, B^j, are called the jth related set of basic variables. The variables that are excluded from the jth set of basic variables are called nonbasic. There are $\prod_{j=1}^{n}(m_j + 1)$ possible related basic matrices associated with system (3) and we shall denote these basic related matrices by $B_\lambda, \lambda \in \left\{1,\cdots,\prod_{j=1}^{n}\left(m_j+1\right)\right\}$.

B_1 will always denote the $m \times m$ horizontal block identity matrix. This is equivalent to requiring that z_j be the nonbasic variable for $\lambda = 1, j = 1,\cdots,n$. We now consider the solutions corresponding to the $\prod_{j=1}^{n}\left(m_j+1\right)$ related basic matrices associated with the system (3).

If a solution exists to the following system

$$B_\lambda r_\lambda = q, \quad \lambda \in \left\{1,\cdots,\prod_{j=1}^{n}\left(m_j+1\right)\right\}$$

we will call the solution a basic related point, and denote it by r_λ. The vector $r_\lambda \in R^m$ is subdivided in accordance with B_λ, *i.e.* $r_\lambda = \left(r_\lambda^1,\cdots,r_\lambda^n\right)^t$ and $r_\lambda^j \in R^{m_j}, \left(j=1,\cdots,n\right)$.

Definition 7. A basic related point is called degenerate if at least one of its components is zero.

Consider the related problem (3). To satisfy the related condition,

$$z_{\lambda,j}\prod_{i=1}^{m_j} w_{\lambda,i}^j = 0$$

at least one component of the jth ordered related $\left(m_j+1\right)$ -tuple, s_λ^j, must be assigned the value zero.

We call this component the related nonbasic variable associated with s_λ^j, and we will denote it by $t_{\lambda,j}$. If each s_λ is an ordered related vector, *i.e.* satisfies the related condition for each $\lambda \in \left(1,\cdots,\prod_{j=1}^{n}\left(m_j+1\right)\right)$, we must have for each $j=1,\cdots,n$ and some $i \in \left\{1,\cdots,m_j\right\}$

$$t_{\lambda,j} = s_{\lambda,i}^j = w_{\lambda,i}^j = 0$$

or

$$t_{\lambda,j} = s_{\lambda,m_j+1}^j = z_{\lambda,i} = 0$$

We denote the related nonbasic vector associated with λ by

$$t_\lambda = \left(t_{\lambda,1},\cdots,t_{\lambda,n}\right)^t$$

The components of s_λ^j that are left if we eliminate $t_{\lambda,j}$ are called the related basic variable of s_λ^j and denoted by r_λ^j. The jth ordered block of related columns associated with s_λ^j is denoted by:

$$C^j = \left(I_{.1}^j,\cdots,I_{.m_j}^j\right)$$

For each λ and each $j \in \left\{1,\cdots,n\right\}$, we denote the columns associated with r_λ^j by B_λ^j. If we eliminate the columns of B_λ^j from the columns of C^j, we are left with the column that is considered nonbasic. We will denote this column by $D_{\lambda,j}$, and this column will be associated with the nonbasic variable $t_{\lambda,j}$.

Using this notation, we can rewrite Equations (2) as follows:
For any given $q \in R^m$, find $\lambda \in \left\{1,\cdots,\prod_{j=1}^{n}\left(m_j+1\right)\right\}$ such that

$$B_\lambda r_\lambda = q,\ r_\lambda \geq 0, t_\lambda = 0 \tag{4}$$

If B_λ is nonsingular, we can find an explicit expression for r_λ and a solution to Equation (4) would have to satisfy

$$r_\lambda = B_\lambda^{-1} q \geq 0,\ t_\lambda = 0$$

3. The Algorithm

The algorithm that we prepose is described as follows:

Step 1: If $q \geq 0$, then $B_1 = I, r_1 = w = q \geq 0, t_1 = z = 0$ is the related solution to Equations (2). Terminate.

Step 2: Suppose $q \ngeq 0$. Start the scheme by picking w as the initial related basic vector, r_1. Then $B_1 = I, r_1 = w = q, t_1 = z = 0$. Go to Step 3.

Step 3: All the matrices obtained during the scheme will be basic related matrices, $B_\lambda, \lambda \in \left\{1, \cdots, \prod_{j=1}^{n}(m_j + 1)\right\}$. In a general stage of the scheme, suppose that $B_{\bar{\lambda}}$ is the present basic related matrix. If $r_{\bar{\lambda}} \geq 0, t_{\bar{\lambda}} = 0$, we are done. The basic related vector $r_{\bar{\lambda}}$ represents the basic related variables and $t_{\bar{\lambda}}$ represents the nonbasic related variables of the solution of Equations (2). Terminate.

Step 4: If $r_{\bar{\lambda}} \ngeq 0$ or $t_{\bar{\lambda}} \neq 0$, find

$$k = \min\left\{ j : r^j_{\bar{\lambda},i} < 0, i \in \{1, \cdots, m_j\}, j = 1, \cdots, n \right\}$$

$$l = \min\left\{ i : r^k_{\bar{\lambda},i} < 0, i \in \{1, \cdots, m_k\} \right\}$$

Interchange the related basic variable represented by $r^k_{\bar{\lambda},l}$ and the related nonbasic variable represented by $t_{\bar{\lambda},k}$. This is equivalent to interchanging the columns $B^k_{\bar{\lambda},l}$ and $D_{\bar{\lambda},k}$. After rearranging the columns of the result matrix, if necessary, to conform with Definition 3, denote the resulting related basic matrix by $B_{\bar{\lambda}+1}$, that is, increase $\bar{\lambda}$ by 1. Continue the scheme as above until there exits a related basic matrix $B_\mu, \mu \geq \bar{\lambda} + 1$, such that

$$B_\mu r_\mu = q$$

$$r_\mu \geq 0, \quad t_\mu = 0$$

Definition 8. If N is a vertical block matrix of type $(m_1, \cdots, m_n)$, then H is defined to be the $(m - m_n) \times (n-1)$ submatrix of type $(m_1, \cdots, m_{n-1})$ if H is the matrix that results from eliminating the nth block and the nth column of N.

Definition 9. Let

$$\psi = \left(w^1_1, \cdots, w^1_{m_1}, \cdots, w^{n-1}_1, \cdots, w^{n-1}_{m_n - 1}\right)^t$$

$$\xi = (z_1, \cdots, z_{n-1})^t$$

$$\gamma = \left(q^1_1, \cdots, q^1_{m_1}, \cdots, q^{n-1}_1, \cdots, q^{n-1}_{m_n - 1}\right)^t$$

The generalized vertical linear complementarity problem for the $(m - m_n) \times (n-1)$ leading submatrix H is:

Given $\gamma \in R^{m - m_n}$, find $\psi \in R^{m - m_n}, \xi \in R^{n-1}$ such that

$$\begin{aligned}
&(1) \quad \psi - H\xi = \gamma \\
&(2) \quad \psi \ge 0, \xi \ge 0 \\
&(3) \quad \xi_j \prod_{i=1}^{m_j} \psi_i^j = 0,\ j = 1,\cdots,n-1
\end{aligned} \tag{5}$$

Problem (5) is called the leading subproblem of Equations (2).

The related basic matrices B_λ associated with (5) are the $(m-m_n)\times(m-m_n)$ matrices given by Definition 2. The associated related basic and nonbasic vectors are denoted by r_λ and ρ_λ, respectively.

Lemma 1 *Suppose* $(\hat{w},\hat{z})$ *is a solution of Equations* (2) *and that* $\hat{z}_n = 0$. *Let*

$$\hat{\psi} = \left(\hat{w}_1^1,\cdots,\hat{w}_{m_1}^1,\cdots,\hat{w}_1^{n-1},\cdots,\hat{w}_{m_n-1}^{n-1}\right)^t$$

$$\hat{\xi} = \left(\hat{z}_1,\cdots,\hat{z}_{n-1}\right)^t$$

Then $(\hat{\psi},\hat{\xi})$ is a solution of problem (5).

Proof: Since $\hat{z}_n = 0$, we have that

$$\hat{\psi}^j = \hat{w}^j = N^j\hat{z} + q^j = H^j\hat{\xi} + \gamma^j,\ j = 1,\cdots,n-1$$

The positivity and satisfied related condition for $(\hat{\psi},\hat{\xi})$ follows from the definition of $(\hat{\psi},\hat{\xi})$.

Lemma 2 *If* $(\bar{\psi},\bar{\xi})$ *is a solution to problem* (5), *let* $\bar{z} = (\bar{\xi},0)^t$. *Suppose*

$$\bar{w}^n = N^n\bar{z} + q^n \ge 0$$

Then $(\bar{w},\bar{z})$ is a solution to Equations (2), where $\bar{w} = (\bar{\psi},\bar{w}^n)$.

Lemma 3 *If N is a vertical block matrix of type* $(m_1,\cdots,m_n)$, *then* H *is vertical block* $(m-m_n)\times(n-1)$ *P-matrix of type* $(m_1,\cdots,m_{n-1})$ *and the leading subproblem has a unique solution.*

Proof: Any representative submatrix of H is a leading submatrix of a representative submatrix of N. Every leading submatrix of N is an $(n-1)\times(n-1)$ P-matrix.

Therefore, H is a vertical block $(m-m_n)\times(n-1)$ P-matrix of type $(m_1,\cdots,m_{n-1})$ and therefore, a unique solution exists for Equations (5).

Lemma 4 *Let* N *be a vertical block P-matrix of type* $(m_1,\cdots,m_n)$ *and let* $(\hat{w},\hat{z})$ *be the unique solution of Equation (2). Suppose* $\hat{z}_n = 0$. *For some* $\lambda \in \left\{1,\cdots,\prod_{j=1}^{n-1}(m_j+1)\right\}$, *let*

$$\rho = \left(\rho_{\lambda,1}^1,\cdots,\rho_{\lambda,m_1}^1,\cdots,\rho_{\lambda,1}^{n-1},\cdots,\rho_{\lambda,m_{n-1}}^{n-1}\right) = \left(\rho_\lambda^1,\cdots,\rho_\lambda^{n-1}\right)^t$$

$$r_\lambda = \left(r_{\lambda,1},\cdots,r_{\lambda,n-1}\right)^t$$

be the related nonbasic and basic vectors associated with the unique solution to Equations (5). Then

$$r_\lambda = \left(\rho_\lambda^1,\cdots,\rho_\lambda^{n-1},\hat{w}^n\right)^t$$

$$t_\lambda = \left(r_{\lambda,1},\cdots,r_{\lambda,n-1},\hat{z}_n\right)^t$$

are the related basic and nonbasic vectors associated with the solution $(\hat{w}, \hat{z})$.

Proof: Let $(\hat{\psi}, \hat{\xi})$ be the unique solution to Equations (5), then ρ_λ and r_λ represent the related nonbasic and basic vectors, respectively of $(\hat{\psi}, \hat{\xi})$.

Since $(\hat{w}, \hat{z})$ is the unique solution to Equations (2) and $\hat{z}_n = 0$, we have $\hat{w}_n \ge 0$ and Lemma 2 implies that

$$\hat{w} = \left(\hat{\psi}^1, \cdots, \hat{\psi}^{n-1}, \hat{w}^n\right)^t, \quad \hat{z} = \left(\hat{\xi}_1, \cdots, \hat{\xi}_{n-1}, 0\right)^t$$

Since the first $n-1$ blocks of $\hat{w}$ and $\hat{\psi}$ are the same and the first $n-1$ components of $\hat{z}$ and $\hat{\xi}$ are the same, we must have

$$r_\lambda = \left(\rho_\lambda^1, \cdots, \rho_\lambda^{n-1}, \hat{w}^n\right)^t, \quad t_\lambda = \left(r_{\lambda,1}, \cdots, r_{\lambda,n-1}, 0\right)^t$$

Theorem 5 *Suppose that the algorithm is applied to the problem in Equations (2), when* N *is a vertical block P-matrix of type* $(m_1, \cdots, m_n)$ *and there exists a* $\lambda \in \left\{1, \cdots, \prod_{j=1}^n (m_j + 1)\right\}$ *such that*

$$r_\lambda = B_\lambda^{-1} q, \quad t_\lambda = 0$$

$$r_\lambda^j \ge 0, \quad j = 1, \cdots, n-1 \tag{6}$$

and there exists an $i \in \{1, \cdots, m_n\}$ such that $r_{\lambda,i}^n < 0$.

Then in any succeeding stage of the scheme, the nonbasic related variable represented by $t_{\lambda,n}$ will always be a basic related variable.

Proof: Without loss of generality, let $\lambda = 1$. Then

$$B_1 = I, \quad r_1 = w, \quad t_1 = z = 0$$

$$w^j \ge 0, \quad j = 1, \cdots, n-1$$

and suppose $w_{1,1}^n < 0$.

The next step in the scheme would be to interchange z_n with $w_{1,1}^n$. Suppose in some succeeding stage of the scheme, we have for some $\sigma, 1 < \sigma \le \prod_{j=1}^n (m_j + 1)$

$$r_\sigma^j \ge 0, \ j = 1, \cdots, n-1, \quad t_\sigma = 0$$

$$z_n = r_{\sigma,k}^n < 0, \quad k \in \{1, \cdots, m_n\}$$

Suppose $k = \min\left\{i : r_{\sigma,i}^n < 0, i \in \{1, \cdots, m_n\}\right\}$. Consider the ordered related $(m_j + 1)$-tuples associated with $r_1, t_1, r_\sigma, t_\sigma$.

$$s_1^j = \left(w_{1,1}^j, \cdots, w_{1,m_j}^{ju}, z_{1,j}\right), \quad j = 1, \cdots, n$$

$$s_\sigma^j = \left(w_{\sigma,1}^1, \cdots, w_{\sigma,m_j}^j, z_{\sigma,j}\right), \quad j = 1, \cdots, n$$

$$s_1^j, s_\sigma^j \ge 0, \ j = 1, \cdots, n-1, \quad s_{1,m_j+1}^j = 0, \ j = 1, \cdots, n$$

$$s_{1,1}^n < 0, \quad s_{\lambda,k}^n < 0$$

We will construct a representative submatrix R of N according to the following criteria:

Case 1: If $s_{\sigma,m_j+1}^j = 0$, then let $R_{j.} = N_{1.}^j, j = 1, \cdots, n$, $h_j = 1$

Case 2: For $j=1,\cdots,n-1$, if $s^j_{\sigma,m_j+1}>0$, find $h_j\in\{1,\cdots,m_j\}$ such that $s^j_{1,h_j}\ge 0$ and $s^j_{\sigma,h_j}=0$.

Let $R_{j.}=N^j_{h_j.}$. For $j=n$, we have $s^n_{1,1}<0, s^n_{1,m_n+1}=0$, and $s^n_{\sigma,m_n+1}=r^n_{\sigma,k}<0$, for some $k\in\{1,\cdots,m_j\}$, where k is the minimum defined above.

