Preprints of the 19th World Congress
The International Federation of Automatic Control
Cape Town, South Africa. August 24-29, 2014

Formalization and Solution of an Optimal Control Problem for Air Quality Planning

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Abstract: In order to define efficient air quality plans, Regional Authorities need suitable tools to evaluate both the impact of emission reduction strategies on pollution indexes and the costs of such emission reductions. Due to difficulty to cope with the complexity of environmental models, decision support systems are essential tools to help Environmental Authorities to plan air quality policies that fulfill EU Directive 2008/50 requirements in a cost-efficient way. Thus, the main concern is to search for policies capable of taking into account both the environmental and the economical problems. This work presents a new formalization and the first results of an optimal control problem, addressing the selection of efficient control policies over a certain time horizon to reduce air quality pollution. Dynamic programming offers a powerful tool that allows an iterative formalization of the environmental problem as a constrained optimal control problem. An objective function has to be minimized along a given finite time horizon. A set of dynamic varying constraints on the applicability thresholds of emission reduction technologies (control variables) is considered. When minimizing the objective function, the nondecreasing property of each technology application level and the maximum feasible reduction levels have been constrained. This approach has been tested over the Lombardia region in northern Italy.

Keywords: Air quality, non-linear control, integrated assessment, optimal control, dynamic programming.

1. INTRODUCTION

The key problem of air quality Decision Makers is to develop suitable emission control strategies, aimed at improving air quality through the reduction of pollutant. Due to the non-linearities involved the pollutant dynamics, it is very challenging to develop sound air quality policies. This task is even more difficult when considering at the same time air quality improvement and policy implementation cost.

In literature the following methodologies, namely based on Integrated Assessment Modeling, are available to evaluate alternative emission reductions: (a) scenario analysis (Thunis et al., 2007), (b) cost-benefit analysis (Rabl et al. (2005), Reis et al. (2005)) (c) cost-effectiveness analysis (Shih et al. (1998), Carslon et al. (2004)) and (d) multi-objective analysis (Guariso et al. (2004), Carnevale et al. (2007)). Scenario analysis is performed by evaluating the effect of an emission reduction scenario on air quality, using modeling simulations. Cost-benefit analysis monetizes all costs and benefits associated to an emission scenario in a target function, searching for a solution that maximizes the objective function. Due to the fact that quantifying costs and benefits of non material issues is strongly affected by uncertainties, the cost-effective approach has been introduced. It searches the best solution considering non monetizable objectives as constraints (without internalizing them in the optimization procedure). Multi-objective analysis selects the efficient solutions, considering both air quality and costs into an objective function, and stressing possible conflicts among them.

The multi-objective analysis has rarely been faced in literature, due to the difficulties to include in the optimization problem the non-linear dynamics involved in ozone formation. The precursors-pollution relationship can be simulated by deterministic 3D modeling systems, describing chemical and physical phenomena generating tropospheric ozone. Such models, due to their complexity, require high computational time and they are not implementable in an optimization problem, which needs thousands of model runs to find solutions. So, it is required to identify simplified models synthesizing the relationship between the precursor emissions and ozone concentrations. In literature source-receptor relationships have been described using ozone isopleths (Shih et al., 1998), or with reduced form models such as (a) simplified photochemical models, adopting semi-empirical relations calibrated with experimental data (Venkatram et al., 1994), and (b) statistical models, identified on the results of complex 3D Chemical Transport Models (Friedrich and Reis (2000), Ryoke et al. (2000), Guariso et al. (2004)). Therefore, all of these approaches do not consider the strategic issue due to the fact that different decisions can be taken in different times, making the optimization, essentially static. In this paper, a new integrated assessment methodology is proposed. The problem has been defined at the beginning as a nonlinear programming problem, taking into account the time, so, the decision can be taken due to *i.e.* time varying budget limits. In this way, air quality plans become dynamic strategies: a series of different decisions that, every year, have to be taken to reach the final air quality objective.

The paper is organized as follows: in Section 2 the problem is formulated and in Section 3 it is recast as an optimal control problem. Section 4 is devoted to the presentation of a computationally feasible approach and, in section 5, a case study is presented and discussed. Finally, conclusions are drawn in section 6.

