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Optimization of SO₂ and NO_x emissions in Thermal Plants

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Abstract

This paper presents an environmental dispatch algorithm in a hydrothermal system and addresses the problem of minimization of emissions of SO₂ and NO_x caused by the operation of thermal plants. Several models have been used to represent the emissions function. In this paper we first construct a quadratic model for both emissions: $E(P) = \alpha + \beta P + \gamma P^2$ where P is the power generated and the parameters were computed via the least square criteria from several tests at thermal plants. We shall see that the problem consists in the minimization of a functional $F(z)$ within the set of piecewise C^1 functions that satisfy boundary conditions and non-holonomic inequality constraints. An optimal control technique is applied and Pontryagin's theorem is employed. The algorithm proposed is easily implemented using the Mathematica © Package and is applied to a sample system to illustrate the results obtained. *Key words: Emissions, Optimization, Control Problem, Hydrothermal MSC 2000: 49J24*

1 Introduction

Electric power systems are traditionally operated in such a way that the total fuel cost is minimized regardless of the emissions produced. Subsequent to the coming into force of the Kyoto Protocol of the UNO Framework Agreement on Climatic Change on February 16 2005, increasing requirements aimed at environmental protection have given rise to the need for alternative strategies. For our hydrothermal problem, it is well known (Table I) that the most important pollutant emissions are: sulphur dioxide (SO₂) and, to a lesser degree,

oxides of nitrogen emissions (NO_x).

Table I. Emissions of 1000 *Mw* thermal plant (thousands of *Tn/year*).

Pollutant	Coal	Oil	Gas
Particles	5	0.8	0.5
SO ₂	150	60	0.015
NO _x	23	25	13
CO	0.25	0.009	—

Henceforth, we shall refer to coal- and oil-fired thermal plants, considering those that employ gas to a lesser extent, since they pollute much less. In this study, we shall minimize the emissions of SO₂ and NO_x, the reactions of which we shall now go on to analyze.

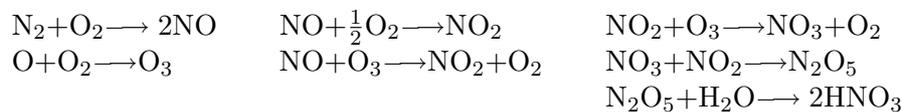
Sulphur dioxide (SO₂). This is formed by the combustion of the S present in the coal and fuel oil in percentages that vary between 0.1 and 5%. SO₂ is a colorless gas that is an irritant at concentrations above 3 *ppm*. SO₂ may form SO₃ in the atmosphere as a result of photochemical action, as well as owing to the catalysis of particles in suspension. Together with atmospheric humidity, SO₂ makes up between 5 and 20% of urban aerosols, thus increasing the corrosive power of the atmosphere, reducing visibility and provoking acid rain. It is thought that more than 90% of the production of sulphur oxides in the northern hemisphere is anthropogenic in origin, the global amount of yearly emissions being 100 – 1000 *GKg*. More than 50% of SO₂ is produced in thermal power plants, the main reactions being:



Fe and Mn chlorides and sulphates acting as a catalyser in (*).

Oxides of Nitrogen (NO_x). The emission of oxides of nitrogen is even more difficult to control and avoid than that of sulphur oxides. NO_x refers to all the existing oxides of Nitrogen, although the major percentage corresponds to NO, approximately 90%. Almost all the remaining 10% is NO₂, since N₂O is present in insignificant amounts. NO is a colorless, odorless gas that is toxic at high concentrations and is present in the air at less than 0.50 *ppm*. Although its tolerance by human beings at low concentrations is acceptable, it is nevertheless a precursor of NO₂ and therefore partly responsible for photochemical pollution. Around 67% of NO_x emissions (total emissions 25 – 99 *GKg/year*) are anthropogenic in origin, of which more than 90% originate in high temperature combustions, from both stationary and mobile sources. The majority of the chemical reactions of these compounds lead to the obtaining of HNO₃,

which falls as acid rain. The main reactions of nitrogen (both from the air as well as that present in fuel) are:



These emissions are currently regulated (Official Journal of the European Communities, Directive 2001/80/CE of the European Parliament and the Council of 23 October 2001), and limit values are imposed on SO_2 and NO_x emissions from large combustion facilities.