If $k=1$, this implies that $s^n_{\sigma,1}=t_{\sigma,n}=0$. If $k>1$, then $s^n_{\sigma,1}>0$. In either case, fix $R_{n.}=N^n_{1.}$, where $h_n=1$. Let

$$y=\begin{pmatrix} s^1_{1,h_1}\\ \vdots \\ s^n_{1,h_n}\end{pmatrix},\quad \bar{y}=\begin{pmatrix} s^1_{\sigma,h_1}\\ \vdots \\ s^n_{\sigma,h_n}\end{pmatrix}$$

$$x=\begin{pmatrix} s^1_{1,m_1+1}\\ \vdots \\ s^n_{1,m_n+1}\end{pmatrix},\quad \bar{x}=\begin{pmatrix} s^1_{\sigma,m_1+1}\\ \vdots \\ s^n_{\sigma,m_n+1}\end{pmatrix},\quad p=\begin{pmatrix} q^1_{h_1}\\ \vdots \\ q^n_{h_n}\end{pmatrix}$$

Since the components of $y,\bar{y}$ and p are chosen to correspond with the rows of R, we have

$$y-Rx=p$$
$$\bar{y}-R\bar{x}=p$$

Therefore,

$$y-Rx=\bar{y}-R\bar{x}$$

or

$$(y-\bar{y})=R(x-\bar{x})$$

and

$$(y_j-\bar{y}_j)(x_j-\bar{x}_j)\le 0,\quad j=1,\cdots,n$$

We conclude that R cannot be a *P*-matrix by Gale and Nakaido [18]. Therefore, k does not equal the minimum subscript such that $r^n_{\sigma,i}<0$, for some $i\in\{1,\cdots,m_n\}$. Therefore, the basic variable z_n is not a candidate to be interchanged with $t_{\sigma,n}$ in any succeeding step of the scheme for $1<\sigma\le\prod_{j=1}^n(m_j+1)$ such that the conditions of Equations (6) are met.

Theorem 6. *If N is a vertical block P-matrix of type $(m_1,\cdots,m_n)$, the algorithm when applied to Equations (2) will terminate with a solution in a finite number of steps. A related basic matrix that appears once in the scheme will not reappear in any succeeding steps.*

Proof: If $n=1$, then N is a vertical block *P*-matrix of type (m_1), and by Theorem 5, we see that a solution will be found in at most (m_1+1) steps. Also once a nonbasic variable becomes basic, it cannot become nonbasic in subsequent steps. Hence, a related basic matrix can appear at most one time in the course of the scheme.

Suppose $n>1$ and the theorem holds for all generalized linear complementarity problems such that N is an $m\times K$ vertical block *P*-matrix of type $(m_1,\cdots,m_K), 1 \le K \le n-1$. Let $(\hat{w},\overline{z})$ be the unique solution of Equations (2).

Case 1: If $z_n = 0$, then by Lemma 1, $(\hat{\psi},\hat{\xi})$ is the unique solution to Equations (5). Since H is a $m \times (m-m_n)$ vertical block P-matrix of type $(m_1,\cdots,m_{n-1})$, Theorem 5 applies and the scheme terminates in a finite number of steps with a solution. Any related basic matrix that appears once in the scheme will nor re-appear again. Let the sequence of related basic vectors that appear when the system is applied to H be $\rho_\lambda, \lambda = 1$ to K, where

$$B\rho_\lambda = \gamma, \quad r_\lambda = 0$$

and ρ_K and r_K represent the basic and nonbasic variables of the unique solution to (5), $(\hat{\phi},\hat{\xi})$.

When the scheme is applied to (2), w^n is a related variable. The question of interchanging w_i^n for some $i \in \{1,\cdots,m_n\}$ will not be considered in the scheme until we come upon λ such that

$$r_\lambda^j \ge 0, t_{\lambda,j} = 0, \ j = 1,\cdots,n-1$$

$$r_\lambda^n = w_\lambda^n, \quad t_{\lambda,n} = z_n = 0$$

The first K related basic and nonbasic vectors must be

$$r_\lambda = \left(\rho_\lambda^1,\cdots,\rho_\lambda^{n-1},w_\lambda^n\right)^t$$

$$t_\lambda = \left(r_{\lambda,1}\cdots,r_{\lambda,n-1},z_{\lambda,n}\right)^t$$

for $\lambda = 1$ to K. Lemma 4 and the fact that $\hat{z}_n = 0$ imply that r_K, t_K are the basic and nonbasic variables $(\hat{w},\hat{z})$. Therefore, the theorem applies to the algorithm if $\hat{z}_n = 0$.

Case 2: If $\hat{z}_n > 0$ and $\hat{w}_{\hat{i}}^n = 0$ for some $\hat{i} \in \{1,\cdots,m_n\}$, then every related basic vector $\left(r_\lambda^1,\cdots,r_\lambda^{n-1},w_\lambda^n\right)$ cannot be a solution to (2) since $t_{\lambda n} = z_n = 0$.

Apply the scheme to (5). By the induction process, we have a sequence of related basic vectors $\rho_\lambda, \lambda = 1$ to k_1, and if a basic matrix appears once in the scheme it does not reappear, k_1 is some finite number and ρ_{k_1}, r_{k_1} are the related basic and nonbasic vectors associated with the unique solution to (5).

When we apply the scheme to (2), the first k_1 related basic and nonbasic vectors must be

$$r_\lambda = \left(\rho_\lambda^1,\cdots,\rho_\lambda^{n-1},w_\lambda^n\right)^t$$

$$t_\lambda = \left(r_{\lambda,1},\cdots,r_{\lambda,n-1},z_{\lambda,n}\right)^t$$

for $\lambda = 1$ to k_1. The hypothesis that $\hat{z}_n > 0$ leads to

$$r_{k_1} = B_{k_1}^{-1}q, \ t_{k_1} = 0, \ r_{k_1}^j \ge 0, \ j = 1,\cdots,n-1$$

and there exists an h_1 such that

$$h_1 = \min\left\{i : r_{k_1,i}^n < 0, i \in \{1,\cdots,m_n\}\right\}$$

The next related basic vector to appear in the scheme would be

$$r_{k_1+1} = \left(\rho_{k_1+1}^1, \cdots, \rho_{k_1+1}^{n-1}, r_{k_1+1}^n\right)$$

where the basic variables associated with $\rho_{k_1+1}^j$ are the same basic variables associated with $\rho_{k_1}^j$ for $j = 1, \cdots, n-1$, and $r_{k_1+1,\hat{i}}^n$ represents the variable z_n. The related nonbasic variables would be

$$t_{k_1+1} = \left(r_{k_1+1,1}, \cdots, r_{k_1+1,n-1}, w_{\hat{i}}^n\right)^t$$

Let $y = \left(\rho_{k_1+1}^1, \cdots, \rho_{k_1+1}^{n-1}, r_{k_1+1}^n\right)^t$. Let B be the associated related basic matrix and let $x = \left(r_{k_1+1,1}, \cdots, r_{k_1+1,n-1}, w_{\hat{i}}^n\right)^t$. Let D be the associated related nonbasic matrix. That is, those columns associated with the components of *t*. Then

$$By + Dx = q$$

Multiplying both sides of the above equation on the left by B^{-1}, we have

$$y + \tilde{N}x = \tilde{q}$$

$\tilde{N}$ is a vertical block *P*-matrix of type $(m_1, \cdots, m_n)$, since it is the result of a sequence of principal pivots on *N*. The generalized linear complementarity problem with respect to $\tilde{N}$ is:

For $\tilde{q} \in R^m$, find $y \in R^m, x \in R^n$ such that

$$y - \tilde{N}x = \tilde{q}$$

$$y \geq 0, \ x \geq 0$$

$$x_j \prod_{i=1}^{m_j} y_i^j = 0, \quad j = 1, \cdots, n \tag{7}$$

By our assumptions, (7) has a unique solution in which $w_{\hat{i}}^n = 0$. If $h_1 = \hat{i}$, then the unique solution to (7) is $(\hat{y}, \hat{x})$ and $\hat{x}_n = w_{\hat{i}}^n = 0$. The subsequent related basic vectors for solving (2) are exactly those related basic vectors which will be obtained by applying the scheme to (7) with y as the initial related basic vector.

We showed in Case 1 that a generalized linear complementarity problem like (7) with unique solution $(\hat{r}, \hat{t})$ and $\hat{t}_n = 0$ is solved by applying the scheme to (7) and a solution will be obtained in a finite number of steps without a related basic matrix appearing more than once. All these basic matrices will have z_n as a basic variable of the nth block of basic variables and $x_n = w_{\hat{i}}^n$ will be nonbasic.

If $h_1 \neq \hat{i}$, we apply the scheme to (7). When applying the scheme to (7), we can argue just as we did when we first applied the scheme to (2). If our transformed system (7) has the unique solution $(\hat{y}, \hat{x})$ such that $\hat{x}_n > 0$, then after k_2 steps in the scheme, we arrive at a related basic and nonbasic vector r_{k_2} and t_{k_2}, respectively, where

$$t_{k_2} = 0, \ r_{k_2}^j \geq 0, \ j = 1, \cdots, n-1$$

and there exists an

$$h_2 = \min\left\{r_{k_2,i}^n < 0, i \in \{1, \cdots, m_n\} - \{h_1\}\right\}$$

By the way the scheme continues, we must eventually reach a transformed system

$$\omega^k - P^k \eta^k = b^k$$

$$\omega^k \geq 0, \eta^k \geq 0$$

$$\eta_j^k \prod_{i=1}^{m_j} \left(\omega^k\right)_i^j = 0, \quad j = 1, \cdots, n$$

that will have as its unique solution $\left(\hat{\omega}^k, \hat{\eta}^k\right)$ and $\hat{\eta}_n^k = 0$. Theorem 5 assures us that a related basic matrix that appears once in the scheme will not re-appear in the scheme. This proves that the theorem must hold if the scheme is applied to (2). Since the theorem is true for $n = k$, it holds for all n.

4. Discussion and Conclusions

The vertical generalized linear complementarity Problem is very general and useful; and it can be applied to many problems in engineering, science, and economics. As such, it may be compared with systems of linear equations, the eigenvalue problem, and linear programming. Thus, it is desirable to have reliable and fail-safe algorithms to obtain a solution. Under the assumption of vertical block *P*-matrix, such a solution exists and is unique. Thus the algorithm takes the input data (N, q) and returns $z \in R^n$, the unique solution. When this occurs, a mapping $F: R^{m\times n} \times R^m$ is defined and this mapping can be used to explore the nature of the VGLP and gain many insights which the researcher desires. An example of this is illustrated in the paper by Oh [10].

Further research might involve investigating the performance of the algorithm under random input data (N, q), measuring the number of iterations taken on average, etc., and the number of arithmetic operations necessary to obtain a solution. These investigations are in lieu of knowledge of a fixed number of iterations and arithmetic operations.

An alternative approach might be to examine a limited set of solutions (say 10 - 50) using a restricted set of points in order to answer some specific questions. This may represent a set of "what if" questions and may satisfy the requirement of this type of study. It is easy to see the appeal of this type of analysis.

Finally, one may envision the algorithm in use as an embedded system, in a vehicle, an industrial machine or a video game. It is quite likely that the model mentioned in Oh [10] would be used in such applications with models of motion, contact (or collision), fluid flow, cooling, etc. In all these cases, the use of direct algorithm will provide efficient, reliable solutions which are necessary for the application of the system in which it is embedded.

The direction of future research will be motivated by all of the above instances of the applications of the vertical generalized linear complementarity problem, and by the discovery of new application areas, which seems to be increasing, as the understanding of this problem continues to develop.

The direct algorithm presented in this paper has certain features not present in other algorithms. It converges in a finite number of steps, and each step consists of only a unique principal pivot. No anti-cycling device is necessary, even if there is degeneracy in the defining equations. Since the choice of pivot rule is discrete, rather than continuous (such as in the minimum ratio test), no ties are possible. If desired, the use of pre-existing linear algebra software enables the solution of the linear equations, which is required for each iteration of the algorithm.

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Mathematical Model of the Criterion of Optimization by Compensation for Designing Commercial Bottles with Lateral Surfaces of Revolution and a Straight Section along Its Silhouette

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Abstract

In this article, the mathematical foundations of the so called Criterion of Optimization by Compensation for designing commercial bottles with a straight section along its silhouette and with lateral surfaces of revolution is presented. Such mathematical model uses as main tools, Lagrange polynomial interpolation and Newton's Method for Nonlinear Systems being first necessary to formulate and demonstrate a theorem. It was redesigned and manufactured a bottle of a half-liter of Fanta soda of the well-known Coca Cola Company, which uses 18.86% more material that such criterion establishes. It was expected that the redesigned bottle use 4.91% more of material with respect to what is established by the Criterion of Optimization by Compensation. However, it was reported a 13% of mistake due to important limitations that must be overcome.

Keywords

Optimization, Modelling, Bottle Design, Environmental Pollution, Solid Residues

1. Introduction

During the production stages of a bottle until being finally sent to the consumers, the manufacturers and merchants must confront a more exigent market and society every day. The bottle has to satisfy not only the necessity of containing, protecting, preserving, commercializing and distributing merchandise, if not also, of retraining, decrease of the ecological impacts and minimization of costs. Therefore, it is necessary to design appropriate bottles according to necessities above indicated, making this evident the necessity of generating and transmitting the knowledge of science and technology, in which the concept of optimization is of great importance. For instance, Fletcher [1] and Pierre [2] describe optimization methods that are currently most valuable in solving real-life problems.

Up to now, there has not been found studies about a clear mathematical model of an optimization method of a bottle with a lateral surface of revolution and a straight section along its silhouette. In the case of PET bottles, there are some studies about optimizing and redesigning the whole or part of the body of them by using different software programs. Masood and KeshavaMurthy [3] have reported the process, design and optimization of a bottle shape using Pro/Engineer Parametric Modelling Software and Pro/Mechanica Finite Element Software (FES); Demeril and Dave [1] have used numerical modelling with finite element analysis (FEA) techniques to redesign the petaloid base of bottles to improve stress-crack resistance. An experimental design based on an algorithmic partial cubic method was employed. Quinchung *et al.* [4] have optimized the structure of the PET bottle in order to increase the buckling load, based on the Abaqus/Explicit computer program. Moreover, according to the stress contour of PET bottle obtained by Abaqus, plastic distribution of PET bottle was optimized in order to improve the efficiency of PET material and reduce the weight of the PET bottle. In addition, Mohammad [5] described the formulation of the mathematical model of the PET thermoplastic material for FEA drop-test simulation. Finally, Silva *et al.* [6] have designed and optimized a PET bottle through parametric computer aided design software (solidworks) and finite element method analysis, allowing the simulation of the blowing process from data input to the process variables listed in the available literature.