2. PROBLEM FORMULATION

Consider a given domain, divided, for the sake of environmental modeling, into a given number n of cells (Carnevale et al., 2012b).
Consider a set of m given technologies, each of them characterized by an application level between 0% and 100% and a vector u containing all the application levels that characterizes all the technologies that can be applied to reduce emission levels over the domain at a certain time.
Also, consider an environmental model which relates technology application levels u to a given air quality index x (*e.g.*, PM10). Vector x has n elements, one for each cell of the studied domain.
Finally, consider a cost function $\mathrm{g}(u)$, that express the annual cost for a given application level vector u.
As said before, the aim of this work is to plan an optimal air quality policy over a finite time horizon of T years, considering both economical and technical aspects. In the next subsections we will formalize all the elements needed in order to correctly state the problem.

2.1 The environmental model

The environmental model that adopted for this work, given a certain application level vector $u(t)$, generates the air quality index vector $x(t+1)$ for the considered domain and for the following year; that is:

$$x(t+1) = \mathrm{f}(\mathrm{e}(u(t))), \tag{1}$$

where $\mathrm{e}(\cdot)$ is a the application levels-to-emissions function and $\mathrm{f}(\cdot)$ is the emissions-to-air quality indexes function.
In this paper, according to (Carnevale et al., 2012b), $\mathrm{e}(\cdot)$ is a linear application, basically an $n \times m$ matrix. Conversely, $\mathrm{f}(\cdot)$ should take into account all the complex and non linear characteristics of secondary pollution. Nevertheless, considering that the devised model will run into an optimization procedure, $\mathrm{f}(\cdot)$ should not be excessively computationally demanding. In oder to meet these requirements, here, surrogate models based on artificial neural networks (ANNs) are employed. The choice of ANNs instead of more complex deterministic models is due to the need to reduce the computational burden without losing the non-linear relations between the control variables and the output variables. A detailed explanation of the employed artificial neural network is out of the scope of the paper, the reader may conveniently refer to (Carnevale et al., 2012a) for details. It is worth to stress that the choice of one year as time step is due to the fact that budget allocation is made once in a year by the policymaker.
Finally, to find a cost-effective solution to the environmental problem, the technologies-to-cost relation has been modeled leading to

$$c(t) = \mathrm{g}(u(t)), \tag{2}$$

where, $c(t)$ is the annual cost of the environmental policy at the y year and, again, $\mathrm{g}(\cdot)$ is a linear application, that is, a $1 \times m$ matrix (Carnevale et al., 2012b).

2.2 Constraints

In order to achieve a cost-effective and technically feasible solution, the optimization problem must be constrained.In particular, in this work, two sets of constraints are taken into account: one considers the technological aspects of the problem, while, the other, states that the problem must be solved under a given annual budget.

Technological constraints Technological constraints are the most complex ones. They require to enlarge the state vector in order to obtain a technically sound solution.
The first set of (static) technological constraints is given by

$$u(t) \in \mathcal{U}, \tag{3}$$

where $\mathcal{U}$ is a set that describes the maximum and the minimum application level of each technology. This set of non dynamic constraints, allows the decision variable to assume values only in a certain range, fixing for each of them the lower bound LB and the upper bound UB and takes into account the unfeasibility of solutions allowing to reduce more than the emission due to a certain activity or the application of two competitive technologies. Even if the number of this constraints can be quite high (hundreds), their formalization is quite easy, as they can be expressed as a linear inequality system.
The second set of technological constraints is dynamic varying and considers that, evidently, for technological and social reasons, the application level of each technology should never decrease along the decision horizon. In order to formalize this constraint, the state vector has been enlarged to $[x, u_{min}]^T$. The non decreasing constraints are automatically embedded into the state transition by using the $\max(\cdot)$ function leading to

$$\begin{cases} x(t+1) = \mathrm{f}(\mathrm{e}(\max(u(t), u_{min}(t)))) \\ u_{min}(t+1) = \max(u(t), u_{min}(t)), \end{cases} \tag{4}$$

where $u_{min}(t)$ is a $m \times 1$ vector and represents the minimum application level of each technology in order to obtain a non-decreasing solution and its initial value is equal to the application level at $t = 0$

Remark 1. It is worth noting that the model (1) is a multidimensional moving average system. Because of the enlarged state vector, now (4) has an autoregressive part, so, (4) is an autoregressive moving average model.

