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Designing an ecologically optimized road corridor surrounding restricted urban areas: A mathematical methodology

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Abstract

The use of optimization techniques for the optimal design of roads and railways has increased in recent years. The environmental impact of a layout is usually given in terms of the land use where it runs (avoiding some ecologically protected areas), without taking into account air pollution (in these or other sensitive areas) due to vehicular traffic on the road. This work addresses this issue and proposes an automatic method for obtaining a specific corridor (optimal in terms of air pollution), where the economically optimized road must be designed in a later stage. Combining a 1D traffic simulation model with a 2D air pollution model, and using classical techniques for optimal control of partial differential equations, the problem is formulated and solved in the framework of Mixed Integer Nonlinear Programming. The usefulness of this approach is shown in a real case study posed in a region that suffers from serious episodes of environmental pollution, the Guadalajara Metropolitan Area (Mexico).

Keywords: Road corridor, Urban air pollution, Restricted areas, Optimal design, Mixed integer nonlinear optimization.

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1. Introduction

In general, the optimal design of highways is a very complex and challenging topic in Civil Engineering still subject to intensive research [1]. The first step of this design process deals with the selection of an initial corridor in which to

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construct the new road [2]. A road corridor can be identified with a polygonal chain, and within the corridor a complete horizontal alignment must be designed. This alignment is usually formed by several line segments appropriately joined by horizontal curves -composed by a circular arc and two transition curves (generally clothoid arcs)- whose curvature varies continuously and smoothly [3]. In the early stage of highway planning, this preliminary alignment is generally determined by considering economic costs and environmental impact [4]. Economic costs can include location-dependent costs, length-dependent costs, earthwork costs and user costs [5], while environmental impact usually consists of avoiding ecologically-sensitive regions (see, for instance, [6, 7, 8]). Additionally, other factors such as safety [9] or animal migration dynamics [10] have been also taken into account in the design of the optimal alignment. However, as far as we know, ecological aspects related with atmospheric pollution have hardly been considered, and this will be our main interest in the present work.

In recent literature related to the optimal design of roads, initial corridors have been considered as input data [11, 12, 13], either obtained in a random way [6, 14] or in an automatic manner by exploring the area under study and minimizing a simplified cost [3, 15, 2]. In this paper we also propose an automatic method to obtain an initial corridor linked to an optimization process. However, our innovative method presents an important novelty with respect to other papers, since our main objective at this early stage of highway planning is not related to economic costs, but to ecological costs. So, we take into account air pollution due to vehicular traffic through the whole road network (including the new road), and we seek for a road corridor avoiding forbidden areas (forests, parklands, lagoons...) and minimizing atmospheric pollution in sensitive zones. Within this ecologically optimized road corridor, an economically optimized road must be designed in a later stage using, for instance, models from [6, 11, 12, 13] or therein references.

In particular, large cities have traffic congestion as one of their major problems with economical, ecological, and health costs. Concerning ecological cost, this consists of high levels of air pollution due to vehicular traffic emissions of pollutants as $\mathrm{NO_x}$, $\mathrm{CO_x}$, particulate matters (PM) and others. Nevertheless, air pollution levels are not homogeneous due to land use, urban morphology, and location of pollutant sources, being main roads and highways the major contributors [16]. In other words, there are urban zones sensibles to pollution that requires special attention.

Different studies and empirical evidences have been analyzed to define strategies in order to mitigate high levels of pollution: urban highway tolls [17], restriction on road network capacity [18], variable speed limits [19], gasoline taxes, vehicle purchase limits and other restrictions on private vehicles [20], and road network expansions to release traffic congestion [21]. In the context of the optimal design of roads, we will focus our attention on the last strategy: the urban highways as a means of networks' expansion.

Urban highways present the following usual characteristics: these are large scale constructions changing drastically the urban space and needing to be tolled in order to finance its construction and maintenance [21]. The impact of an existing urban highway on air pollution, noise and health have been extensively studied (see [22, 23, 24] and references therein), meanwhile the problem of finding the optimal toll and its environmental implications can be seen in [17, 21, 25]. Thus, a new urban highway needed a previous design of its layout, considering not only economical costs, land use and its future toll [21], but also its implications on air pollution.