For all the above reasons, we consider the minimization of SO_2 and NO_x presented in this paper to be of vital importance. The problem basically consists in finding, given a hydrothermal system composed of thermal and hydraulic plants (in which pollutant emissions may have been reduced to a certain degree by means of other procedures, such as desulfurization of the fuel, fluid bed combustion, selective catalytic reduction - SCR procedure -, etc.), the powers that the plants must generate for the SO_2 and NO_x emissions from the thermal plants in the system during a certain time interval to be minimum, bearing in mind the numerous system constraints. The paper is organized in the following way. In Section 2, the emission of pollutants is modeled by means of the measurements carried out at the thermal plants. Subsequently, in Section 3, we set out the corresponding mathematical problem and, in order to simplify its exposition, we do so in two steps: first considering one single hydro-plant to then go on to generalize to n hydro-plants. Section 4 summarizes the mathematical fundamentals employed in the solution of the problem and the obtaining of the optimum solution. Finally, the results obtained in an example are presented in Section 5 and the conclusions reached in this study are discussed in Section 6.

2 Emissions Model

Several models have been used to represent the emissions function [1]. In this paper we construct a quadratic model for both emissions: $E(P) = \alpha + \beta P + \gamma P^2$, where E is the unit emission and P is the power generated, and the parameters were computed via the least square criteria from several tests at thermal plants.

From an optimization viewpoint, the model commonly employed in power plants is that of fuel cost - power, the fuel cost usually being considered a smooth curve that may be approximated by a second degree polynomial. In

contrast, the unit emission of pollutant - power is not usually employed; environmental departments are usually content to control the emitted pollution by means of continuous measurements at the stack outlet. Therefore, a study was first carried out to test whether this relation is actually maintained appreciably constant by each plant and operating conditions. Measurements were carried out for 3 weeks with the data supplied by the company *HC* (Asturias, Spain). We shall estimate the unit emission E and the existing relation in each plant to the generated power P , studying whether this may be approximated by another second degree polynomial in a similar way to the fuel cost.

The unit emission $E \left(\frac{Kg}{h} \right)$ is calculated knowing:

- The Net Consumption NC , obtained by multiplying the net specific consumption curve R of the plant (data supplied by the manufacturer) by P .

$$R \left(\frac{Kcal}{hKw} \right) \cdot P(Mw) \rightarrow NC \left(\frac{Kcal}{h} \right)$$

- The average amount of coal EQ consumed at the plant.

- The concentration C of the pollutant as a function of the power P , which is obtained by continuous measurement at the stack outlet.

- The production of smoke S for the average amount of coal consumed.

We thus obtain the unit emission of pollutant

$$NC \left(\frac{Kcal}{h} \right) \cdot \frac{1}{EQ} \left(\frac{Kg}{Kcal} \right) \cdot S \left(\frac{m^3}{Tn} \right) \cdot C \left(\frac{mg}{m^3} \right) \rightarrow E \left(\frac{Kg}{h} \right)$$

Given that the power at which this pollution is emitted is known, it is possible to build point graphs like those in Fig. 1 (for NO_x) or Fig. 2 (for SO₂) and to perform the least square approximation over these. Data was collected over 3 weeks, for both SO₂ and NO_x, and was comprised of some 150 measurements per week, the r^2 (correlation ratio) obtained always being higher than 0.96.

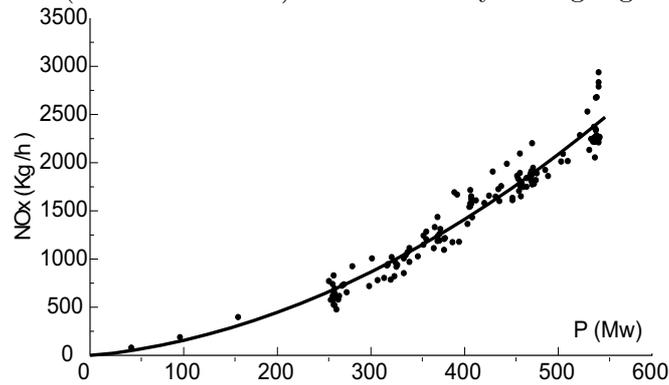


Figure 1. Least square approximation to NO_x emissions (week 1).