Economical constraints These constraints are responsible for the achievement of a cost-effective solution. An annual budget $b(t)$, that annually increases of a quantity $\Delta b(t)$ along the environmental policy time horizon is considered, that is

$$b(t+1) = b(t) + \Delta b(t). \tag{5}$$

The economical policy, also considering the second part of (4), is described by the following equality constraint

$$b(t) = \mathrm{g}(\max(u(t), u_{min}(t))). \tag{6}$$

In turn, the previous constraints state that the annual budget must be completely used in such a way that, at

year t, the application levels are higher than those of the previous year.
Note that, once defined the annual budget increase $\Delta b(t),\ t = 0, \dots, T-1$, the economical policy is completely defined. This information is supposed to be known. Also note that the level of use of a given technology cannot decrease in order to be realistic. As a consequence, the budget allocated at a given year on a given technology cannot be reallocated on new ones the next years.

Remark 2. Reducing the level of use of a given technology is not feasible since it means to dismiss a technology in few years from the investment, usually before the end of its service life.

The constrained problem Now we are ready to formalize the model and the constraints in a compact form. Putting together equations (1)-(6) we finally obtain (Carnevale et al., 2013)

$$\begin{cases} x(t+1) = \mathrm{f}(\mathrm{e}(\max(u(t), u_{min}(t)))) \\ u_{min}(t+1) = \max(u(t), u_{min}(t)) \\ b(t+1) = b(t) + \Delta b(t), \end{cases} \tag{7}$$

subject to

$$\begin{aligned} & u(t) \in \mathcal{U}; \\ & b(t) = \mathrm{g}(\max(u(t), u_{min}(t))); \\ & t \le T; \end{aligned} \tag{8}$$

where the last constraint define the policy time horizon T.

3. THE OPTIMAL CONTROL PROBLEM

In order to completely setup the optimal control problem we must formalize an objective function to be minimized. We use here a dynamic programming approach (Luenberger, 1979). Accordingly, the objective function to be minimized subject to (8) is:

$$\begin{aligned} \mathrm{J}(u) &= \mathrm{l}(x, u_{min}, u) + \Psi(x(T)) \\ &= \sum_{t=0}^{T-1} \mathrm{h}(x(t)) + \mathrm{g}(u(t)) + \Psi(x(T)). \end{aligned} \tag{9}$$

where $\mathrm{h}(\cdot)$ is the air quality improvement objective function, $\mathrm{g}(\cdot)$ is the cost function and $\Psi(\cdot)$ is a function of the final state.
The $\mathrm{h}(\cdot)$ function can be defined in several ways (*e.g.* the average air quality index over the considered domain or the numbers of peaks of pollutants over the considered domain and so on). Note that, depending on the way $\mathrm{h}(\cdot)$ and $\Psi(\cdot)$ are defined, the previous objective function allows the designer to deal the trade-off between costs and air quality improvements.
Nevertheless, since the cost problem is addressed in the constraints, the cost function is not needed into the problem constraints, because the value of $\mathrm{g}(u(t))$ along the policy horizon is imposed by the second of (8). A further simplification can be obtained considering that, in order to obtain a reasonable solution, $\mathrm{h}(\cdot)$ and $\Psi(\cdot)$ should not operate against each other. Bearing the previous reasoning, a possible simple solution is to chose $\mathrm{h}(\cdot) = \Psi(\cdot)$ leading to the following objective function

$$\mathrm{J}(u) = \mathrm{l}(x) = \sum_{t=0}^{T} \mathrm{h}(x(t)), \tag{10}$$

The previous objective function has to be minimized considering the dynamic model (7) subject to the set of constraints (8).

3.1 Optimal return function

In order to solve an optimal control problem, the general approach is to define an optimal return function associated to it (Luenberger, 1979). The general structure of the optimal return functions, to be used for the optimization, is