On the other hand, for aluminum bottles, Han *et al.* [7] have used numerical simulation and mathematical programming to optimized a cylindrical shell body of an aluminum can (volume: 500 ml), which was triangulated as one of the expectant choices of crushable cans for being folded down easily and safely for recycling. At the same way, Han *et al.* [8] have applied the structural optimization technique, to aluminum beverage bottle design, based on nonlinear finite element analyses to know the influence of the design parameters on the buckling strength and the stiffness of the bottom under an axial load and internal pressure, respectively. Similarly, Han *et al.* [9] have also performed multi-objective optimization of a two-piece aluminum beverage bottle considering tactile sensation of heat and embossing formability. Karl *et al.* [10] have performed simulation of the filling of PET bottles with a volumetric swirl chamber valve on the basis of calculations models and experiments. Hopmann *et al.* [11] have provide a sism tiao mulative approach to determine a well-adapted preform and bottle design as well as corresponding process parameters. For this, a three-dimensional simulation of the stretch-blow molding process was used within an iterative optimization routine. At the same way, numerical modelling and optimization of the production process of glass bottles have been the topic of several papers [12] [13] [14] [15] [16] [17].

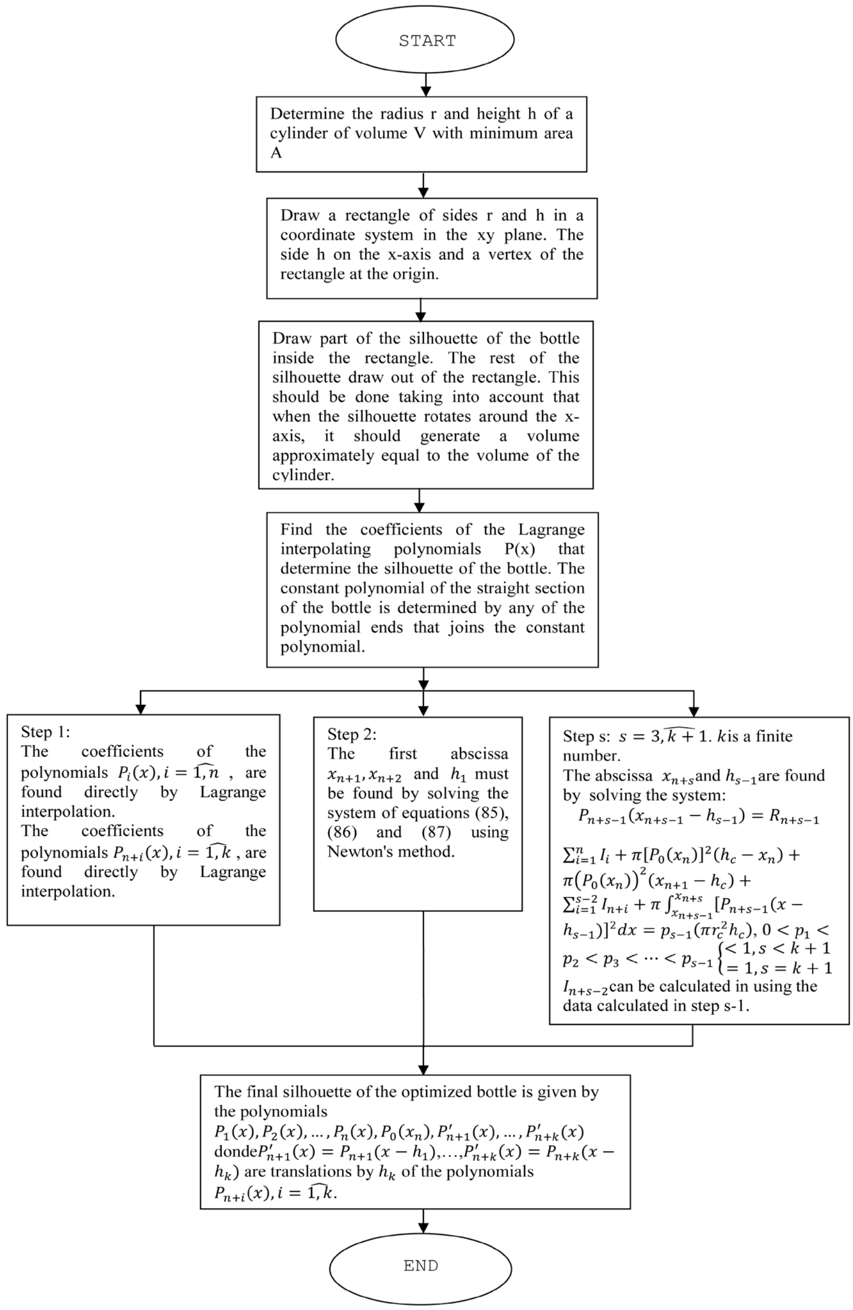
Therefore, since most containers whose shapes are determined by surface of revolution and manufactured from plastic or metal material, the enterprises that decide to apply criterion of optimization on its manufacture, could try to reach the following achievements: reduction of rubbish, saving energy, decrease of the negative environmental impact and hence a friendly environmental image.

In this work, we report a mathematical model of the Criterion of Optimization by Compensation proposed by Reyna and Moore [18] in order to design commercial bottles with lateral surfaces of revolution and a straight section along its silhouette. With the aim of designing and manufacturing bottles using the less amount of material in their fabrication, it can avoid so environmental pollution by solid residues. Since the expenditure of material is proportional to the area of a bottle, to design a bottle by using the lesser as amount of material as possible, means that the superficial area of the bottle have to be minimized. For example, to design a cylinder of minimal area is very easy since it is possible to find its area as a function of its radius and then in using differential calculus to get the radius and height of the cylinder that makes the area of the cylinder a minimum. In the case of any container (bottle in particular) with lateral surface of revolution and a predetermined silhouette, to get a mathematical relation similar to the case of the cylinder, in general is not possible. In this case, that the Criterion of Optimization by Compensation becomes appropriate.

Such Criterion of Optimization by Compensation tells us that in order to design a bottle with a minimal total superficial area, it must first design a cylinder with a minimal total superficial area. From the cylinder, it must be get the shape of the bottle by removing certain solid parts of the cylinder. With the solid parts removed, it must be formed a cylinder whose volume is equal to the sum of the volumes of the solid parts removed from the initial cylinder. The lateral surface area of the formed cylinder must be equal to or less than the sum of the outer surface areas of the solid parts removed from the initial cylinder. This new formed cylinder has to fit the straight section of the bottle that is being designing. Since de cylinder has a minimal area, it is optimized, and at a beginning, the superficial area of the bottle is optimized too. Indeed, theorem 2.1 (see below) shows that the area of the bottle results to be less than that of the cylinder. However, this is only a descriptive fact and a mathematical modelling turns out to be necessary. Then, this work presents a mathematical modelling as the one required, according to the Criterion of Optimization by Compensation.

2. Theory

Flow diagram of the Optimization method for designing an optimized bottle of volume V. The starting point is a cylinder of minimal area of volume V. Following the Criterion of Optimization by Compensation according to steps 1, 2,…, $s = \widehat{3, k+1}$, where k is a finite number, the final silhouette of the optimized bottle can be found. From this, the three dimensional bottle is obtained.



2.1. Criterion of Optimization of Containers with a Straight Cylindrical Shape

To design a container with a straight cylindrical shape and of a certain volumetrically capacity in using a smaller amount of material, lead us to determine a minimum of the following function

$$A(r) = 2\pi r^2 + \frac{2V}{r} \tag{1}$$

where V, A and r are the volume, total area and radius of the cylinder respectively.

Deriving the function $A(r)$ with respect to r and equaling to zero we have that

$$4\pi r - \frac{2V}{r^2} = 0$$

Solving this equation with respect to r

$$r = \sqrt[3]{\frac{V}{2\pi}} \tag{2}$$

Which is a critical point for the function given in Equation (1)

But

$$\frac{\mathrm{d}^2 A(r)}{\mathrm{d}r^2} = 4\pi + \frac{4V}{r^3} \tag{3}$$

By replacing (2) in (3)

$$\frac{\mathrm{d}^2 A\left(\sqrt[3]{\frac{V}{2\pi}}\right)}{\mathrm{d}r^2} = 12\pi$$

Which is major than zero. This means that the value of r given by Equation (2) corresponds to a minimum and which let us determine the height h of the cylinder in using $V = \pi r^2 h$, equal to

$$h = \sqrt[3]{\frac{4V}{\pi}} \tag{4}$$

As it can be seen in this case, it is not difficult to get the values of r given by Equation (2) and h given by Equation (4) which let us minimize the area of a cylinder for a given value of its volume V. Furthermore Equation (3) tell us that Equation (1) is always concave above because $4\pi + \frac{4V}{r^3} > 0$, $\forall r > 0$. This means that r given by Equation (2) corresponds to a global minimum.

2.2. Criterion of Optimization by Compensation

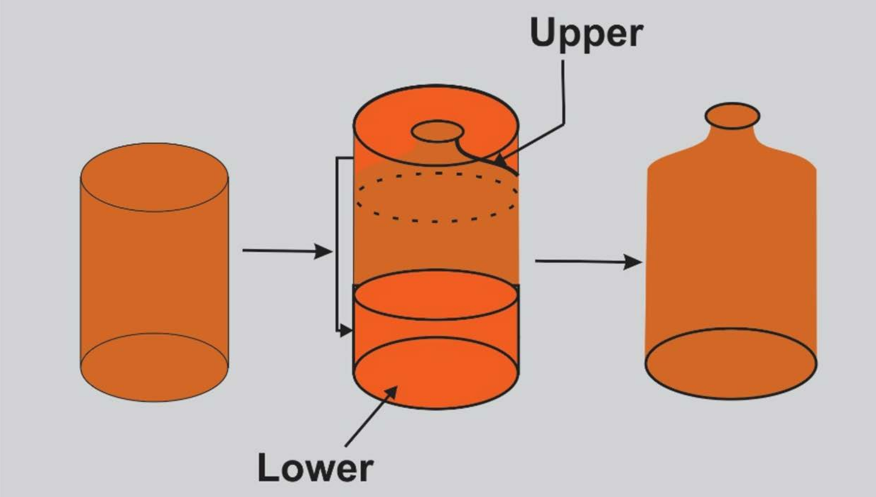
In the case of designing containers with a non-cylindrical shape as it can be the general case, of a bottle, its silhouette could result whimsical due to aesthetic considerations as many others, so it is impossible to write an Equation (function), as in the case of the cylinder discussed in Section 2.1. Therefore, in order to solve this apparent difficult, we will use the Criterion of Optimization by Compensation proposed by Reyna and Moore [18]. This optimization criterion consists in designing first a cylinder with a minimal area for a given volume in using Equations (2) and (4) and then redistributes the total volume and area that will be removed from de cylinder in order to get the desired shape of the bottle that we wish to manufacture. At the end of the process, the volume of the resultant bottle must be equal to that of the original cylinder, where the area of the resultant bottle could be less than that of the cylinder, as it is shown in theorem 2.1 below. Now, the unique proposition given in [19] tell us that the area of a cylinder of minimal area is among the area of a sphere and the area of a cube having all of them the same volume. But, the area of the bottle turns out to be less than that of the cylinder of minimal area, so we have the area of a bottle closer to the area of a sphere than the area of a cylinder of minimal area. Of course, the volumes of the bottle, cylinder of minimal area and sphere are the same. Since the sphere is considered as a geometric object with maximum volume and lesser area, the Criterion of Optimization by Compensation turns out to be a good method for optimizing.

An outline of the Criterion of Optimization by Compensation, in order to minimize the area of a bottle, keeping a constant volume is as follow:

1) Know the volumetric capacity V of the bottle that will be optimized;

2) Optimize the total area of a cylinder whose volumetric capacity is V;

3) In each zone of the optimized cylinder where will be modified (**Figure 1(a)**) in order to get the desired shape of the bottle, it must be removed a solid which is enclosed by an external surface, the surface of the cylinder, and internal surface, the surface of revolution that will give the shape to the bottle. See in the upper part of **Figure 1(b)** signed with the arrow. Calculate the difference of areas between the cylindrical surface and the surface of revolution that both enclose the solid that was removed. With this difference must be formed a cylinder without bases whose volume must be equal approximately to the volume that was removed (see **Figure 1(b)**);



(a) (b) (c)

Figure 1. (a) Optimized cylinder with a volume V from which an optimized bottle will be obtained; (b) Cylinder with an upper region that will be lost and recovered in the lower region; (c) Bottle after the application of the optimization criterion. Adapted with permission from Reyna and Moore [18]. Copyright 2016 ECI.

4) Fit the cylinder without bases, obtained in the step 3, in the cylindrical zone of the optimized cylinder. In this way, it is possible to obtain an optimized bottle with lateral surface of revolution (see Figure 1(c)).

The theorem below is based on the Criterion of Optimization by Compensation. This theorem tell us that it is possible to deform a cylinder of volume V_c and minimal area A_c to a solid of revolution of volume V_s and area A_s such that $V_c = V_s$ and $A_s < A_c$. This theorem is formulated in order to show in particular that the area of a bottle could be less than the corresponding minimal area of a cylinder, both enclosing the same volume, so that the optimization of the bottle is better.

Theorem 2.1 *There exists a solid of revolution of the non-convex type whose surface is less than the surface of a right circular cylinder of minimal area, keeping both of them the same volume.*

Proof

Figure 2 shows the scheme to be used in order to prove the theorem given above.