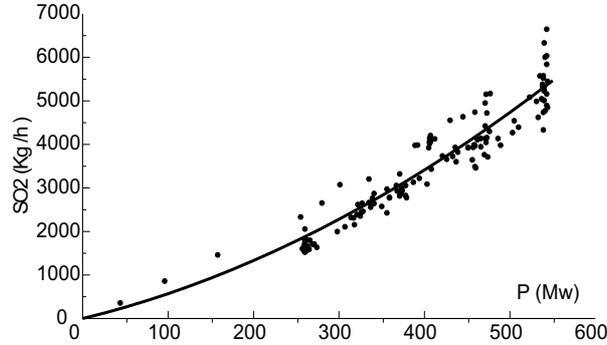
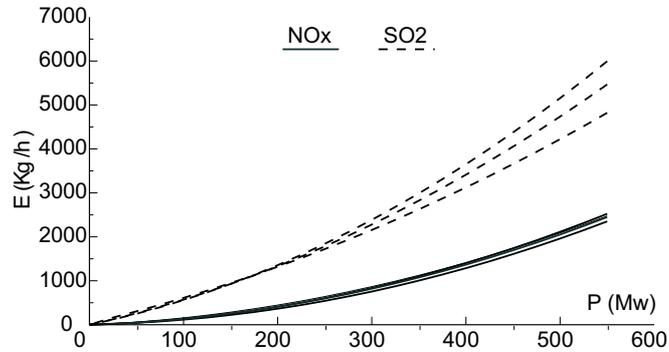
Figure 2. Least square approximation to SO_2 emissions (week 1).

Figure 3. Comparison between three weeks.

It should be noted that data were taken during plant shut-down, measurements that confirm the form of the curve when approaching low power (unusual in ordinary functioning). We may thus conclude that a quadratic model is appreciated that relates pollutant emissions with the generated power, in which the parameters that are obtained are also appreciably similar in the different observations carried out at the same plant. Although, of course, operating conditions such as meteorological conditions, temperature of the fumes at the boiler outlet or operating conditions in the burners exert a greater or lesser influence on the production of pollution, in a first approximation we may modelize the sum of SO_2 and NO_x by

$$\Psi(P) = \alpha + \beta P + \gamma P^2$$

3 Statement of the Hydrothermal Problem

We consider a hydrothermal system with m thermal power plants and n hydroplants ($H_n - T_m$ Problem). The hydrothermal problem consists in minimizing

the emissions of SO₂ and NO_x of thermal plants to satisfy a certain power demand during the optimization interval $[0, T]$. Although diverse authors have previously addressed this problem using varied techniques, such as, for instance, neural networks [2], calculus of variations [3], or linear programming [4], they introduce notable simplifications in the modelization of the system so as to facilitate its solution. In this paper, however, we shall modelize the system in all its details, formulating and resolving a complex mathematical problem. The first step, already presented in previous papers [5-6] and fundamental in the setting out of the problem, is to substitute the m thermal power plants by one single thermal power plant, called the *thermal equivalent*.

In the present paper, we first of all consider a simple hydrothermal system with 1 hydro-plant and m thermal power plants that have been substituted by their thermal equivalent ($H_1 - T_1$ Problem). We shall next go on to discuss the general case with n hydro-plants ($H_n - T_1$ Problem). The $H_1 - T_1$ problem is to minimize the functional

$$F(P) = \int_0^T \Psi(P(t)) dt$$

where Ψ is the emissions function of the thermal equivalent and $P(t)$ is the power generated by said plant at the instant t . Moreover, the following equilibrium equation of active power will have to be fulfilled

$$P(t) + H(t, z(t), z'(t)) = P_d(t), \quad \forall t \in [0, T]$$

where $P_d(t)$ is the power demand and $H(t, z(t), z'(t))$ is the power contributed to the system at the instant t by the hydro-plant, $z(t)$ being the volume that is discharged up to the instant t by the plant, and $z'(t)$ the rate of water discharge of the plant at the instant t .