In order to estimate the implications of a new highway on air pollution, we need to couple a road traffic model -providing traffic quantities such as density and velocity of vehicles- with a convection-reaction-diffusion model for the spread of traffic-related atmospheric pollutants. For the former item, since we will only need vehicular velocities, we propose the use of the first order Lighthill-Whitham-Richards model [26, 27]. However, if vehicular acceleration would be necessary for pollution estimates, second order models -such as the well-known Aw-Rascle-Zhang model [28, 29]- could be also employed. With respect to the latter item, we propose the use of a partial differential equation -including the effects of chemical reactions, molecular diffusion and wind dispersion- with a source term depending linearly on traffic flow [30], but other alternative approaches could be addressed (for instance, the quadratic estimate for traffic emissions given in [31]).

The remaining of this article is organized as follows. In section 2 we introduce the details of the real-world problem, we fix some notation related to the different elements involved in its mathematical setting, and we formulate the mixed integer nonlinear optimization problem to be solved. In section 3 we deal with the novel numerical algorithm proposed to solve the optimization problem, including the suitable discretization of the cost functions and the delicate choice of the minimization method. Section 4 is devoted to present two different sets of numerical experiences, with their corresponding tables and figures, both posed in a road network for the Guadalajara Metropolitan Area (Mexico). Finally, in last section, and based on the computational results in section 5, we derive some concluding remarks.

color

2. Formulation of the problem

This section is devoted to present in detail the physical real-world problem we are dealing with, and also to translate it into a manageable mathematical formulation of all the elements appearing in the environmental problem (variables, models, constraints, objective functions and so on), allowing us an effective analytical/numerical process in order to compute the optimized design of the road corridor.

2.1. Physical description

In this subsection, the environmental problem related to the ecological cost of road network expansion with a new urban highway will be detailed.

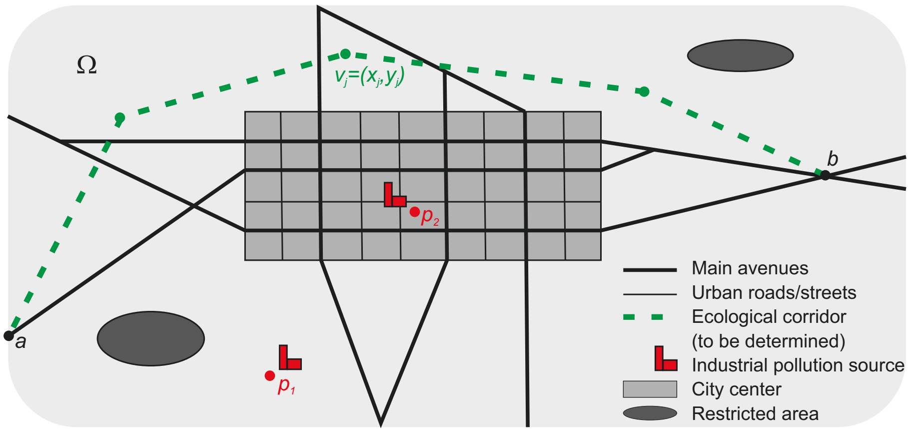

Figure 1 Scheme of a typical domain Ω showing the whole road network, the restricted zones, the city center (as a sensitive area needing to be protected), and a possible "ecological" road corridor joining end-points a and b.

Let us consider a bi-dimensional domain $\Omega \subset \mathbb{R}^2$ representing a metropolitan area, where we can distinguish the four main issues of our problem (a simple scheme of a standard domain of this type can be seen in figure 1):

- a road network formed by different avenues connected to each other through several junctions, where vehicle traffic causes an increase in already existing air pollution, which affects the quality of life of the city's inhabitants,
- a set of urban areas especially sensitive to contamination, which we want to protect from this increase of traffic-related air pollution,
- a set of restricted zones, which cannot be crossed by any avenue, due to its prohibitive character as residential, industrial or recreational areas, and
- a road corridor (to be optimally designed) consisting of a piecewise linear line, verifying some technological constraints to be a preliminary road horizontal alignment. This corridor connects two given points in the road network, so that the diversion of traffic through that corridor minimizes the impact of pollution on sensitive areas and, at the same time, avoids above mentioned forbidden zones.

So, our main interest focuses on obtaining the optimal design of this ecologically optimized corridor, that is, finding the locations and lengths of the different sections of this "ecological" road corridor satisfying above commented conditions.