From scheme of Figure 2 we have:

$$V_c = \sum_{i=1}^{6} V_i \tag{5}$$

Due to the Criterion of Optimization by Compensation,

$$V_7 = \sum_{i=4}^{6} V_i \tag{6}$$

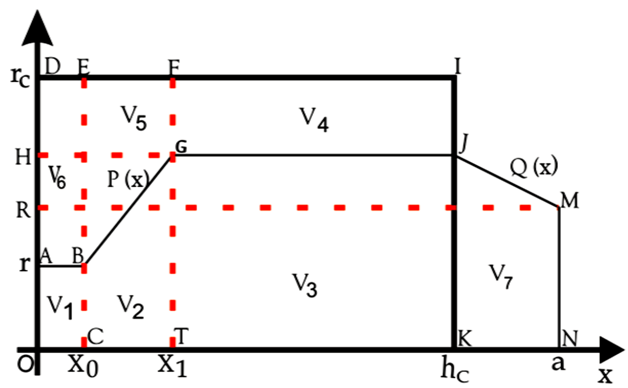


Figure 2. Schema according to the criterion of optimization by compensation. h_c and r_c correspond to the height and radius of a cylinder of volume V_c and minimal area A_c which is generated when the rectangle *ODIK* rotates around the x-axis. From Equations (2) and (4), we have that $r_c = \frac{h_c}{2}$. $P(x)$ and $Q(x)$ are polynomials of first degree whose coefficients must be found. $V_i, i = \widehat{1,7}$ are the volumes generated when the regions given by the correspondent closed polygons *OABC*, *CBGT*, *TGJK*, *GFIJ*, *BEFG*, *ADEB* and *KJMN*, rotate around the x-axis. A_i, $i = \widehat{0,5}$ are the areas generated when the correspondent segments *OA*, *AB*, *BG*, *GJ*, *JM* and *MN*, rotate around the x-axis. The value of a must be found. H, r, R, x_0 and x_1 are values that must be freely given in such a way as to allow us to determine an acceptable value for a.

replacing Equation (6) in (5)

$$V_c = \sum_{i=1}^{3} V_i + V_7 \tag{7}$$

We have as well that,

$$V_c = \pi r_c^2 h_c \tag{8}$$

$$V_1 = \pi r^2 x_0 \tag{9}$$

$$V_2 = \pi \int_{x_0}^{x_1} \left[P(x) \right]^2 \mathrm{d}x \tag{10}$$

$$V_3 = \pi H^2 \left(h_c - x_1 \right) \tag{11}$$

$$V_7 = \pi \int_{h_c}^{a} \left[Q(x) \right]^2 \mathrm{d}x \tag{12}$$

$$P(x) = \alpha_1 x + \alpha_2 \tag{13}$$

$$Q(x) = \beta_1 x + \beta_2 \tag{14}$$

By replacing Equation (13) in (10)

$$V_2 = \pi \int_{x_0}^{x_1} \left[\alpha_1 x + \alpha_2 \right]^2 \mathrm{d}x$$

$$V_2 = \pi \left[\alpha_1^2 \frac{\left(x_1^3 - x_0^3 \right)}{3} + \alpha_1 \alpha_2 \left(x_1^2 - x_0^2 \right) + \alpha_2^2 \left(x_1 - x_0 \right) \right] \tag{15}$$

Then,

$$V_2 = V_2 \left(\alpha_1, \alpha_2 \right) \tag{16}$$

By replacing Equation (14) in (12),

$$V_7 = \pi \int_{h_c}^{a} \left[\beta_1 x + \beta_2 \right]^2 \mathrm{d}x$$

$$V_7 = \pi \left[\beta_1^2 \frac{\left(a^3 - h_c^3 \right)}{3} + \beta_1 \beta_2 \left(a^2 - h_c^2 \right) + \beta_2^2 \left(a - h_c \right) \right] \tag{17}$$

Then,

$$V_7 = V_7 \left(\beta_1, \beta_2, a \right) \tag{18}$$

By replacing Equations. (8), (9), (11), (16) and (18) in (7),

$$\pi r_c^2 h_c - \pi r^2 x_0 - V_2 \left(\alpha_1, \alpha_2 \right) - \pi H^2 \left(h_c - x_1 \right) - V_7 \left(\beta_1, \beta_2, a \right) = 0 \tag{19}$$

Let A_c be such that,

$$A_c = \sum_{i=0}^{5} A_i \tag{20}$$

Where,

$$A_0 = \pi r^2 \tag{21}$$

$$A_1 = 2\pi r x_0 \tag{22}$$

$$A_2 = 2\pi \int_{x_0}^{x_1} P(x) \sqrt{1 + \left[P'(x) \right]^2} \mathrm{d}x \tag{23}$$

$$A_3 = 2\pi H \left(h_c - x_1 \right) \tag{24}$$

$$A_4 = 2\pi\int_{h_c}^{a} Q(x)\sqrt{1+\left[Q'(x)\right]^2}\,\mathrm{d}x \tag{25}$$

$$A_5 = \pi R^2 \tag{26}$$

$$A_c = 2\pi r_c h_c + 2\pi r_c^2 \tag{27}$$

Deriving Equation (13),

$$P'(x) = \alpha_1 \tag{28}$$

Deriving Equation (14),

$$Q'(x) = \beta_1 \tag{29}$$

Replacing Equations (13) and (28) in (23) and integrating,

$$A_2 = 2\pi\sqrt{1+\alpha_1^2}\left[\alpha_1\frac{x_1^2}{2} + \alpha_2 x_1 - \alpha_1\frac{x_0^2}{2} - \alpha_2 x_0\right] \tag{30}$$

Then,

$$A_2 = A_2(\alpha_1, \alpha_2) \tag{31}$$

Replacing Equations (14) and (29) in (25) and integrating,

$$A_4 = 2\pi\sqrt{1+\beta_1^2}\left[\beta_1\frac{a^2}{2} + \beta_2 a - \beta_1\frac{h_c^2}{2} - \beta_2 h_c\right] \tag{32}$$

Then,

$$A_4 = A_4(\beta_1, \beta_2, a) \tag{33}$$

Replacing Equations (21), (22), (24), (26), (31) and (33) in (20),

$$2\pi r_c h_c + 2\pi r_c^2 - \pi r^2 - 2\pi r x_0 - A_2(\alpha_1, \alpha_2) - 2\pi H(h_c - x_1) - A_4(\beta_1, \beta_2, a) - \pi R^2 = 0 \tag{34}$$

Now, the conditions that the polynomials $P(x)$ and $Q(x)$ must satisfy are:

$$P(x_0) = r \tag{35}$$

$$P(x_1) = H \tag{36}$$

$$Q(h_c) = H \tag{37}$$

$$Q(a) = R \tag{38}$$

From Equations (35) and (13),

$$\alpha_1 x_0 + \alpha_2 - r = 0 \tag{39}$$

From Equations (36) and (13),

$$\alpha_1 x_1 + \alpha_2 - H = 0 \tag{40}$$

From Equations (37) and (14),

$$\beta_1 h_c + \beta_2 - H = 0 \tag{41}$$

From Equations (38) and (14),

$$\beta_1 a + \beta_2 - R = 0 \tag{42}$$

Taking into account Equations (19), (34), (39), (40), (41) and (42) we get the following system of equations,

$$\alpha_1 x_0 + \alpha_2 - r = 0 \tag{43}$$

$$\alpha_1 x_1 + \alpha_2 - H = 0 \tag{44}$$

$$\beta_1 h_c + \beta_2 - H = 0 \tag{45}$$

$$\beta_1 a + \beta_2 - R = 0 \tag{46}$$

$$\pi r_c^2 h_c - \pi r^2 x_0 - V_2(\alpha_1, \alpha_2) - \pi H^2 (h_c - x_1) - V_7(\beta_1, \beta_2, a) = 0 \tag{47}$$

$$\begin{aligned} &2\pi r_c h_c + 2\pi r_c^2 - \pi r^2 - 2\pi r x_0 - A_2(\alpha_1, \alpha_2) \\ &-2\pi H (h_c - x_1) - A_4(\beta_1, \beta_2, a) - \pi R^2 = 0 \end{aligned} \tag{48}$$

Hence, we have six equations in five unknowns.

From Equations (43) and (44),

$$\alpha_1 = \frac{H - r}{x_1 - x_0} \tag{49}$$

$$\alpha_2 = \frac{r x_1 - H x_0}{x_1 - x_0} \tag{50}$$

From Equations. (45) and (46),

$$\beta_1 = \frac{R - H}{a - h_c} \tag{51}$$

$$\beta_2 = \frac{Ha - R h_c}{a - h_c} \tag{52}$$

By replacing Equations (15) and (17) in (47),

$$\begin{aligned} &\pi r_c^2 h_c - \pi r^2 x_0 - \pi\left[\alpha_1^2 \frac{\left(x_1^3 - x_0^3\right)}{3} + \alpha_1\alpha_2\left(x_1^2 - x_0^2\right) + \alpha_2^2\left(x_1 - x_0\right)\right] \\ &- \pi H^2\left(h_c - x_1\right) - \pi\left[\beta_1^2 \frac{\left(a^3 - h_c^3\right)}{3} + \beta_1\beta_2\left(a^2 - h_c^2\right) + \beta_2^2\left(a - h_c\right)\right] = 0 \end{aligned} \tag{53}$$

By replacing Equations (49), (50), (51) and (52) in (53) and simplifying,

$$\begin{aligned} &\pi r_c^2 h_c - \pi r^2 x_0 - \pi\left[\left(\frac{H - r}{x_1 - x_0}\right)^2 \frac{\left(x_1^3 - x_0^3\right)}{3} + (H - r)(r x_1 - H r_0)\left(\frac{x_1 + x_0}{x_1 - x_0}\right) + \frac{\left(r x_1 - H x_0\right)^2}{x_1 - x_0}\right] \\ &- \pi H^2\left(h_c - x_1\right) - \pi\left[\left(\frac{R - H}{a - h_c}\right)^2 \frac{\left(a^3 - h_c^3\right)}{3} + (R - H)(Ha - R h_c)\left(\frac{a + h_c}{a - h_c}\right) + \frac{\left(Ha - R h_c\right)^2}{a - h_c}\right] = 0 \end{aligned} \tag{54}$$

Equation (54) is an equation in the unknown parameter *a*.

By replacing Equations (30) and (32) in (48)

$$\begin{aligned} &2\pi r_c h_c + 2\pi r_c^2 - \pi r^2 - 2\pi r x_0 - 2\pi\sqrt{1 + \alpha_1^2}\left[\alpha_1 \frac{x_1^2}{2} + \alpha_2 x_1 - \alpha_1 \frac{x_0^2}{2} - \alpha_2 x_0\right] \\ &- 2\pi H\left(h_c - x_1\right) - 2\pi\sqrt{1 + \beta_1^2}\left[\beta_1 \frac{a^2}{2} + \beta_2 a - \beta_1 \frac{h_c^2}{2} - \beta_2 h_c\right] - \pi R^2 = 0 \end{aligned} \tag{55}$$

By replacing Equations (49), (50), (51) and (52) in (55),

$$2\pi r_c h_c + 2\pi r_c^2 - \pi r^2 - 2\pi r x_0 - 2\pi\sqrt{1+\left(\frac{H-r}{x_1-x_0}\right)^2}\left[\left(\frac{H-r}{x_1-x_0}\right)\frac{x_1^2}{2}+\left(\frac{rx_1-Hx_0}{x_1-x_0}\right)x_1\right.$$
$$\left.-\left(\frac{H-r}{x_1-x_0}\right)\frac{x_0^2}{2}-\left(\frac{rx_1-Hx_0}{x_1-x_0}\right)x_0\right]-2\pi H\left(h_c-x_1\right)-2\pi\sqrt{1+\left(\frac{R-H}{a-h_c}\right)^2} \tag{56}$$
$$\times\left[\left(\frac{R-H}{a-h_c}\right)\frac{a^2}{2}+\left(\frac{Ha-Rh_c}{a-h_c}\right)a-\left(\frac{R-H}{a-h_c}\right)\frac{h_c^2}{2}-\left(\frac{Ha-Rh_c}{a-h_c}\right)h_c\right]-\pi R^2=0$$

Equation (56) as well as Equation (54), is an equation in the unknown parameter *a*.

Since we have a theorem of existence, we solve numerically Equation (54) in the unknown parameter a in using the testing data $r=1.2u$, $r_c=4.43u$, $h_c=8.86u$, $x_0=2u$, $H=4.2u$, $R=2.7u$ and $x_1=4.7u$. Here, from Equations (2) and (4) $r_c=\frac{h_c}{2}$ and the value $h_c=8.86u$ is arbitrary. The rest of values for r, x_0, H and R are given heuristically by looking Figure 2 and according to the Criterion of Optimization by Compensation. This let us find $a=15.1384u$. With this data, the area and volume of the solid of revolution that is generated when the region enclosed by the polygonal *OABGJMN* and x-axis of **Figure 2**, rotates around *x*-axis, are equal to $A_s=360.684u^2$ and $V_s=546.249u^3$ respectively.

The minimal area of the cylinder of revolution that is generated when the region enclosed by the rectangle *ODIK* rotates around the *x*-axis, is equal to $A_c=369.921u^2$, while its volume is equal to $V_c=546.249u^3$ which is the same value for the solid of revolution. So, we have $V_c=V_s$ and $A_s<A_c$ which prove the theorem.

Equation (56) led us to a no wished solution since $a=15.5758u$ increase the volume of the solid of revolution to $V_s=562.862u^3$ such that the surface of minimal area of the cylinder is $A_c=A_s=369.921u^2$. Say, we have $A_c=A_s$ and $V_c<V_s$.

2.3. Mathematical Model of the Criterion of Optimization by Compensation for Designing Commercial Bottles with a Straight Section along Its Silhouette

In this section, the mathematical model of the criterion of optimization by compensation for designing commercial bottles with lateral surfaces of revolution and a straight section along its silhouette is presented. The start point is the schema shown in **Figure 3**, which is based in the criterion of optimization by compensation seen in the *xy*-plane.

The mathematical model taking into account the Criterion of Optimization by Compensation is as follows: consider the schema (shown in **Figure 3**) corresponding to a general bottle with a straight section along its silhouette, where $V_i, i=\widehat{1,n+k}$, are volumes generated when the regions below the curves represented by the non-constant polynomials $P_i(x), i=\widehat{1,n+k}$ of certain

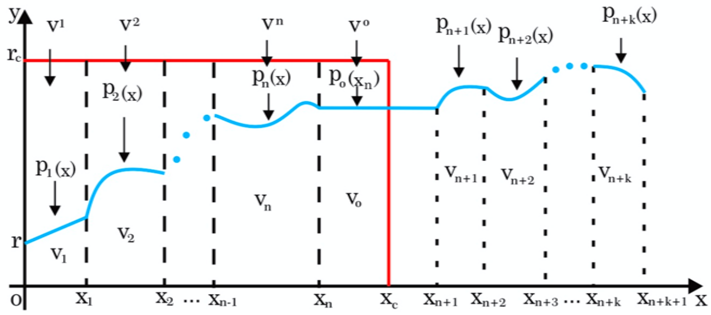


Figure 3. Schema to get a mathematical model in using the Criterion of Optimization by Compensation. When the rectangle with vertices $(0,0),(0,r_c),(h_c,r_c)$ and $(h_c,0)$ rotates around the *x*-axis, the cylinder of minimal area is to be obtained. When the curve described by the polynomials that must be determined in using interpolation when a set of points is given, rotates around the *x*-axis, the bottle must be obtained. Here, r,r_c,h_c and $x_i, i=\widehat{1,n}$ are known constants. $P_i(x), i=\widehat{0,n+k}$ are the polynomials that describe the silhouette of the bottle. V_i and $V^i,\widehat{0,n}$ are described on the text.

degree rotates around the *x*-axis. The value of k depends on the number of polynomials needed to complete the shape of the silhouette of the bottle out of the rectangle with vertices $(0,0)$, $(0,r_c)$, (h_c,r_c) and $(h_c,0)$. $V^i,\widehat{1,n}$ are volumes generated when the regions above of the polynomials $P_i(x),\widehat{1,n}$, rotates around the x-axis. V_0 and V^0 are volumes below and above the constant polynomial $P(x)=P_0(x_n)$. Then, from Figure 3

$$V_c = \sum_{i=0}^{n}\left(V_i + V^i\right) \tag{57}$$

where V_c is the volume of the cylinder of minimal area with radius r_c and height h_c which is generated when the rectangle with vertices $(0,0),(0,r_c),(h_c,r_c)$ and $(h_c,0)$ rotates around the *x*-axis (see Figure 3). By Criterion of Optimization by Compensation

$$\sum_{i=0}^{n} V^i = \pi\left(P_0(x_n)\right)^2\left(x_{n+1}-h_c\right) + \sum_{i=1}^{k} V_{n+i} \tag{58}$$