Taking into account the equilibrium equation, the problem reduces to calculating the minimum of the functional

$$F(z) = \int_0^T \Psi(P_d(t) - H(t, z(t), z'(t))) dt$$

If we assume that b is the volume of water that must be discharged during the entire optimization interval $[0, T]$, the following boundary conditions will have to be fulfilled

$$z(0) = 0, \quad z(T) = b$$

For the sake of convenience, we assume throughout the paper that these are sufficiently smooth and are subject to the following additional assumptions:

Let us assume that the function of emissions $\Psi : \mathbb{R}^+ \longrightarrow \mathbb{R}^+$ satisfies $\Psi'(x) > 0, \forall x \in \mathbb{R}^+$ and is thus strictly increasing. This constraint is absolutely natural; it reads more pollutant to more generated power. Let us assume as well that $\Psi''(x) > 0, \forall x \in \mathbb{R}^+$ and is therefore strictly convex. The models traditionally employed meet this constraint.

Let us assume that the function of effective hydraulic generation $H(t, z, z') : \Omega_H = [0, T] \times \mathbb{R}^+ \times \mathbb{R}^+ \longrightarrow \mathbb{R}^+$ is strictly increasing with respect to the rate of water discharge z' , i.e., $H_{z'} > 0$. Let us also assume that $H(t, z, z')$ is concave with respect to z' , i.e., $H_{z'z'} \leq 0$. The real models meet these two restrictions; the former means more power to a higher rate of water discharge. We see that we only admit non-negative thermal power $P(t)$ and we shall only admit non-negative volumes $z(t)$ and rates of water discharge $z'(t)$.

We may hence expound the mathematical problem in the following terms. We shall call $H_1 - T_1$ the problem of minimization of the functional

$$F(z) = \int_0^T \Psi(P_d(t) - H(t, z(t), z'(t))) dt \quad (3.1)$$

over the set of piecewise C^1 functions $(z \in \widehat{C}^1[0, T])$

$$\Theta_b = \{z \mid z(0) = 0, z(T) = b, 0 \leq H(t, z(t), z'(t)) \leq P_d(t), \forall t \in [0, T]\}$$

If the hydrothermal system accounts for n hydro-plants, the statement will be the same taking $\bar{z}(t) = (z_1(t), z_2(t), \dots, z_i(t), \dots, z_n(t))$ instead of $z(t)$. We shall call $H_n - T_1$ the problem of minimization of the functional

$$F(\bar{z}) = \int_0^T \Psi(P_d(t) - H(t, \bar{z}(t), \bar{z}'(t))) dt \quad (3.2)$$

over the set of piecewise C^1 functions $(\bar{z} \in (\widehat{C}^1[0, T])^n)$

$$\Theta_{\bar{b}} = \{\bar{z} \mid z_i(0) = 0, z_i(T) = b_i, 0 \leq H(t, \bar{z}(t), \bar{z}'(t)) \leq P_d(t), \forall t \in [0, T]\}$$

with $i = 1, \dots, n$.

4 Optimal Solution

Let us now see the fundamental result (*the coordination theorem*), which is the basis for elaborating the optimization algorithm that leads to determination of the optimal solution of the hydrothermal system. An optimal control technique is applied and Pontryagin's Minimum Principle [7] is employed. Let us consider the functional (3.1).

We present the problem considering the state variable to be $z(t)$ and the control variable $u(t) = H(t, z(t), z'(t))$. Moreover, as $H_{z'} > 0$, the equation $u(t) - H(t, z(t), z'(t)) = 0$ allows the state equation $z' = f(t, z, u)$ to be explicitly defined. The optimal control problem is thus:

$$\min_{u(t)} \int_0^T L(t, z(t), u(t)) dt \quad \text{with} \quad \begin{cases} z' = f(t, z, u) \\ z(0) = 0, \quad z(T) = b \\ u(t) \in \Omega(t) = \{x \mid 0 \leq x \leq P_d(t)\} \end{cases}$$

with L having the form

$$L(t, z(t), u(t)) = \Psi(P_d(t) - u(t))$$

It can be seen that from the relations $u(t) - H(t, z(t), z'(t)) = 0$ and $z' = f(t, z, u)$, we easily obtain

$$f_z = -\frac{H_z}{H_{z'}}; \quad f_u = \frac{1}{H_{z'}}$$

Prior to seeing the theorem, we define the following function.