2.2. Mathematical formulation

Once set the physical description of our environmental design problem, we need to translate it into a rigorous mathematical formulation, in order to be able

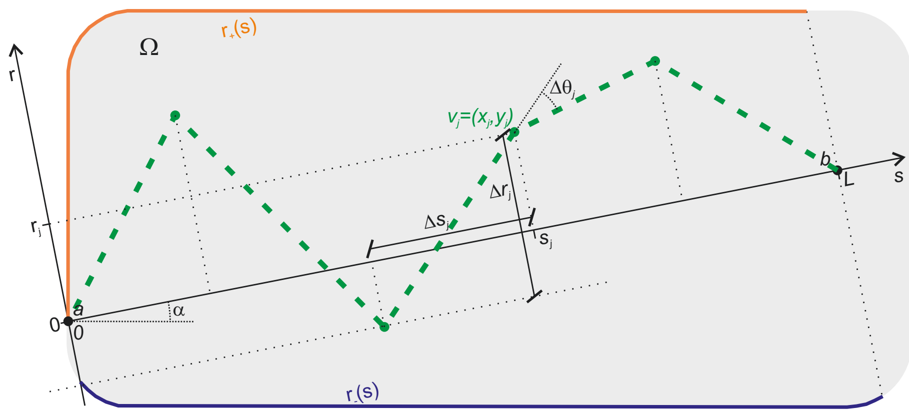

Figure 2 Graphical representation of the decision variables and the polygonal line for the optimal design process of the road corridor.

to apply to its resolution the powerful tools of applied mathematics (mainly, optimal control of partial differential equations, numerical simulation and nonlinear optimization). So, bellow subsections are devote to present the detailed mathematical formulation of the main elements of the problem, that is, the design variables, the control constraints, the mathematical model, the cost functions, and the full optimization problem.

2.2.1. Design variables

In this subsection we will state the decision variables (usually denoted also as design variables or controls) to be changed during the design optimization process, in order to achieve the environmentally optimized road corridor.

Any road corridor connecting point $a = (a_1, a_2)$ to point $b = (b_1, b_2)$ could be seen as a polygonal line (usually known as baseline [12]) being univocally determined by its number of direction changes, $N \in \mathbb{N}$, and the vertices that define it, $v_j \in \Omega,\ j = 1, \ldots, N$. It is worthwhile recalling here that the "corners" of these mean tangents must be later smothered by connection curves (usually clothoid-circular-clothoid curves) with suitable radii [11], as a next step in the horizontal alignment design.

However, for convenience when expressing the geometric constraints, in addition to the Cartesian reference system, we will consider another orthogonal reference system, defined by the point $a = (a_1, a_2)$ and the vector $\mathbf{ab} = (b_1 - a_1, b_2 - a_2)$, which is obtained by translating the origin of coordinates to point a and rotating the axes until OX^+ coincides with vector $\mathbf{ab}$ (see figure 2). So, taking $v_0 = a$, $v_{N+1} = b$, denoting by (s_j, r_j) the coordinates of v_j with respect to this new reference system, and defining $\Delta s_j = s_j - s_{j-1}$ and

$\Delta r_j = r_j - r_{j-1}$, we have that:

$$s_j = \sum_{k=1}^{j} \Delta s_k, \qquad r_j = \sum_{k=1}^{j} \Delta r_k,$$

and the Cartesian coordinates of $v_j = (x_j, y_j)$ -measured in km- are given by:

$$x_j = a_1 + s_j \cos\alpha - r_j \sin\alpha, \tag{1a}$$

$$y_j = a_2 + s_j \sin\alpha + r_j \cos\alpha, \tag{1b}$$

where $\alpha = \arctan((b_2 - a_2)/(b_1 - a_1))$ represents the angle of rotation.

Thus, the vector $\mathbf{u}^N = (N, \Delta s_1, \Delta r_1, \ldots, \Delta s_N, \Delta r_N) \in \mathbb{N} \times \mathbb{R}^{2N}$, which will be denoted as the *decision vector* of the problem, unambiguously determines the road corridor. The length of the corridor is given by $L_{\mathbf{u}^N} = \sum_{j=1}^{N+1} L_j$, where L_j is the length of the j-th section of the polygonal,

$$L_j = \sqrt{\Delta s_j^2 + \Delta r_j^2}, \tag{2}$$

and its parametrization with respect to the arc length, $\sigma_{\mathbf{u}^N} : [0, L_{\mathbf{u}^N}] \longrightarrow \mathbb{R}^2$, is given, in Cartesian coordinates, by expression:

$$\sigma_{\mathbf{u}^N}(\lambda) = (x_{j-1}, y_{j-1}) + \frac{\lambda - L_{j-1}^{ac}}{L_j}(x_j - x_{j-1}, y_j - y_{j-1}), \quad \text{if } \lambda \in [L_{j-1}^{ac}, L_j^{ac}], \tag{3}$$

with $L_0^{ac} = 0$ and $L_j^{ac} = \sum_{k=1}^{j} L_k$, for $j = 1, \ldots, N+1$.