Putting Equation (58) in (57)

$$V_c = \sum_{i=0}^{n} V_i + \pi\left(P_0(x_n)\right)^2\left(x_{n+1}-h_c\right) + \sum_{i=1}^{k} V_{n+i} \tag{59}$$

But,

$$V_c = \pi r_c^2 h_c \tag{60}$$

$$V_1 = \pi\int_0^{x_1}\left[P_1(x)\right]^2 \mathrm{d}x \tag{61}$$

$$V_2 = \pi\int_{x_1}^{x_2}\left[P_2(x)\right]^2 \mathrm{d}x \tag{62}$$

$$\vdots$$

$$V_n = \pi\int_{x_{n-1}}^{x_n}\left[P_n(x)\right]^2 \mathrm{d}x \tag{63}$$

$$V_0 = \pi\left[P_0(x_n)\right]^2\left(h_c - x_n\right) \tag{64}$$

$$\begin{aligned} V_{n+1} &= \pi\int_{x_{n+1}}^{x_{n+2}}\left[P_{n+1}(x)\right]^2 \mathrm{d}x \\ V_{n+2} &= \pi\int_{x_{n+2}}^{x_{n+3}}\left[P_{n+2}(x)\right]^2 \mathrm{d}x \end{aligned} \tag{65}$$

$$\vdots$$

$$V_{n+k} = \pi\int_{x_{n+k}}^{x_{n+k+1}}\left[P_{n+k}(x)\right]^2 \mathrm{d}x \tag{66}$$

Putting Equations (60)–(66) in (59), we have finally,

$$\begin{aligned} \pi r_c^2 h_c &= \pi\int_0^{x_1}\left[P_1(x)\right]^2 \mathrm{d}x + \pi\sum_{i=1}^{n-1}\int_{x_i}^{x_{i+1}}\left[P_{i+1}(x)\right]^2 \mathrm{d}x + \pi\left[P_0(x_n)\right]^2(h_c - x_n) \\ &+ \pi\left(P_0(x_n)\right)^2(x_{n+1} - h_c) + \pi\sum_{i=1}^{k}\int_{x_{n+i}}^{x_{n+i+1}}\left[P_{n+i}(x)\right]^2 \mathrm{d}x \end{aligned} \tag{67}$$

Equation (67) is a fundamental equation derived from the Criterion of Optimization by Compensation.

Now let $P_1(x) = \sum_{i=0}^{m_1} a_1^i x^i$, $P_2(x) = \sum_{i=0}^{m_2} a_2^i x^i$, $\cdots$, $P_n(x) = \sum_{i=0}^{m_n} a_n^i x^i$, $P_{n+1}(x) = \sum_{i=0}^{m_{n+1}} a_{n+1}^i x^i$, $P_{n+2}(x) = \sum_{i=0}^{m_{n+2}} a_{n+2}^i x^i$, $\cdots$, $P_{n+k}(x) = \sum_{i=0}^{m_{n+k}} a_{n+k}^i x^i$ be, the polynomials that are shown in **Figure 3**, where the coefficients of these polynomials are unknowns. Thus, the Optimization problem can be formulated as follows: given the equation

$$\begin{aligned} \pi r_c^2 h_c &= \pi\int_0^{x_1}\left[P_1(x)\right]^2 \mathrm{d}x + \pi\sum_{i=1}^{n-1}\int_{x_i}^{x_{i+1}}\left[P_{i+1}(x)\right]^2 \mathrm{d}x + \pi\left[P_0(x_n)\right]^2(h_c - x_n) \\ &+ \pi\left(P_0(x_n)\right)^2(x_{n+1} - h_c) + \pi\sum_{i=1}^{k}\int_{x_{n+i}}^{x_{n+i+1}}\left[P_{n+i}(x)\right]^2 \mathrm{d}x \end{aligned} \tag{68}$$

Subject to the following conditions:

$$P_1(x_0) = r \tag{69}$$

$$P_1(x_1) = P_2(x_1) = R_1 \tag{70}$$

$$P_2(x_2) = P_3(x_2) = R_2 \tag{71}$$

$$P_{n-1}(x_{n-1}) = P_n(x_{n-1}) = R_{n-1}$$

$$P_n(x_n) = P_0(x_n) = R_n = R_0 \tag{72}$$

$$P_0(x_n) = P_0(x_{n+1}) = P_{n+1}(x_{n+1} - h_1) = R_n = R_0 = R_{n+1} \tag{73}$$

$$P_{n+1}(x_{n+2} - h_1) = P_{n+2}(x_{n+2} - h_2) = R_{n+2} \tag{74}$$

$$P_{n+2}(x_{n+3} - h_2) = P_{n+3}(x_{n+3} - h_3) = R_{n+3} \tag{75}$$

$$P_{n+3}(x_{n+4} - h_3) = P_{n+4}(x_{n+4} - h_4) = R_{n+4} \tag{76}$$

$$\vdots$$

$$P_{n+k-1}(x_{n+k} - h_{k-1}) = P_{n+k}(x_{n+k} - h_k) = R_{n+k} \tag{77}$$

$$P_{n+k}(x_{n+k+1} - h_k) = R_{n+k+1} \tag{78}$$

$$P_1(t_i) = P_1^i,\ 0 \le t_i \le x_1,\ 0 \le i \le m_1 \tag{79}$$

$$P_2(t_i) = P_2^i,\ x_1 \le t_i \le x_2,\ 0 \le i \le m_2 \tag{80}$$

$$\vdots$$

$$P_n(t_i) = P_n^i,\ x_{n-1} \le t_i \le x_n,\ 0 \le i \le m_n \tag{81}$$

$$P_{n+1}(t_i) = P_{n+1}^i,\ x_{n+1} \le t_i \le x_{n+2},\ 0 \le i \le m_{n+1} \tag{82}$$

$$P_{n+2}(t_i) = P_{n+2}^i,\ x_{n+2} \le t_i \le x_{n+3},\ 0 \le i \le m_{n+2} \tag{83}$$

$$\vdots$$

$$P_{n+k}(t_i) = P_{n+k}^i,\ x_{n+k} \le t_i \le x_{n+k+1},\ 0 \le i \le m_{n+k} \tag{84}$$

where $R_i, i = 1,\cdots,n+k$ in Equations (70)-(78) are constant ordinates given by the designer. On the other hand, in order to give the shape of the silhouette of the bottle, (t_i, P_1^i), $0 \le t_i \le x_1$, $0 \le i \le m_1$; (t_i, P_2^i), $x_1 \le t_i \le x_2$, $0 \le i \le m_2$; $\cdots$, (t_i, P_n^i), $x_{n-1} \le t_i \le x_n$, $0 \le i \le m_n$ are also given by the designer such that each of them determines a set of points through which the polynomials obtained by interpolation, $P_i(t), i = \widehat{1,n}$, passes respectively. Similarly, the (t_i, P_{n+1}^i), $x_{n+1} \le t_i \le x_{n+2}$, $0 \le i \le m_{n+1}$; (t_i, P_{n+2}^i), $x_{n+2} \le t_i \le x_{n+3}$, $0 \le i \le m_{n+2}$; $\cdots$, (t_i, P_{n+k}^i), $x_{n+k} \le t_i \le x_{n+k+1}, 0 \le i \le m_{n+k}$; are also given by the designer, such that each of them determines a set of points through which the polynomials obtained by interpolation, $P_{n+i}(t), i = \widehat{1,k}$, passes respectively. These polynomials are such that their corresponding polynomials by translation according to, $P_{n+i}(t - h_i), i = \widehat{1,k}$ fit with the remaining part of the bottle in the interval $x_{n+k} \le t_i \le x_{n+k+1}, k \ge 1$. The r and $x_i, \widehat{1,n}$, are constants given by the designer, while r_c and h_c are the radius and height of a cylinder of minimal area. We must find $a_1^i, 0 \le i \le m_1$; $a_2^i, 0 \le i \le m_2$; $\cdots$; $a_n^i, 0 \le i \le m_n$; $a_{n+1}^i, 0 \le i \le m_{n+1}$; $a_{n+2}^i, 0 \le i \le m_{n+2}$; $\cdots$; $a_{n+k}^i, 0 \le i \le m_{n+k}$; $h_i, 1 \le i \le k$; $x_{n+i}, 1 \le i \le k+1$ such that the area of the bottle of volume V_c is less or equal than the area of a cylinder of minimal area according to the theorem given above.

Solving the Problem of Optimization

We can solve the optimization problem in using Lagrange polynomial interpolation and Newton's Method for Nonlinear Systems according to the following steps:

Step 1 Find the constants $a_1^i, 0 \le i \le m_1$; $a_2^i, 0 \le i \le m_2$; $\cdots$; $a_n^i, 0 \le i \le m_n$; $a_{n+1}^i, 0 \le i \le m_{n+1}$; $a_{n+2}^i, 0 \le i \le m_{n+2}$; $\cdots$; $a_{n+k}^i, 0 \le i \le m_{n+k}$, in using Lagrange interpolation, say, by determining the coefficients of the Lagrange interpolating polynomial in each case respectively. These coefficients are the constants we are trying to find.

Step 2 The x_{n+1}, x_{n+2} and h_1 can be found by solving the system of Equations (85), (86) and (87) given below, in using the Newton's Method.

$$\begin{aligned} &\sum\nolimits_{i=1}^{n} I_i + \pi\left[P_0(x_n)\right]^2 (h_c - x_n) + \pi\left(P_0(x_n)\right)^2 (x_{n+1} - h_c) \\ &+ \pi\int_{x_{n+1}}^{x_{n+2}} \left[P_{n+1}(x - h_1)\right]^2 \mathrm{d}x = p_1\left(\pi r_c^2 h_c\right), 0 < p_1 < 1 \end{aligned} \tag{85}$$

where,

$I_1, I_2, \cdots, I_n$ are integrals that correspond to the polynomials

$P_1(x), P_2(x), \cdots, P_n(x)$, and can be calculated as well as $\pi[P_0(x_n)]^2(h_c - x_n)$.

$$P_{n+1}(x_{n+1} - h_1) = R_n = R_0 = R_{n+1} \quad (86)$$

$$P_{n+1}(x_{n+2} - h_1) = R_{n+2} \quad (87)$$

Step 3 x_{n+3} and1 can be found by solving the system of equations:

$$P_{n+2}(x_{n+2} - h_2) = R_{n+2}$$

$$\sum_{i=1}^{n} I_i + \pi[P_0(x_n)]^2(h_c - x_n) + \pi(P_0(x_n))^2(x_{n+1} - h_c) + I_{n+1}$$
$$+ \pi\int_{x_{n+2}}^{x_{n+3}}[P_{n+2}(x - h_2)]^2 \, dx = p_2(\pi r_c^2 h_c), \ 0 < p_1 < p_2 < 1$$

I_{n+1} can be calculated in using the data calculated in step 2.

Step 4 x_{n+4} and h_3 can be found by solving the system of equations:

$$P_{n+3}(x_{n+3} - h_3) = R_{n+3}$$

$$\sum_{i=1}^{n} I_i + \pi[P_0(x_n)]^2(h_c - x_n) + \pi(P_0(x_n))^2(x_{n+1} - h_c) + I_{n+1} + I_{n+2}$$
$$+ \pi\int_{x_{n+3}}^{x_{n+4}}[P_{n+3}(x - h_3)]^2 \, dx = p_3(\pi r_c^2 h_c), \ 0 < p_1 < p_2 < p_3 < 1$$

I_{n+2} can be calculated in using the data calculated in step 3.

Step *k* x_{n+k} and h_{k-1} can be found by solving the system of equations:

$$P_{n+k-1}(x_{n+k-1} - h_{k-1}) = R_{n+k-1}$$

$$\sum_{i=1}^{n} I_i + \pi[P_0(x_n)]^2(h_c - x_n) + \pi(P_0(x_n))^2(x_{n+1} - h_c) + \sum_{i=1}^{k-2} I_{n+i}$$
$$+ \pi\int_{x_{n+k-1}}^{x_{n+k}}[P_{n+k-1}(x - h_{k-1})]^2 \, dx = p_{k-1}(\pi r_c^2 h_c), \ 0 < p_1 < p_2 < p_3 < \cdots < p_{k-1} < 1$$

I_{n+k-2} can be calculated in using the data calculated in step $k-1$.

Step *k*+1 x_{n+k+1} and h_k can be found by solving the system of equations:

$$P_{n+k}(x_{n+k} - h_k) = R_{n+k}$$

$$\sum_{i=1}^{n} I_i + \pi[P_0(x_n)]^2(h_c - x_n) + \pi(P_0(x_n))^2(x_{n+1} - h_c) + \sum_{i=1}^{k-1} I_{n+i}$$
$$+ \pi\int_{x_{n+k}}^{x_{n+k+1}}[P_{n+k}(x - h_k)]^2 \, dx$$
$$= p_k(\pi r_c^2 h_c), 0 < p_1 < p_2 < p_3 < \cdots < p_k = 1$$

I_{n+k-1} can be calculated in using the data calculated in step *k*.

The number of unknown coefficients of the polynomials depends on the number of points that were arbitrary chosen, in order to get a Lagrange polynomial that must describe the silhouette of the bottle. Hence, we must be careful when the number of points are chosen, since the polynomial in that region could present slight oscillations and not describing the shape of the silhouette of the bottle in that region, as shown in Figure 4. If this were the case, we must try to choose other points by varying slightly some points of the initial set of points until the oscillations have vanished. Polynomial oscillation could be present when a number of chosen points are not appropriated in order to get a Lagrange polynomial interpolation. Therefore, in order to get a desirable solution for the problem of optimization and choose a set of points in such a way that the poly

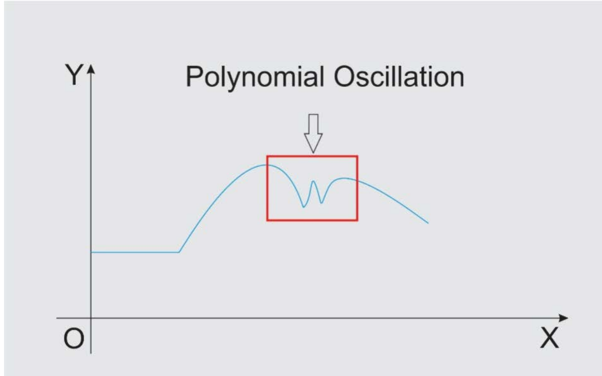


Figure 4. Schema showing the polynomial oscillations when the chosen points are not appropriated to get the Lagrange interpolation. This happens when the number of points chosen is great.

nomials should be free of oscillations, we must use a computer program (optimizer of five sections).