$$\begin{aligned} & \mathrm{V}(x, T-i) = \min_{u(T-i)\in\mathcal{C}} [\mathrm{l}(x(T-i), u(T-i)) \\ & + \min_{u(T-i+1)\in\mathcal{C}} [\mathrm{l}(\mathrm{s}(x(T-i), u(T-i)), u(T-i+1)) \\ & + \min_{u(T-i+2)\in\mathcal{C}} [\mathrm{l}(\mathrm{s}(\mathrm{s}(x(T-i), u(T-i)), u(T-i+1)), \\ & u(T-i+2)) \\ & \vdots \\ & + \min_{u(T-i+m)\in\mathcal{C}} [\mathrm{l}(\mathrm{s}(\dots \mathrm{s}(\mathrm{s}(x(T-i), u(T-i)), u(T-i+1)), \\ & \dots, u(T-i+m-1)), u(T-i+m)) \\ & \vdots \\ & + \min_{u(T-1)\in\mathcal{C}} [\mathrm{l}(\mathrm{s}(\dots \mathrm{s}(\mathrm{s}(x(T-i), u(T-i)), u(T-i+1)), \\ & \dots, u(T-2)), u(T-1)) \\ & + \Psi(\mathrm{s}(\mathrm{s}(\dots \mathrm{s}(\mathrm{s}(x(T-i), u(T-i)), u(T-i+1)), \\ & \dots, u(T-2)), u(T-1)))]]] \dots] \dots], \end{aligned} \tag{11}$$

being $\mathcal{C}$ a generic set of constraints and $\mathrm{s}(\cdot)$ a generic state transition function.
For the proposed problem, considering the model (7) and the objective function (10), the previous equation becomes

$$\begin{aligned} & \mathrm{V}(x, u_{min}, T) = \mathrm{h}(x(T)); \\ & \mathrm{V}(x, u_{min}, T-1) = \min[h(x(T-1)) \\ & + h(\mathrm{f}(\mathrm{e}(\max(u(T-1), u_{min}(T-1)))))]; \\ & \mathrm{V}(x, u_{min}, T-2) = \min[h(x(T-2)) \\ & + \min[h(\mathrm{f}(\mathrm{e}(\max(u(T-2), u_{min}(T-2))))) \\ & + h(\mathrm{f}(\mathrm{e}(\max(u(T-1), \max(u(T-2), u_{min}(T-2))))))]]; \\ & \vdots \end{aligned} \tag{12}$$

subject to the set of constraints (8).
In order to solve the optimal control problem, an expression for the optimal return function (12) has to be obtained.
For very specific problems, in general, it is quite difficult to obtain a closed-form analytic expression for the optimal return function. The best way to solve these problems is to use numerical methods, but this approach requires an enormous computational effort. However, the problem cannot be split into simpler subproblems because of the autoregressive part of the state vector u_{min}, (*i.e.*, the non decreasing constraint). Hence, considering the high number of state variables $(n+m)$ and input variables (m) typical of environmental models, it is not numerically tractable as it is.

4. A FEASIBLE SUBOPTIMAL SOLUTION

In this section we propose an approach to simplify the previous problem and, at the same time we present a criterion to evaluate the distance between the obtained suboptimal solution and the optimal one.
As previously said, in the optimal return function, the autoregressive part only depends on the non decreasing constraint $\max(u(T-i), u_{min}(T-i)),\ i = 1, \dots, T$. In order to reduce the computational burden, we propose here to change the non decreasing constraint into

$$u(t) \le u_{subopt}(t+1),\ t = T-1, \dots, 1, \tag{13}$$

where u_{subopt} is the suboptimal solution of the problem, namely, the solution of the control problem originated from the following model

$$\begin{cases} x(t+1) = \mathrm{f}(\mathrm{e}(\max(u(t), u_{min}(t)))) \\ b(t+1) = b(t) + \Delta b(t), \end{cases} \tag{14}$$

subject to

$$\begin{array}{l} u(t) \in \mathcal{U}; \\ b(t) = \mathrm{g}(u(t)); \\ t \le T; \\ u(t) < u_{subopt}(t+1); \end{array} \tag{15}$$

Starting from (14) and considering the objective function (10), we easily obtain the following return function

$$\begin{array}{l} \mathrm{V}(x, u_{min}, T) = \mathrm{h}(x(T)); \\ \\ \mathrm{V}(x, u_{min}, T-1) = \min[h(x(T-1)) + h(\mathrm{f}(\mathrm{e}(u(T-1))))]; \\ \\ \mathrm{V}(x, u_{min}, T-2) = \min[h(x(T-2)) \\ + \min\left[h(\mathrm{f}(\mathrm{e}(u(T-2)))) + h(\mathrm{f}(\mathrm{e}(u(T-1))))\right]\right]; \\ \vdots \end{array} \tag{16}$$