Definition 1. Let us term the *coordination function* of $q \in \Theta_b$ the function in $[0, T]$, defined as follows

$$\mathbb{Y}_q(t) = -L_{z'}(t, q(t), q'(t)) \cdot \exp \left[- \int_0^t \frac{H_z(s, q(s), q'(s))}{H_{z'}(s, q(s), q'(s))} ds \right]$$

Now, based on Pontryagin's Minimum Principle, it is easy to prove the next theorem.

Theorem 1. (The coordination theorem) *If $q \in \widehat{C}^1$ is a solution of problem $H_1 - T_1$, then there exists a constant $K \in \mathbb{R}^+$ such that*

- i) If $0 < H(t, q(t), q'(t)) < P_d(t) \implies \mathbb{Y}_q(t) = K$.*
- ii) If $H(t, q(t), q'(t)) = P_d(t) \implies \mathbb{Y}_q(t) \geq K$.*
- iii) If $H(t, q(t), q'(t)) = 0 \implies \mathbb{Y}_q(t) \leq K$.*

If we did not have the constraints $0 \leq H(t, z(t), z'(t)) \leq P_d(t)$, we could use the shooting method to resolve the problem. In this case, we would use the *coordination equation*, $\forall t \in [0, T]$

$$\mathbb{Y}_z(t) = -L_{z'}(0, z(0), z'(0)) = K \tag{4.1}$$

Varying the initial condition of the derivative $z'(0)$ (initial flow rate), we would search for the extremal that fulfils the second boundary condition $z(T) = b$ (final volume). However, we cannot use this method in our case, since, owing to the restrictions, the extremals may not admit bilateral variations, i.e. they may present boundary arcs. We use the same framework in the present case,

but the variation of the initial condition for the derivative, which now need not make sense, is substituted by the variation of the coordination constant K . The problem will consist in finding for each K the function q_K that satisfies $q_K(0) = 0$ and the conditions of the main coordination theorem, and from among these functions, the one that gives rise to an admissible function ($q_K(T) = b$).

From the computational point of view, the construction of q_K can be performed with the same procedure as in the shooting method, with the use of a discretized version of the coordination equation (4.1). The exception is that at the instant when the values obtained for z and z' do not obey the constraints, we force the solution q_K to belong to the boundary until the moment when the conditions of leaving the domain (established in Theorem 1) are fulfilled.

Having resolved the $H_1 - T_1$ problem, we now generalize the study to the $H_n - T_1$ problem. Let us assume that a hydrothermal system accounts for n hydro-plants. The problem of optimization of a hydrothermal system that involves n hydro-plants is highly complicated, since the associated variational problem is related to solving a boundary-value problem for a system of differential equations. We now present an algorithm of its numerical resolution using a particular strategy related to the *cyclic coordinate descent method* [8]. With this method, a problem of the type $H_n - T_1$ could be solved, under certain conditions, if we start out from the resolution of a sequence of problems of the type $H_1 - T_1$.

Let the function $G : \mathbb{R}^n \rightarrow \mathbb{R}$, $G \in C^1(\mathbb{R}^n)$, and $\bar{\mathbf{x}} = (x_1, \dots, x_j, \dots, x_n)$. The idea behind the coordinate descent method is to use the coordinate axes as descent directions. The method sequentially searches for the minimum of G in all the directions $\bar{\mathbf{e}}_j$. Descent with respect to the x_j coordinate means that $G(x_1, \dots, x_j, \dots, x_n)$ is minimized with respect to x_j , while the rest remain fixed.

Now we adapt the finite-dimensional version of this algorithm to our functional. The algorithm for the $H_n - T_1$ problem carries out several iterations and at each k -th iteration calculates n stages, one for each hydro-plant. At each stage, it calculates the optimal functioning of a hydro-plant, while the behavior of the rest of the plants is assumed fixed. For every $\bar{\mathbf{q}} = (q_1, \dots, q_n) \in \Theta_{\bar{\mathbf{b}}}$, we consider the functional $F_{\bar{\mathbf{q}}}^i$ defined by

$$F_{\bar{\mathbf{q}}}^i(z_i) = \int_0^T \Psi (P_d(t) - H_{\bar{\mathbf{q}}}^i(t, z_i(t), z_i'(t))) dt$$