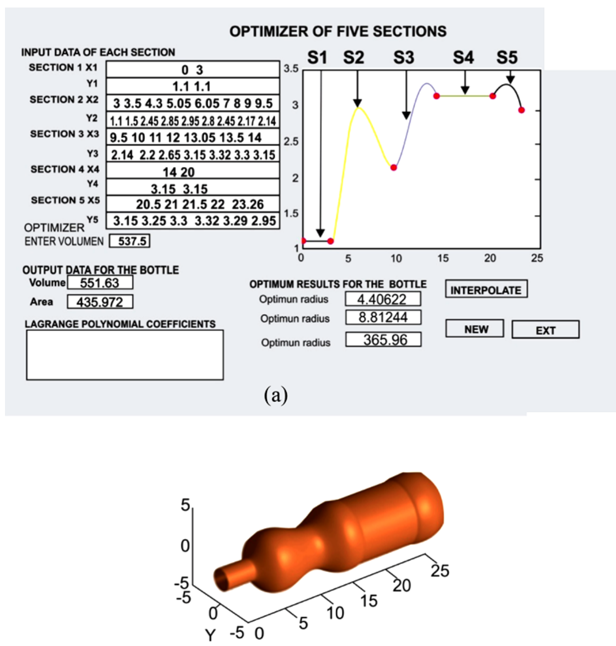
2.4. Application of the Criterion of Optimization by Compensation

As an application of the criterion by compensation, a bottle of Fanta soda of the Coca Cola Company was considered, as shown in **Figure 5**. The characteristics of the bottle are: Type of the product that it contains: carbonated drink; Factory: Coca Cola company; volume of the bottle: 537.5 ml; weight of the empty bottle without its cap: 25.18 g; material from which the bottle is manufactured: Polyethylene terephthalate (PET); base of the bottle: petaloid base of five cavities.

We first analyse the real bottle, in order to determine its superficial area mainly. In fact, after cutting along the bottle through the middle and putting half of it in a coordinate system, previously drawn on a millimetered paper, the x and y coordinates of the silhouette of the real bottle are shown in **Table 1**:

Figure 6(a) shows for the real bottle, the interface of the computer program elaborated in the high-level programming language MATLAB. This computer program has five options: interpolate, volume, area, surface of revolution and optimize in order to perform the tasks. The calculations are performed by considering the bottle with a flat base. Adjustments are made in Input Data of each section. In this case, it was considered five sections $\left(S_i, i=\widehat{1,5}\right)$ for the bottle. In Optimizer, the volume of the bottle to be optimized must be entered. As a result, in using Equations (2)-(4), we get optimum results for the cylinder, such as: radio, height and area. In Output Data of **Figure 6(a)** are shown the results of the volume and area of the bottle, according to the adjustments that were made in Input data of each section. When the optimization is being performed the value of the area varies until get approximately the value of the area obtained in Optimum results for the cylinder, keeping approximately constant the value of the volume in Optimizer (see **Figure 6(a)**). In using the computer program and with the data of the **Table 1**, the real bottle in three dimensions is shown in **Figure 6(b)**. As, it can be seen from the results of the calculations in using the

Figure 5. Bottle of Fanta soda, from the Coca-Cola Company, used to apply the application of the Criterion of Optimization by Compensation.



(b)

Figure 6. Real bottle, (a) Silhouette of the real bottle according to the data of the **Table 1**. It is shown the sections S1, S2…S5, according to data in Input Data of Each Section in Optimizer of Five Sections. In Optimizer, the volume V of the bottle is entered in order to obtain the optimum radius, optimum height and optimum area of the cylinder which are visualized in Optimum Results for the Bottle. In Output Data, for the bottle, the volume and area of the bottle are visualized when the curves in corresponding sections S1, S2…S5 rotates around the x- axis and which generate the bottle; (b) view of the real bottle in three dimensions.

Table 1. Coordinates of the silhouette of the real bottle seen in a Cartesian coordinate system of the *xy* plane. Section 1 (S1), corresponds to the lip of the bottle, Section 2 (S2), section 3 (S3), section 4 (S4) and section 5 (S5) correspond to the form of the bottle.

Section 1		Section 2		Section 3		Section 4		Section 5	
x	*y*	*x*	*y*	*x*	*y*	*x*	*y*	*x*	*y*
0.00	1.10	3.00	1.10	9.50	2.14	14.00	3.15	20.00	3.15
3.00	1.10	3.50	1.50	10.00	2.20	20.00	3.15	20.50	3.25
		4.30	2.45	11.00	2.65			21.00	3.30
		5.05	2.85	12.00	3.15			21.50	3.32
		6.05	2.95	13.05	3.32			22.00	3.29
		7.00	2.80	13.50	3.30			23.26	2.95
		8.00	2.45	14.00	3.15				
		9.00	2.17						
		9.50	2.14						

computer program, the optimum area of the bottle according to the Criterion of Optimization by Compensation must be 365.96 cm^2 when the base of the bottle is flat.

It is worth to emphasize that, the volume of 551.63 cm^3 in Output Data, of **Figure 6(a)**, for the bottle exceeds 537.5 cm^3 because the program calculates the volume of the bottle with flat base. By measuring the volume of the cavities of the petaloid base (base of the real bottle) in laboratory by using water for filling such cavities, it is found a total volume of 14 cm^3 approximately that have to be subtracted from 551.63 cm^3. So we have 537.63 cm^3 which is a good approximation of the volume of the real bottle. Similarly, the area 435.972 cm^2 in Output Data for the bottle is due to fact that the program calculates the area of the bottle by considering it with flat base. By calculations made apart in the zone of the petaloid base in order to determine its area by approximation by triangles and circles as shown in **Figure 7**, we find that the area of the bottle with petaloid base is 435.23 cm^2, so that the difference in areas between the bottle with flat base and petaloid base is not significant.

In order to redesign the bottle, it is necessary to give some points through which the silhouette of the redesigned bottle passes. These points are given by the designer and are shown in **Table 2**, being shown a set of them in **Figure 8** by circles in sections S1, S2, S3, S4 and S5. The task is to determine by Lagrange interpolation the polynomials that pass through these points. The number x_4 in the *x*-axis, is the right extreme of the section S4 which is a straight line, and left extreme of section S5 represented by the polynomial $P_4(x)$. This number must be determined by moving section S5 to the right or left according to the sign of h_1, positive or negative in $P_4(x-h_1)$ as it is shown in **Figure 8**. These polynomials are the starting points to get the final polynomials that determine the silhouette of the redesigned bottle and hence optimized. As it can be seen

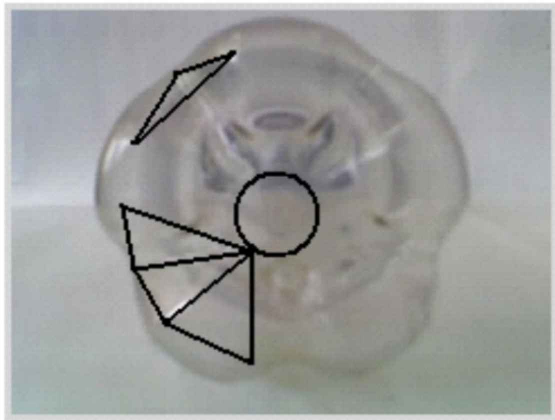


Figure 7. Approximation by triangles and circles in order to determine the area of the petaloid base of the bottle.

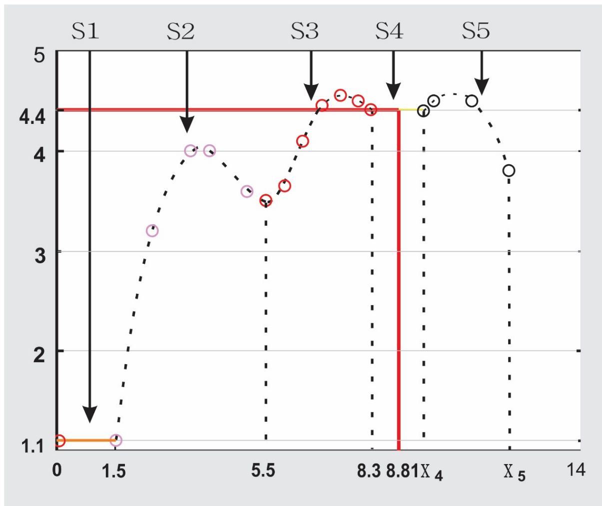


Figure 8. Silhouette of the redesigned bottlein using a set of pointsof Section 1 (S1), Section 2 (S2)… Section 5 (S5) shown in Table 2.

Table 2. Coordinates of the silhouette of the redesigned bottle seen in a Cartesian coordinate system of the *xy* plane. Section 1 (S1) corresponds to the lip of the bottle; Section 2 (S2), Section 3 (S3), and Section 5 (S5) correspond to the form of the bottle.

Section 1		Section 2		Section 3		Section 4		Section 5	
x	*y*	*x*	*y*	*x*	*y*	*x*	*y*	*x*	*y*
0.00	1.10	1.50	1.10	5.50	3.50	8.30	4.40	9.71	4.40
1.50	1.10	2.50	3.20	6.00	3.65	9.71	4.40	10.01	4.50
		3.50	4.00	6.50	4.10			11.01	4.50
		4.00	4.00	7.00	4.45			12.01	3.80
		5.00	3.60	7.50	4.55				
		5.50	3.50	8.00	4.50				
				8.30	4.40				

according to the development of the model in Section 2.3, in general the polynomials $P_{n+i}(x), i=\widehat{1,k}$ are susceptible of changing, depending if some of $h_1, h_2, \cdots, h_k$ are zero or different of zero. In this particular case we have only $P_4(x-h_1)$ from $P_4(x)$ and we will find that $h_1 \approx 0$, so that the Lagrange polynomials of the redesigned bottle will be equal to the Lagrange polynomials of the optimized redesigned bottle.

It is worth to emphasize that, the coefficients of the polynomials, in Table 3, are expressed in the form of decimals in order to decrease distortions in the design of the bottle, optimization and during passing data to the CNC lathe. Greater the number of considered decimal places better will be the design. These criteria are taken into account in all the calculations that are made in all the process of optimization and must be presented in this way.

In order to get the optimized redesigned bottle, rest to find the polynomial $P_4(x-h_1)$ from $P_4(x)$ that fit correctly with the design of the silhouette of the bottle. To do this we put in Table 2, x_4 instead of 9.71 and x_5 instead of 12.01 and a new Table with new values for x_4 and x_5 must be found.

Equations (73) and (74) with $R_4 = 4.4$, $R_5 = 3.8$ where $n=3$, and in using the polynomial $P_4(x)$ become,

$P_4(x_5 - h_1) - 3.8 = 0$, from Equation (74),

$$-0.0406912(x_5-h_1)^3 + 0.99403(x_5-h_1)^2 - 7.40008(x_5-h_1) + 15.9863 = 0 \quad (88)$$

$P_4(x_4 - h_1) - 4.4 = 0$, from Equation (73),

$$-0.0406912(x_4-h_1)^3 + 0.99403(x_4-h_1)^2 - 7.40008(x_4-h_1) + 15.3863 = 0 \quad (89)$$

By looking Figure 8 we see that $P_1(x) = 1.1$, $P_4(x) = 4.4$, $x_1 = 1.5$ and $r = 1.1$, $h_c = 8.81$, $r_c = 4.41$. In using the data of Table 3, Equation (67) can be written as,

$$\begin{aligned}531.798009333735 = {} & \pi\int_{1.5}^{5.5}\left[P_2(x)\right]^2 \mathrm{d}x + \pi\int_{5.5}^{8.3}\left[P_3(x)\right]^2 \mathrm{d}x \\ & + \pi\left[P_3(8.3)\right]^2 (x_4 - 8.3) + \pi\int_{x_4}^{x_5}\left[P_4(x-h_1)\right]^2 \mathrm{d}x\end{aligned}$$

where $P_3(8.3) = P_4(x_4) = 4.4$.

By numerical integration of the first two integrals and taking into account that $P_3(8.3) = 4.4$, we have,

Table 3. Polynomials according to the points given in Table 2 corresponding to Section 1 (S1), 2 (S2), 3 (S3), 4 (S4) and 5 (S5) of the redesigned bottle.

Section	Lagrange polynomials of the redesigned bottle
S1	$P_1(x) = 1.1$
S2	$P_2(x) = 0.0034921x^5 - 0.040476x^4 + 0.21706x^3 - 1.3089x^2 + 5.7384x - 5.1167$
S3	$P_3(x) = -0.036829113x^6 + 1.4915791x^5 - 24.923167x^4 + 219.65835x^3$ $-1075.681x^2 + 2772.3003x - 2931.6348$
S4	$P_0(x) = 4.4$ (Straight section)
S5	$P_4(x) = -0.0406912x^3 + 0.99403x^2 - 7.40008x + 19.7863$

$$225.332507809904 = \pi\left(x_4 - 8.3\right)\left(4.4\right)^2 + \pi\int_{x_4}^{x_5}\left[P_4\left(x - h_1\right)\right]^2 \mathrm{d}x$$

From which

$$730.148748129941 = 60.8212337734984 x_4 + \pi\int_{x_4}^{x_5}\left[P_4\left(x - h_1\right)\right]^2 \mathrm{d}x \tag{90}$$

Since

$$\begin{aligned}
&\pi\int_{x_4}^{x_5}\left[P_4\left(x-h_1\right)\right]^2 \mathrm{d}x \\
&= \pi\left(0.00165577375744\frac{\left(x_5-h_1\right)^7}{7} - 0.080896547072\frac{\left(x_5-h_1\right)^6}{6}\right. \\
&\quad +1.590331911492\frac{\left(x_5-h_1\right)^5}{5} - 16.32205962592\frac{\left(x_5-h_1\right)^4}{4} \\
&\quad \left. +94.0975355844\frac{\left(x_5-h_1\right)^3}{3} - 292.840405808\frac{\left(x_5-h_1\right)^2}{2} + 391.49766769 x_5\right) \\
&\quad -\pi\left(0.00165577375744\frac{\left(x_4-h_1\right)^7}{7} - 0.080896547072\frac{\left(x_4-h_1\right)^6}{6}\right. \\
&\quad +1.590331911492\frac{\left(x_4-h_1\right)^5}{5} - 16.32205962592\frac{\left(x_4-h_1\right)^4}{4} \\
&\quad \left. +94.0975355844\frac{\left(x_4-h_1\right)^3}{3} - 292.840405808\frac{\left(x_4-h_1\right)^2}{2} + 391.49766769 x_4\right)
\end{aligned}$$

where integration was performed analytically, Equation (90) becomes finally,

$$\begin{aligned}
&60.8212337734984 x_4 + \pi\left(0.00165577375744\frac{\left(x_5-h_1\right)^7}{7} - 0.080896547072\frac{\left(x_5-h_1\right)^6}{6}\right. \\
&+1.590331911492\frac{\left(x_5-h_1\right)^5}{5} - 16.32205962592\frac{\left(x_5-h_1\right)^4}{4} \\
&\left. +94.0975355844\frac{\left(x_5-h_1\right)^3}{3} - 292.840405808\frac{\left(x_5-h_1\right)^2}{2} + 391.49766769 x_5\right) \\
&-\pi\left(0.00165577375744\frac{\left(x_4-h_1\right)^7}{7} - 0.080896547072\frac{\left(x_4-h_1\right)^6}{6}\right. \\
&+1.590331911492\frac{\left(x_4-h_1\right)^5}{5} - 16.32205962592\frac{\left(x_4-h_1\right)^4}{4} \\
&\left. +94.0975355844\frac{\left(x_4-h_1\right)^3}{3} - 292.840405808\frac{\left(x_4-h_1\right)^2}{2} + 391.49766769 x_4\right) \\
&-730.148748129941 = 0
\end{aligned} \tag{91}$$

Now, must be solved the system of Equations (88), (89) and (91).