subject to (15).
The previous optimization problem can be solved numerically in an iterative way. Indeed, by defining

$$u_{subopt}(T+1) := UB \tag{17}$$

and by backward solving the problem, the optimal value at a given time $T-i,\ i = 0, \dots, T$ only depends on the actual state $x(T-i)$ and on the actual constraints $u(T-i) \in \mathcal{U}$, $b(T-i) = g(u(T-i))$. Basically, the dynamic programming problem reduces to solving T algebraic optimization problems, that is, the optimal control problem can be divided into simpler subproblems. Thus, the numerical burden only shows a linear increase with respect to the time horizon. Note that, despite being suboptimal, the obtained solution remains economically and technically sound. Indeed, substituting the non decreasing constraint with (13) guarantees anyway monotonicity, hence technical feasibility of solution u_{subopt}.

4.1 Performance evaluation

Clearly, we must be able to quantitatively evaluate how far the obtained solution is from the optimal one. In order to do that, we note that if we simply remove the nondecreasing constraint, we can define a third optimal control problem: minimize (10) with the model (14) subject to the constraints

$$\begin{array}{l} u(t) \in \mathcal{U}; \\ b(t) = \mathrm{g}(u(t)); \\ t \le T. \end{array} \tag{18}$$

Apart from a missing non decreasing constraint (the fourth of (15)), the previous optimal control problem is exactly the same as the one that leads to (16), hence, the optimal return function is identical, as well as the reduced computational burden.
Nevertheless, because of the missing constraints, the objective function obtained with the solution of this new control problem (called unconstrained optimal solution), has always lower values than the ones that would have been obtained by solving the original problem (called optimal solution). Moreover, since the new problem leads to an algebraic optimization for each year in the policy horizon, the optimization function remains lower (or equal) for each time instant along the policy horizon.
Conversely, being the suboptimal solution monotonic and, again, being algebraically solvable for each time instant, the optimization function remains, by construction, higher (or equal) than the one that would have been obtained by solving the original problem. Hence, it has to be that

$$\begin{array}{l} \mathrm{h}(\mathrm{f}(\mathrm{e}(u_{opt}(t)))) \le \mathrm{h}(\mathrm{f}(\mathrm{e}(u_{constropt}(t)))) \\ \le \mathrm{h}(\mathrm{f}(\mathrm{e}(u_{subopt}(t)))), \end{array} \tag{19}$$

being u_{opt} the unconstrained optimal solution and $u_{constropt}$ the solution of the original problem. $u_{constropt}$ is unknown, otherwise all the solutions would be meaningless, but u_{opt} and u_{subopt} can be obtained through numerically tractable optimization and they give quantitative information by upper bounding the distance between the suboptimal solution and the the optimal one.
Finally, note that, if the unconstrained optimal solution is already non decreasing in each components of the vector u, the non decreasing constraint can be dropped, considerably simplifying the optimization problem, because, in this case, $u_{opt} = u_{constropt} = u_{subopt}$.

5. A CASE STUDY: PM10 OVER LOMBARDIA

The proposed methodology has been tested over Lombardia region in northern Italy. The data used to identify the neural network models has been provided by a set of 20 simulations computed through the TCAM (Transport Chemical Aerosol) model (Carnevale et al., 2008). The Internal Cost Index (CI) describes the cost to implement a particular emission reduction policy. This index is computed by means of ANNs linking emission

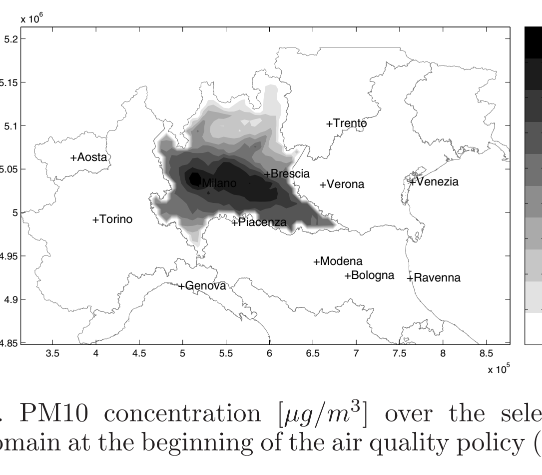

Fig. 1. PM10 concentration $[\mu g/m^3]$ over the selected domain at the beginning of the air quality policy (year 0).