with

$$H_{\bar{\mathbf{q}}}^i(t, z_i, z_i') = H(t, q_1, \dots, q_{i-1}, z_i, q_{i+1}, \dots, q_n, q_1', \dots, q_{i-1}', z_i', q_{i+1}', \dots, q_n')$$

where $H_{\bar{\mathbf{q}}}^i$ represents the power generated by the hydraulic system as a function of the rate of water discharge and the volume turbined by the i -th plant, under the assumption that the rest of the plants behave in a definite way. We call the i -th *minimizing mapping* the mapping $\Phi_i : \Theta_{\bar{\mathbf{b}}} \rightarrow \Theta_{\bar{\mathbf{b}}}$, defined in the following way: for every $\bar{\mathbf{q}} \in \Theta_{\bar{\mathbf{b}}}$

$$\Phi_i(q_1, \dots, q_i, \dots, q_n) = (q_1, \dots, q^*, \dots, q_n)$$

where q^* minimizes $F_{\bar{\mathbf{q}}}^i$. Beginning with some admissible $\bar{\mathbf{q}}^0 = (q_1^0, \dots, q_n^0)$, we construct a sequence of $\bar{\mathbf{q}}^k$ via successive applications of $\{\Phi_i\}_{i=1}^n$. If we set

$$\Phi = (\Phi_n \circ \Phi_{n-1} \circ \dots \circ \Phi_2 \circ \Phi_1) \implies \bar{\mathbf{q}}^k = \Phi(\bar{\mathbf{q}}^{k-1})$$

the algorithm will search

$$\lim_{k \rightarrow \infty} \bar{\mathbf{q}}^k$$

Under appropriate conditions in the admissible set (bounded derivatives), the convergence of the above algorithm may be assured using *Zangwill's global convergence theorem of algorithms* [8].

5 Example

A program that solves the optimization problem was elaborated using the Mathematica © package and was then applied to one example of a hydrothermal system made up of 3 thermal plants and 3 hydro-plant of variable head. The emissions function Ψ_i for each thermal plant is a quadratic model, the sum of the two aforementioned emissions (SO₂ and NO_x)

$$\Psi_i(P) = \alpha_i + \beta_i P + \gamma_i P^2$$

and we consider Kirchmayer's model for the transmission losses: $l_i \cdot P^2$, where l_i is termed the loss coefficient. The data are summarized in Table II.

Table II: Coefficients of the thermal plants.

Plant i	α_i	β_i	γ_i	l_i
1	0	5.475	0.013	0.00010
2	0	5.150	0.010	0.00007
3	0	5.765	0.015	0.00015

The units for the coefficients are: α_i in (Kg/h), β_i in (Kg/h.Mw), γ_i in (Kg/h.Mw²), and l_i in (1/Mw). We construct the equivalent thermal plant as we saw in [5-6], obtaining: $\alpha_{eq} = 757.193$; $\beta_{eq} = 3.63155$; $\gamma_{eq} = 0.00561797$.

We use a complex variable head model, and for each hydro-plant the active power generation P_{hi} (variable head) is a function of $z_i(t)$ and $z'_i(t)$

$$P_{hi}(t, z_i(t), z'_i(t)) := \frac{R_i}{G_i}(S_i + t \cdot n_i) \cdot z'_i(t) - \frac{R_i}{G_i} \cdot z_i(t) \cdot z'_i(t)$$

In variable head models, the negative term represents the negative influence of the consumed volume and reflects the fact that consuming water lowers the effective height and hence the performance of the plant. We consider the transmission losses for the hydro-plant to be also expressed by Kirchmayer's model. Hence, the function of effective hydraulic generation is

$$H_i(t, z_i(t), z'_i(t)) := P_{hi}(t, z_i(t), z'_i(t)) - l_i P_{hi}^2(t, z_i(t), z'_i(t))$$