Since a system of three nonlinear equations in three unknowns has been obtained, must be solved numerically in using the Newton's Method for Nonlinear Systems, whose interface Solver For System of Nonlinear Equations (SNLEs) shows us the results of the values for the unknowns after perform 5 iterations (see **Figure 9**). To solve the system, Equations (88), (89) and (91) are renamed as f_1, f_2 and f_3, where:

$$f_1 = -0.0406912(x_5 - h_1)^3 + 0.99403(x_5 - h_1)^2 - 7.40008(x_5 - h_1) + 15.9863$$

$$f_2 = -0.0406912(x_4 - h_1)^3 + 0.99403(x_4 - h_1)^2 - 7.40008(x_4 - h_1) + 15.3863$$

$$\begin{aligned} f_3 = 60.8212337734984 x_4 + \pi \Bigg(& 0.00165577375744 \frac{(x_5 - h_1)^7}{7} - 0.080896547072 \frac{(x_5 - h_1)^6}{6} \\ & + 1.590331911492 \frac{(x_5 - h_1)^5}{5} - 16.32205962592 \frac{(x_5 - h_1)^4}{4} \\ & + 94.0975355844 \frac{(x_5 - h_1)^3}{3} - 292.840405808 \frac{(x_5 - h_1)^2}{2} + 391.49766769 x_5 \Bigg) \\ - \pi \Bigg(& 0.00165577375744 \frac{(x_4 - h_1)^7}{7} - 0.080896547072 \frac{(x_4 - h_1)^6}{6} \\ & + 1.590331911492 \frac{(x_4 - h_1)^5}{5} - 16.32205962592 \frac{(x_4 - h_1)^4}{4} \\ & + 94.0975355844 \frac{(x_4 - h_1)^3}{3} - 292.840405808 \frac{(x_4 - h_1)^2}{2} + 391.49766769 x_4 \Bigg) \\ - 730.148748129941 & \end{aligned}$$

Additionally, we need the elements of the Jacobian matrix, which are:

$$f_{1x} = -0.1220736(x_5 - h_1)^2 + 1.98806(x_5 - h_1) - 7.40008$$

$$f_{1y} = 0$$

$$f_{1z} = 0.1220736(x_5 - h_1)^2 - 1.98806(x_5 - h_1) + 7.40008$$

$$f_{2x} = 0$$

$$f_{2y} = -0.1220736(x_4 - h_1)^2 + 1.98806(x_4 - h_1) - 7.40008$$

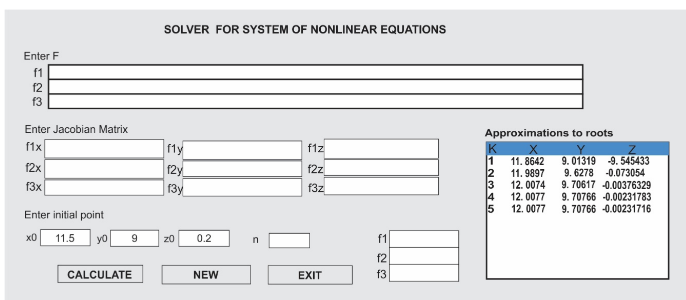


Figure 9. Solver for System of Nonlinear Equations based on Newton–Raphson numerical method to find the unknowns parameters of Equations. (88), (89) and (91). These Equations were renamed as f_1, f_2 and f_3 (see Enter F). This figure also show the Enter Jacobian Matrix (f_{1x}, f_{2x}, f_{3x}, f_{1y}, f_{2y}, f_{3y}, f_{1z}, f_{2z} and f_{3z}); Enter initial points (x_o, y_o and z_o) as well as the Approximations to roots.

$$f_{2z} = 0.1220736(x_4 - h)^2 - 1.98806(x_4 - h) + 7.40008$$

$$f_{3x} = \pi\Big(0.00165577375744(x_5 - h_1)^6 - 0.080896547072(x_5 - h_1)^5 + 1.590331911492(x_5 - h_1)^4 - 16.32205962592(x_5 - h_1)^3 + 94.0975355844(x_5 - h_1)^2 - 292.840405808(x_5 - h_1) + 391.49766769\Big)$$

$$f_{3y} = -\pi\Big(0.00165577375744(x_4 - h_1)^6 - 0.080896547072(x_4 - h_1)^5 + 1.590331911492(x_4 - h_1)^4 - 16.32205962592(x_4 - h_1)^3 - 94.0975355844(x_4 - h_1)^2 - 292.840405808(x_4 - h_1) + 391.49766769\Big) + 60.8212337734984$$

$$f_{3z} = \pi\Big(-0.00165577375744(x_5 - h_1)^6 + 0.080896547072(x_5 - h_1)^5 - 1.590331911492(x_5 - h_1)^4 + 16.32205962592(x_5 - h_1)^3 - 94.0975355844(x_5 - h_1)^2 + 292.840405808(x_5 - h_1)\Big) - \pi\Big(-0.00165577375744(x_4 - h_1)^6 + 0.080896547072(x_4 - h_1)^5 - 1.590331911492(x_4 - h_1)^4 + 16.32205962592(x_4 - h_1)^3 - 94.0975355844(x_4 - h_1)^2 + 292.840405808(x_4 - h_1)\Big)$$

In order to enter Equations (88), (89), (91) and the elements of the Jacobian matrix to the SNLEs, in Matlab language, we change to an equivalent form. Then, taking into account $x = x_5, y = x_4$ and $z = h_1$, we have

$$f_1 = \frac{92501*z}{12500} - \frac{92501*x}{12500} + 99403*\frac{(x-z)^2}{100000} - \frac{3179*(x-z)^3}{78125} + \frac{22498717100947801}{1407374883553280}$$

$$f_2 = \frac{92501*z}{12500} - \frac{92501*y}{12500} + 99403*\frac{(y-z)^2}{100000} - \frac{3179*(y-z)^3}{78125} + \frac{21654292170815833}{1407374883553280}$$

$$f_3 = \frac{484*\pi y}{25} - \frac{3101764083969877660917925914 2809*\pi*(x-z)}{79228162514264337593543950336} - \frac{(31017640839698776609179259142809*\pi*(y-z))}{79228162514264337593543950336} - \frac{51517029002966159255 3*\pi*(x-z)^2}{3518437208883200000} + \frac{13794844602681830518141 77*\pi*(x-z)^3}{43980465111040000000000} - \frac{\left(224328679349402861263 31*\pi*(x-z)^4\right)}{5497558138880000000000} + \frac{\left(397582977873*\pi*(x-z)^5\right)}{1250000000000} - \frac{\left(316002137*\pi*(x-z)^6\right)}{23437500000} + \frac{\left(10106041*\pi*(x-z)^7\right)}{42724609375} + \frac{\left(515170290029661592553*\pi*(y-z)^2\right)}{3518437208883200000}$$

$$-\frac{\left(1379484460268183051814177*\pi*(y-z)^3\right)}{43980465111040000000000}$$
$$+\frac{\left(2243286793494028612633 1*\pi*(y-z)^4\right)}{549755813888000000000}$$
$$-\frac{\left(397582977873*\pi*(y-z)^5\right)}{1250000000000}+\frac{\left(316002137*\pi*(y-z)^6\right)}{23437500000}$$
$$-\frac{\left(10106041*\pi*(y-z)^7\right)}{42724609375}-\frac{6422456308599681}{8796093022208}$$

$$f_{1x}=\frac{99403*x}{50000}-\frac{99403*z}{50000}-9537*\frac{(x-z)^2}{78125}-\frac{92501}{12500}$$

$$f_{1y}=0$$

$$f_{1z}=\frac{99403*z}{50000}-\frac{99403*x}{50000}-9537*\frac{(x-z)^2}{78125}-\frac{92501}{12500}$$

$$f_{2x}=0$$

$$f_{2y}=\frac{99403*y}{50000}-\frac{99403*z}{50000}-9537*\frac{(y-z)^2}{78125}-\frac{92501}{12500}$$

$$f_{2z}=\frac{99403*z}{50000}-\frac{99403*y}{50000}-9537*\frac{(y-z)^2}{78125}-\frac{92501}{12500}$$

$$f_{3x}=\frac{31017640839698776609179259142809*\pi}{79228162514264337593543950336}$$
$$-\frac{515170290029661592553*\pi*(2x-2z)}{3518437208883200000}$$
$$+\frac{4138453380804549155442531*\pi*(x-z)^2}{43980465111040000000000}$$
$$-\frac{2243286793494028612633 1*\pi*(x-z)^3}{137438953472000000000}$$
$$+\frac{397582977873*\pi*(x-z)^4}{250000000000}-\frac{316002137*\pi*(x-z)^5}{3906250000}$$
$$+\frac{10106041*\pi*(x-z)^6}{6103515625}$$

$$f_{3y}=\frac{515170290029661592553*\pi*(2y-2z)}{3518437208883200000}$$
$$-\frac{73709459033556547583420620660 7601*\pi}{198070406285660843983859875840 0}$$
$$-\frac{4138453380804549155442531*\pi*(y-z)^2}{43980465111040000000000}$$
$$+\frac{2243286793494028612633 1*\pi*(y-z)^3}{137438953472000000000}$$
$$-\frac{397582977873*\pi*(y-z)^4}{250000000000}+\frac{316002137*\pi*(y-z)^5}{3906250000}$$

$$-\frac{10106041*\pi*(y-z)^6}{6103515625}$$

$$f_{3z}=\frac{51517029002966159 2553*\pi*(2x-2z)}{3518437208883200000}$$
$$-\frac{4138453380804549155442531*\pi*(x-z)^2}{439804651110400000000}$$
$$+\frac{22432867934940286126331*\pi*(x-z)^3}{13743895347200000000}$$
$$-\frac{397582977873*\pi*(x-z)^4}{250000000000}+\frac{316002137*\pi*(x-z)^5}{3906250000}$$
$$-\frac{10106041*\pi*(x-z)^6}{6103515625}-\frac{515170290029661592553*\pi*(2y-2z)}{3518437208883200000}$$
$$+\frac{4138453380804549155442531*\pi*(y-z)^2}{439804651110400000000}$$
$$-\frac{22432867934940286126331*\pi*(y-z)^3}{13743895347200000000}$$
$$+\frac{397582977873*\pi*(y-z)^4}{250000000000}-\frac{316002137*\pi*(y-z)^5}{3906250000}$$
$$+\frac{10106041*\pi*(y-z)^6}{6103515625}$$

Figure 9 shows the SNLEs, where it is possible to see the entry functions f_1, f_2 and f_3; Jacobian matrix f_{1x}, f_{2x}, f_{3x}, f_{1y}, f_{2y}, f_{3y}, f_{1z}, f_{2z} and f_{3z}; initial points x_o, y_o and z_o as well as the approximations to roots.

In Approximations to roots of the Solver for System of Nonlinear Equations, we can see that $x_5=12.0077\approx 12.01$, $x_4=9.70766\approx 9.71$ and $h_1=-0.00231716\approx -0.0023$. The values of $x_5=12.0077\approx 12.01$, $x_4=9.70766\approx 9.71$, $x_3=8.3$, $x_2=5.5$ and $x_1=1.5$, in **Figure 9**, are similar to values of **Table 2**; and $P_4(x-h_1)=P_4(x+0.0023)\approx P_4(x)$, $P_3(x)$, $\cdots$, $P_1(x)$ similar to values of **Table 3**. With these results, and in using the Optimizer of Five Sections, we get the polynomials for the optimized redesigned bottle shown in Lagrange polynomial coefficients of **Figure 10**, and which are shown in **Table 4**.

Therefore, with the data of **Table 2** where $x_5=12.007\approx 12.01$ and $x_4=9.70766\approx 9.71$ and following the same procedure that was made for the real bottle, the results for the redesigned bottle, after applying criterion of optimization by compensation, are shown in **Figure 10**.

In Output data of this figure, we can see that we can manufacture a bottle with an area of 363.588 cm^2 less than 365.96 cm^2 specified in optimum area of optimum results for the bottle, which is in accordance with theorem 2.1 and similar results reported by Reyna and Morales [19].

When considering a petaloid base for the bottle of **Figure 10**, and according to the design of a new petaloid base following similar calculations to that made

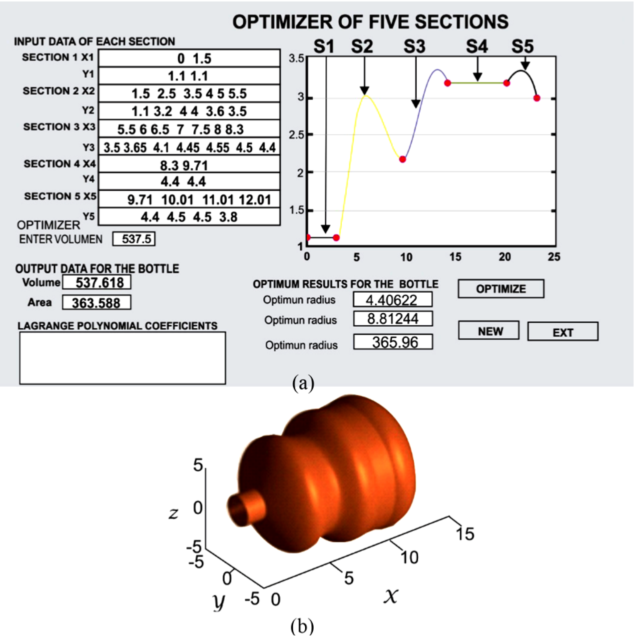


Figure 10. Optimized redesigned bottle with flat base, (a) Silhouette of the optimized redesigned bottle according to the data of Table 2. It is shown the sections S1, S2… S5, according to data in Input Data of Each Section in Optimizer of five Sections. In Optimizer, the volume V of the bottle is entered in order to obtain the optimum radius, optimum height and optimum area of the cylinder which are visualized in Optimum Results for the Bottle. In Output Data for the bottle the volume and area of the bottle are visualized when the curves in corresponding sections S1, S2…S5 rotates around the x-axis and which generate the bottle. The coefficients of the polynomials that represent each curve of each section S1, S2…S5 are placed on the Lagrange Polynomial Coefficients (shown in Table 4). Theseresults were obtained following the Flow diagram of the Optimization method for designing an optimized bottle of volume V; (b) view of the optimized redesigned bottle in three dimensions.