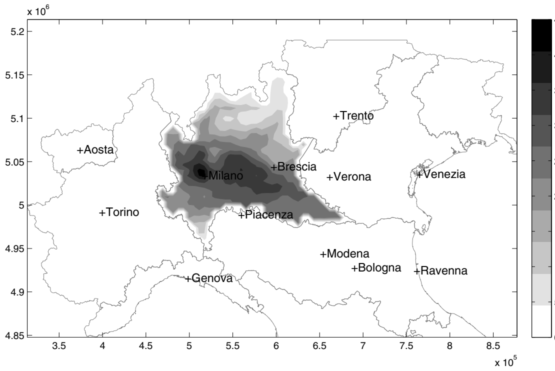

Fig. 2. PM10 concentration $[\mu g/m^3]$ over the selected domain at the middle of the air quality policy (year 5) using the unconstrained optimal solution.

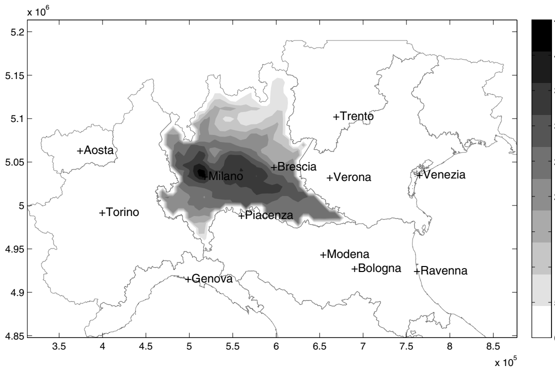

Fig. 3. PM10 concentration $[\mu g/m^3]$ over the selected domain at the middle of the air quality policy (year 5) using the suboptimal solution.

reductions and their relative implementation cost, for different CORINAIR macro sectors. The data used to identify the emission-to-cost models have been provided by IIASA through GAINS Europe database (Carnevale et al., 2012b). The solutions of the decision problem are shown for Lombardia region, one of the most polluted areas in Europe, with a delta budget of $\Delta b(t) = 50MEuros$ per year has been considered over a time horizon of $T = 10$ years.
The computation of the suboptimal solution over a set of approximately 130 technologies together with the computation of the unconstrained optimal solution has required less than 580 s, using Matlab on a commercial quadcore processor.

Figure 1 shows the PM10 distribution over Lombardia at the beginning of the air quality improvement policy, while Figures 2 and 3 show the PM10 distribution using, respectively, the unconstrained optimal and the suboptimal solution. It can be noticed that the two PM10 distributions are not distinguishable. This means that, for the proposed case study, it holds f(e($u_{opt}(5)$)) = f(e($u_{constropt}(5)$)) = f(e($u_{subopt}(5)$)). It is worth stressing that this set of equalities implies (19), but, in general, the contrary is not true. Finally, Figure 4 shows the PM10 distribution over Lombardia at the end of the air quality

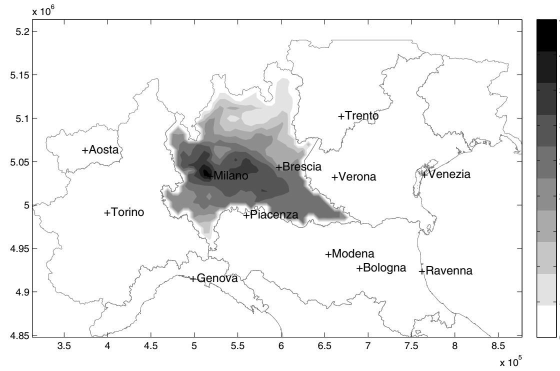

Fig. 4. PM10 concentration $[\mu g/m^3]$ over the selected domain at the end of the air quality policy (year 10) using the suboptimal solution or the unconstrained optimal solution.