For the n hydro-plants without hydraulic coupling, we consider

$$H(t, \bar{z}(t), \bar{z}'(t)) = \sum_{i=1}^n H_i(t, z_i(t), z'_i(t))$$

Taking the function $\min\{H_{\max}, P_d(t)\}$ as the upper limit for $H(t, z(t), z'(t))$ at any instant, technical constraints of the type $P_h(t, z(t), z'(t)) \leq P_{h \max} \implies H(t, z(t), z'(t)) \leq H_{\max}$ may also be considered in the set Θ_b . The data of the hydro-plants are summarized in Table III. The units for the coefficients of the hydro-plant are: the efficiency G_i in ($m^4/h.Mw$), the constraint on the volume b_i in ($10^6 m^3$), the loss coefficient l_i in ($1/Mw$), the natural inflow n_i in ($10^6 m^3/h$), the initial volume S_i in ($10^9 m^3$), the coefficient R_i (a parameter that depends on the geometry of the tanks) in ($10^{-12} m^{-2}$) and the maximum hydraulic generation $P_{hi \max}$ in (Mw).

Table III. Hydro-plant coefficients.

Plant	G_i	b_i	l_i	n_i	S_i	R_i	$P_{hi \max}$
1	526315	20	0.00031	10.18	200.	149.5	120
2	496221	35	0.00029	10.99	150.	144.5	120
3	555315	50	0.00028	1.019	450.	150.2	290

We consider a short-term hydrothermal scheduling (24 hours) with an optimization interval $[0, 24]$ and we consider a discretization of 96 subintervals. The optimal power for the hydro-plants, $P_h(t)$, is shown in Fig. 4, and the optimal power for the three thermal plants, $P_{th}(t)$, in Fig. 5. As can be seen in Fig. 4, the power generated by hydro-plant 3 is limited by its technical maximum $P_{h \max} = 290$. Hydro-plants 1 and 2, however, are limited by their technical minimum $P_{h \min} = 0$. The algorithm of coordinate descent shows a

rapid convergence to the optimal solution. The secant method was used to calculate the value of K , given by the coordination theorem, for each hydro-plant. In the example, we need 4 iterations and the time required by the program was 115 s on a personal computer (Pentium IV/2GHz).

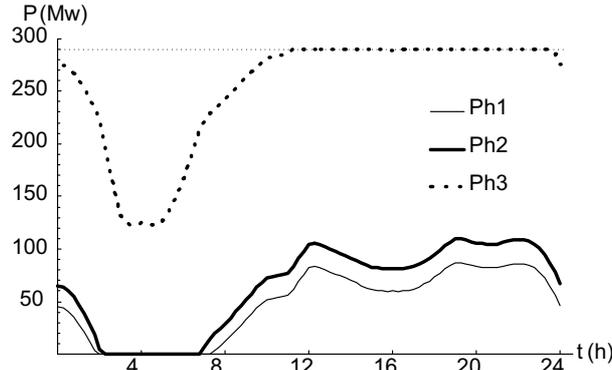


Fig. 4. Optimal power for the hydro-plants.

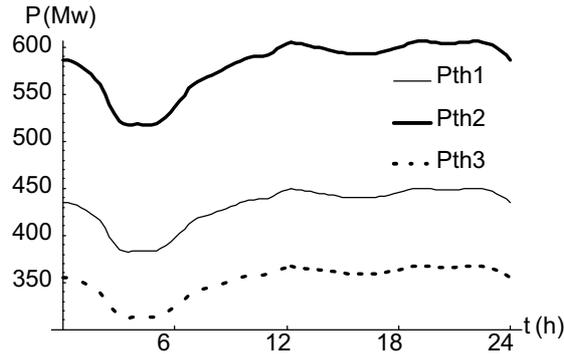


Fig. 5. Optimal power for the thermal plants.

As can be seen in Fig. 5, the power generated by thermal plant 3 is the lowest, due to it being the plant that pollutes the most and that also has the highest transmission losses.

6 Conclusions

This paper presents an environmental dispatch algorithm in a hydrothermal system and solves the problem of minimization of emissions of SO₂ and NO_x caused by the thermal plants based on Pontryagin's Minimum Principle and an algorithm related to the cyclic coordinate descent method. The chemical problem was modeled in the utmost detail and this leads us to a difficult-to-solve mathematical problem: the problem of minimization of a functional

within the set of piecewise C^1 functions that satisfy boundary conditions and non-holonomic inequality constraints. We have developed a novel application of familiar mathematical techniques, and simulation results show that the proposed method has enough efficiency for its practical application in a problem that will be of tremendous importance in the years to come.

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