Table 4. Section 1 (S1), 2 (S2), 3 (S3), 4 (S4), and 5 (S5) of the optimized redesigned bottle with its corresponding Lagrange Polynomials that draw the silhouette of the bottle according to Table 2, where $x_5 = 12.0077 \approx 12.01$ and $x_4 = 9.70766 \approx 9.7$.

Section	Lagrange polynomials of the optimized redesigned bottle
S1	$P_1(x) = 1.1$
S2	$P_2(x) = 0.0034921x^5 - 0.040476x^4 + 0.21706x^3 - 1.3089x^2 + 5.7384x - 5.1167$
S3	$P_3(x) = -0.036829113x^6 + 1.4915791x^5 - 24.923167x^4 + 219.65835x^3$ $-1075.681x^2 + 2772.3003x - 2931.6348$
S4	$P_0(x) = 4.4$
S5	$P_4(x) = -0.0406912x^3 + 0.99403x^2 - 7.40008x + 19.7863$

for the real bottle (see Figure 6), the area of the bottle is modified from 365.96 cm^2 to 366.17 m^2.

Table 4 shows the Lagrange polynomials, of each section, of the optimized redesigned bottle. We can see similar results to that given in Table 3, which means that the optimization criterion by compensation works very well.

3. Results and Discussions

On the basis of the Criterion of Optimization by Compensation it was obtained a mathematical model that let us optimize (minimize) the superficial area of a bottle with a straight section along its silhouette. The minimal area that this mathematical model let us obtain is in the sense that it tends to the area of the sphere which is considered as geometric object with maximal volume and less area. Say, in general the area of the bottle is between the area of the sphere and the area of the cylinder. This is not difficult to show in using proposition presented in [11] that establishes the inequality $A_{\text{sphere}} < A_{\text{cylinder}} < A_{\text{cube}}$ enclosing these areas the same volume. If we build a bottle from a cylinder of minimal area according to the Criterion of Optimization by Compensation we obtain the inequality $A_{\text{sphere}} < A_{\text{bottle}} < A_{\text{cyliner}}$. In this sense, we are optimizing. We really don't know the absolute minimum for the area of the bottle being this an open problem.

Results of the application of the Criterion of Optimization by Compensation for the case of the half-liter bottle of the Fanta soda, are summarized in **Table 5**. It can be seen that the real bottle is made in using 25.18 g of PET plastic to enclose a volume of 537.5 cm^3 with a superficial area of 435.23 cm^2 approximately. However, in using the Criterion of Optimization by Compensation for almost the same volume (537.63 cm^3), the area can be reduced to 366.17 cm^2 (with petaloid base) so that it is necessary only 21.185 g of PET plastic keeping the original thickness of the wall of the bottle. It is worth to emphasize that 21.185 g was obtained using a rule of three with the data of **Table 5** keeping constant the thickness of the bottle, which is not considered as a parameter of design. It was optimized the given geometric shape of the bottle. Consequently, the real bottle of Fanta soda has a mistake of 18.86 % (This value was obtained by using the relation $\frac{\text{area of the bottle} - \text{area of the optimized bottle}}{\text{area of the optimized bottle}} \times 100$) respecting to what is established by the Criterion of Optimization by Compensation and, it has 69.06 cm^2 more superficial area or it uses 3.995 g more of PET plastic. In indications such as * and ** are specified that the results 366.17 cm^2 and 537.63 cm^3 are

Table 5. Comparison between the results of the real and the optimized bottle.

Real		Optimum		Deviation		Volume-real	
area	weight	area	weight	area	weight	Water	Matlab
(cm^2)	(g)	(cm^2)	(g)	(cm^2)	(g)	(cm^3)	(cm^3)
435.23	25.18	366.17	21.185	69.06	3.995	537.5	537.63
* with non-flat base		* with non-flat base		18.86%			** It was Subtracted 14 cm^3 due to non-flat base

due to the petaloid base of the bottle. The difference in areas between the bottle-with flat base and petaloid base is not significant in the present work.

The cost that it is paid when the optimization is achieved in using the Criterion of Optimization by Compensation is that the height of the bottle diminishes and a widening happens. The view at scale of the real bottle and the redesigned bottle optimized in extreme is shown in Figure 11. It can be seen that the height of the redesigned bottle is almost half of the real bottle, but fatter in order to compensate the loss of volume, keeping so the same volume of the real bottle.

Since no necessarily, an optimization in extreme must be achieved, it was attempted to manufacture a bottle with a mistake of 4.91% considered arbitrarily by the designer, say, with an area of 383.916 cm^2 (This value is obtained by using the relation $\frac{\text{area of the bottle} - \text{area of the optimized bottle}}{\text{area of the optimized bottle}} \times 100 = 4.91$, where the area of the optimized bottle is 365.96 cm^2). Such attempt of manufacturing the bottle was achieved with certain limitations such as:

1) It was impossible to find preforms of PET plastic of 23.25 g approximately, as it was required by calculations.

2) It was impossible to find preforms of PET plastic whose design must be according to the

length of the lip of the bottle as it is required in the design.

3) The mechanism of exportation of data, to the numerical control lathe distorted the data. So, volume and area of the bottle were slightly altered.

Table 6 shows coordinates of the silhouette of the manufactured bottle in a Cartesian coordinate system of the xy plane. The process to obtain this Table is the same fallowed to obtain Table 2 and Table 4.

In Figure 12 we can see in Output data that the area of the bottle to be manufactured is 383.916 cm^2, while the area of the bottle in Optimum results is

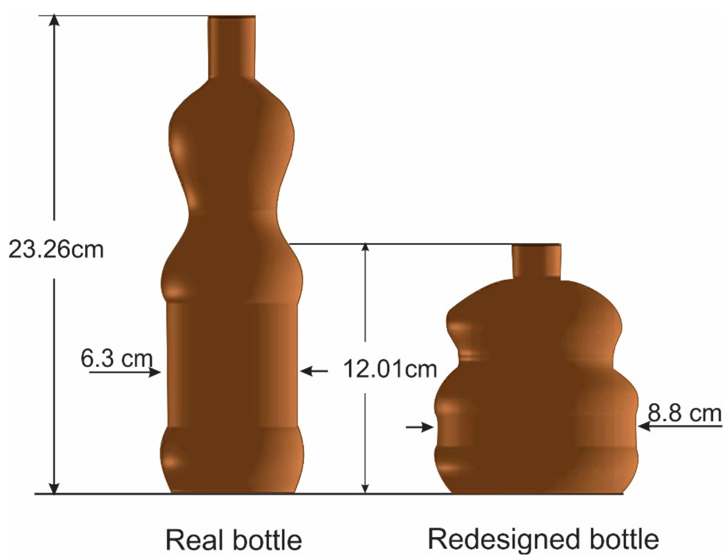
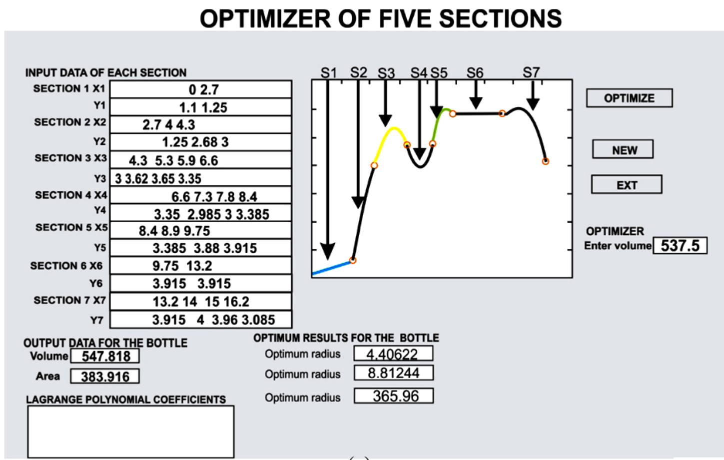
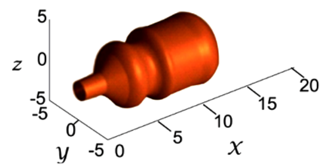


Figure 11. View at scale of the real and redesigned bottle. Adapted with permission from Reyna and Moore [18]. Copyright 2016 ECI.



(a)



(b)

Figure 12. Manufactured bottle, (a) Silhouette of the manufactured bottle according to the data of **Table 6**. It is shown the sections S1, S2…S7, according to data in Input Data of Each Section in Optimizer of Seven Sections. In Optimizer, the volume V of the bottle is entered in order to obtain the optimum radius, optimum height and optimum area of the cylinder which are visualized in Optimum Results for the Bottle. In Output Data, for the bottle, the volume and area of the bottle are visualized when the curves in corresponding sections S1, S2…S7 rotates around the x-axis and which generate the bottle. The coefficients of the polynomials that represent each curve of each section S1, S2…S5 are placed on the Lagrange Polynomial Coefficients (shown in **Table 7**). These results were obtained following the Flow diagram of the Optimization method for designing an optimized bottle of volume V; (b) view of the manufactured bottle in three dimensions.

Table 6. Coordinates of the silhouette of the manufactured bottle seen in a Cartesian coordinate system of the *xy* plane. Section 1 (S1) corresponds to the lip of the bottle, Section 2 (S2), Section 3 (S3)…Section 7 (S7) correspond to the form of the bottle.

Section 1		Section 2		Section 3		Section 4		Section 5		Section 6		Section 7	
x	*y*	*x*	*y*	*x*	*y*	*x*	*y*	*x*	*y*	*x*	*y*	*x*	*y*
0.0	1.10	2.70	1.25	4.30	3.00	6.60	3.35	8.40	3.385	9.75	3.915	13.20	3.915
2.7	1.25	4.00	2.68	5.30	3.62	7.30	2.985	8.90	3.88	13.2	3.915	14.00	4.00
		4.30	3.00	5.90	3.65	7.80	3.00	9.75	3.915			15.00	3.96
				6.60	3.35	8.40	3.385					16.20	3.085

365.960 cm² being in both cases when the base of the bottle is flat. This means that there is a mistake of 4.91% with respect to optimum results. As a consequence of inserting to the bottle a petaloid base plus the limitations stated above the mistake increase as it is indicated below.

Table 7 shows the Lagrange polynomials, of each section, of the manufactured bottle which were obtained following the same procedure to obtain **Table 4**.

The above last limitation (number 3) allowed us to obtain a bottle whose geometric design had a mistake of 13% (This value was obtained by direct measurement of the area of the mold of the bottle and by using the formula $\frac{\text{area of the mold of the bottle} - \text{area of the optimized bottle}}{\text{area of the optimized bottle}} \times 100$, where the area of the optimized bottle is 365.96 cm^2 according to Optimum results for the bottle of **Figure 12**). The limitation, numbered as 1, caused that the thickness of the wall of the bottle resulted be 75% of that of the real bottle because a preform of 22 g of PET plastic was used. In spite of the limitations, a good bottle was obtained as shown in **Figure 13**. In this Figure we can see: a) the corresponding mold that was fabricated to manufacture the redesigned Fanta soda bottle of the Coca Cola company, b) comparison between the real (higher) and redesigned (smaller) bottle. Our results are in accordance with the literature, for instance, Silva *et al.* [6] have reported a reduction of 21% of PET material (weight of 4.6 g) of a bottle of 22 g, using simulations based on finite element method (FEM). On the other hand, Hung *et al.* [20] have reported a reduction of the weight of a bottle, with a volume of 500 ml, from 27 g to 22.3 g using numerical simulations, where thickness and pattern of the bottle were changed in order to reduce the weight of the bottle. At the same way, Hopmann *et al.* [11] have also reported a reduction of the weight of a 0.5 liter PET bottle of Krones AG, Neutraubling, Germany, from 18.5 g to 15.5 g. For this aim, they have developed a simulative approach to determine a well-adapted preform and bottle design with its corresponding process parameters. Therefore, a three-dimensional simulation of the stretch-blow molding process was used within an iterative optimization routine. Their bottles were manufactured on a stretch-blow molding machine LB1 (Krones AG, Neutraubling, Germany), with a changed wall thickness.

Therefore, according to this reports, we can note that, in all cases the wall

Table 7. Lagrange polynomials of the manufactured bottle obtained via interpolation according to data of **Table 6** and in using Optimizer of seven sections.

Section	Lagrange polynomials of the manufactured bottle
S1	$P_1(x) = 0.0\hat{5}x + 1.1$
S2	$P_2(x) = -0.020833333333335x^2 + 1.239583333333336x - 1.945000000000007$
S3	$P_3(x) = -0.005166029622552x^3 - 0.276176540850457x^2 + 3.629662267080676x - 7.090307990922156$
S4	$P_4(x) = 0.053631553631554x^3 - 0.704280904280836x^2 + 1.489891774891476x + 8.776333333333241$
S5	$P_5(x) = -0.702832244008714x^2 + 13.148997821350747x - 57.474738562091602$
S6	$P_0(x) = 3.915$
S7	$P_6(x) = -0.0773358585859x^3 + 0.031823232323232x^2 - 0.435284469696971x + 2.018724999999995$

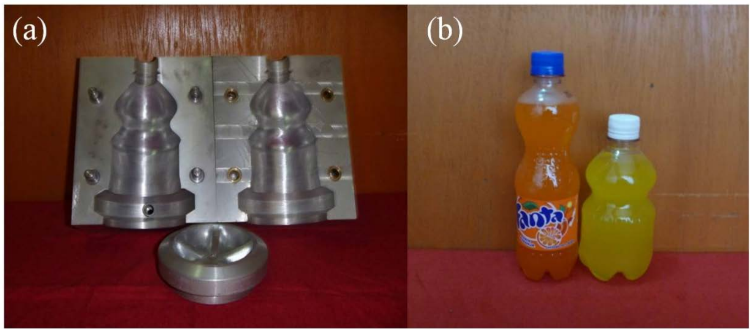


Figure 13. (a) Mold used to manufacture the redesigned bottle of Fanta soda, and (b) comparison between the real (higher) and redesigned (smaller) bottle.

thickness of the bottles was changed, and the weight of the bottle reduced in average~4.0 g, similarly to the found results in this work. However, in this work the wall thickness of the bottle have to remain unchanged.

4. Conclusion

In summary, we propose the mathematical foundations of the so-called Criterion of Optimization by Compensation and in using this, an optimized and redesigned half-liter bottle of Fanta soda of the well-known Coca Cola Company, was manufactured. This manufactured bottle was designed with a mistake of 4.91% with respect to what such criterion of optimization stablishes. However, it was reported a mistake of 13% in each manufactured bottle due to important technical limitations listed above that must be overcome. In general, in spite of such limitations a good bottle was obtained with such 13% of mistake, resulting the thickness of the wall of the bottle 75% of that of the real bottle because a preform of 22 g of PET plastic was used, instead of a preform of 23.25 g as it was required.

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