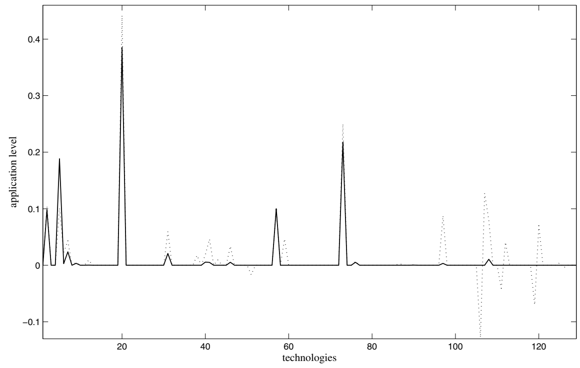

Fig. 5. Technology application level increments (or decrements) between year 1 and year 2 of the air quality policy horizon using the unconstrained optimal (dotted line) and the suboptimal (solid line) solutions.

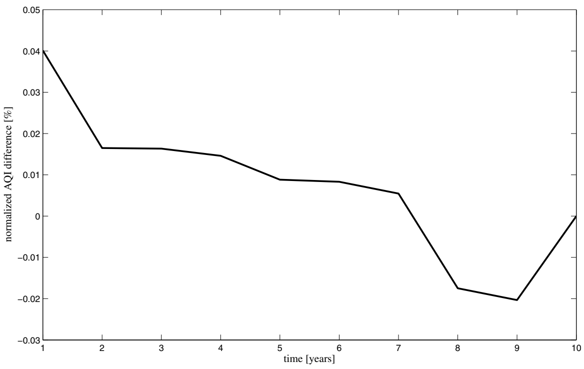

Fig. 6. Average air quality index difference in percentage using the unconstrained optimal and the suboptimal solutions.

improvement strategy. At t=T=10 it always holds, by construction and independently from the considered case, that $u_{opt}(T) = u_{constropt}(T) = u_{subopt}(T)$. Indeed, the suboptimal solution is obtained by backward solving the dynamic programming problem. Hence, it holds that at t=T all the solutions lead to the same technology application level. Note that this set of equalities stronger implies the previous one and, in general, only holds $t = T$.
It is interesting to analyze the technology application levels

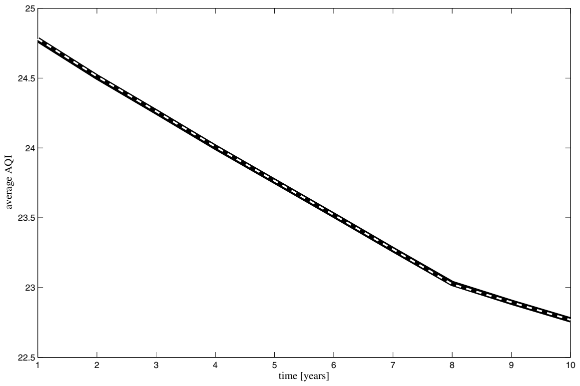

Fig. 7. Average air quality index (PM10 concentration $[\mu g/m^3]$) using the optimal (dotted line) and the suboptimal (solid line) solutions.

differences between two consecutive years. For the sake of brevity only the changes between the first and the second year of the control horizon are considered here, as Figure 5 shows. It immediately appears that at $t = 2$ $u_{opt}(2) \neq u_{subopt}(2)$. It can be also noticed that, the differences between the technology application levels change in sign using the unconstrained optimal solution, while the suboptimal solution, as expected, guarantees a monotonic behavior.

Finally, Figures 6 and 7 show that, for the proposed case, the values of the air quality indexes (*i.e.*, average PM10 over Lombardia) are the same both using the unconstrained optimal and the suboptimal solutions, even though the technology application levels are different. This allows the user to quantify the loss of performance obtained with the suboptimal solution with respect to the (unknown) constrained optimal one. For the proposed case study the set of inequalities (19) is practically a set of equalities.

Remark 3. The negative values in Figure 6 depend on the numerical optimization process and they are not inconsistent with (18) because of their negligible entity (lower than 0.02%).

6. CONCLUSION

In this work, an air quality control problem has been formalized and solved as a non-linear dynamic programming problem. The general structure of the optimal return function for the stated problem has been defined and the approximation leading to a computationally sustainable suboptimal solution has been presented. Moreover, the differences between the computed suboptimal solution and the optimal one have been investigated. The methodology has been applied to the PM10 control problem over the Lombardia region in the northern Italy domain with a time horizon of 10 years. The results show that the application of the control strategy leads to an improvement of air quality, in particular in the central part of Lombardia region.

This work is a first step for the implementation of a suitable long-term planning decision support system that could help Regional Authorities in the selection of optimal (in terms of both cost and air quality) emission control strategies.

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