2.2.2. Constraints

This subsection is devoted to fix the admissibility ranges for shape design variables in the optimization process.

First of all we will require that the road corridor be contained in the domain Ω. For this, it is enough to ask, for example, that all the vertices belong to a convex subset of Ω. In that sense, we will demand that

$$0 \leq s_j \leq ||\mathbf{ab}||, \quad j = 1, \ldots, N, \tag{4}$$

$$r_-(s_j) \leq r_j \leq r_+(s_j), \quad j = 1, \ldots, N, \tag{5}$$

where $r_-(s)$ and $r_+(s)$ are functions (convex and concave, respectively) that delimit the area in which the corridor is searched (cf. figure 2). In particular, the options $r_-(s) = 0 < r_+(s)$ and $r_-(s) < 0 = r_+(s)$ correspond to the search for north and south corridors, respectively.

Finally, as previously commented, in order to guarantee that the sections of the polygonal can be linked with curves with sufficiently large radii, we must require that (see [14]):

- the direction changes (azimuth variations $\Delta\theta_j$ -measured in radians) are bounded,

$$\Delta\theta_{min} \leq \Delta\theta_j = \left| \arctan\left(\frac{\Delta r_{j+1}}{\Delta s_{j+1}}\right) - \arctan\left(\frac{\Delta r_j}{\Delta s_j}\right) \right| \leq \Delta\theta_{max}, \quad (6)$$

for given values $0 < \Delta\theta_{min} < \Delta\theta_{max} < \pi$. The lower bound avoids zigzagging paths, and the upper bound preserves from too sharp bends.

- the lengths of the polygonal sections are large enough,

$$\Delta s_j^2 + \Delta r_j^2 \geq L_{min}^2, \quad (7)$$

for a given value $L_{min} > 0$. This constraint is related to the necessity of sufficiently large sections allowing suitable connection curves.

2.2.3. Traffic model

The traffic flow and density are fundamental elements to define the environmental cost of the optimal road corridor. To get them it will be necessary solve numerically the traffic model that is formulated in this subsection.

In the context of our environmental problem, several scenarios could be posed. In this work, the ecologically optimized corridor lies in a domain Ω that also contains an urban zone with a road network, and several restricted areas to be protected. Obviously, there exist some road junctions where the converging (diverging) avenues allow the inlet (outlet) vehicles flow to (from) the road corridor. Thus, a suitable model for vehicular densities and velocities in the whole network -including the road corridor- is needed. This partial differential equations model was formulated by the authors in recent papers [30, 32] as a Lighthill-Whitamm-Richardson (LWR) type model considering a supply-demand rule for an estimate of the flow-through junctions, a coupled queue length model, and also flow conditions at the network ends.

However, since our priority is related to evaluating the environmental services of the ecologically optimized road corridor, the LWR model will be formulated exclusively for the road corridor, but including conservative flow conditions on corridor's ends (corresponding to road network junctions) as functions of known traffic densities along the roads of the network. So, let $\mathcal{I}^{in}$ the set of indexes of convergent avenues to the corridor and $\mathcal{I}^{out}$ the set of indexes of divergent avenues from the corridor. Then, given the densities ρ_k, ρ_l, for $k \in \mathcal{I}^{in}$, $l \in \mathcal{I}^{out}$, in the urban road network, we are looking for a function $\rho_c(\lambda, t)$, with $(\lambda, t) \in [0, L_{\mathbf{u}^N}] \times [0, T]$, such that satisfies the following LWR type model with conservative flows on its ends:

$$\frac{\partial \rho_c}{\partial t} + \frac{\partial f_c(\rho_c)}{\partial \lambda} = 0 \quad \text{in } (0, L_{\mathbf{u}^N}) \times (0, T), \quad (8)$$

$$\rho_c(., 0) = \rho_c^0 \quad \text{in } [0, L_{\mathbf{u}^N}], \quad (9)$$

$$f_c(\rho_c(0, .)) = \sum_{k \in \mathcal{I}^{in}} \min\{\alpha_{ck} D_k(\rho_k(b_k, .)), \beta_{kc} S_c(\rho_c(0, .))\} \quad \text{in } [0, T], \quad (10)$$

$$f_c(\rho_c(L_{\mathbf{u}^N}, .)) = \sum_{l \in \mathcal{I}^{out}} \min\{\alpha_{lc} D_c(\rho_c(L_{\mathbf{u}^N}, .)), \beta_{cl} S_l(\rho_l(a_l, .))\} \quad \text{in } [0, T], \quad (11)$$

where:

- ρ_c [number of cars/km] is the traffic density on the road corridor,
- f_c represents the static relation giving the flux Q_c [number of cars/h] as a function of density: $Q_c = f_c(\rho_c)$,
- α_{ck} is the rate of vehicles from the convergent avenue k that are going to take the corridor,
- $D_k(\rho_k(b_k, .))$ is the demand function giving the potential flux from the avenue k to the corridor,
- β_{kc} is the rate of vehicles that, coming from convergent avenue k, can enter the corridor,
- $S_c(\rho_c(0, .))$ is the supply function giving the corridor capacity against the potential flow from the convergent avenues,
- α_{lc} is the rate of vehicles from the corridor that are going to take the divergent avenue l,
- $D_c(\rho_c(L_{\mathbf{u}^N}, .))$ is the demand function giving the potential flux from the corridor to the divergent avenue l,
- β_{cl} is the rate of vehicles from the corridor that can enter the divergent avenue l, and
- $S_l(\rho_l(a_l, .))$ is the supply function giving the capacity of divergent avenue l against the potential flow from the corridor.

As it seems obvious, parameters α_{lc} and β_{ck} are normalized, that is, they must satisfy that:

$$0 \leq \alpha_{lc} \leq 1, \quad \sum_{l \in \mathcal{I}^{out}} \alpha_{lc} = 1 \tag{12}$$

$$0 \leq \beta_{ck} \leq 1, \quad \sum_{k \in \mathcal{I}^{in}} \beta_{ck} = 1. \tag{13}$$

We also remark here that the model only focuses on the road corridor, meanwhile traffic dynamics in other junctions and roads are not considered. However, it is clear that the complete mathematical model for the whole network including the road corridor needs to be solved numerically and its results will be showing below.

2.2.4. Objective functionals

In this subsection we will formulate the objective functionals related to the optimal road corridor, taking into account pollution at sensible zones, forbidden zones and corridors' length restriction.

The most natural (and simplest) choice for the ecological cost of the corridor consists in measuring, in terms of pollution due to vehicles emissions along the time interval $[0,T]$, its impact on the sensitive zones $C_k \subset \Omega$, $k = 1,\ldots,N_Z$. So, we have the following cost functional, representing the mean pollution in protected areas:

$$J_E(\mathbf{u}^N) = \sum_{k=1}^{N_Z} \frac{\omega_k}{T|C_k|} \int_0^T \int_\Omega 1_{C_k}(x)\, \phi(x,t)\, dx\, dt \tag{14}$$

where ω_k, $k = 1,\ldots,N_Z$ denotes normalized weight parameters for each protected area C_k, $|C_k|$ stands for its Euclidean measure, 1_{C_k} represents its indicator function given by

$$1_{C_k}(x) = \begin{cases} 1 & \text{if } x \in C_k, \\ 0 & \text{if } x \in \Omega \setminus C_k, \end{cases}$$

and ϕ denotes the pollutant concentration (for instance, $\mathrm{CO_x}$ or $\mathrm{NO_x}$) in the whole domain Ω.

However, in order to avoid the computation of this pollutant concentration and to link the ecological cost with the sensitive zones, the authors have proven recently that, given the vehicular density in the corridor ρ_c as solution of (8)-(11), its associated traffic flux $Q_c = f_c(\rho_c)$, and a bounded wind velocity $\mathbf{v} : (x,t) \in \bar{\Omega} \times [0,T] \longrightarrow \mathbb{R}^2$ such that $\nabla \cdot \mathbf{v} = 0$, then, the ecological cost of the corridor could be rewritten (see Theorem 3.1 of [30]), using adjoint-state classical techniques, as the following expression:

$$\begin{aligned} J_E(\mathbf{u}^N) = \int_0^T \int_0^{L_{\mathbf{u}^N}} \{\gamma f_c(\rho_c(\lambda,t)) + \eta \rho_c(\lambda,t)\}\, g(\sigma_{\mathbf{u}^N}(\lambda),t)\, d\lambda\, dt \\ + \int_\Omega \phi^0(x)\, g(x,0)\, dx, \end{aligned} \tag{15}$$

where $\gamma > 0$ [kg/number of cars/km] and $\eta > 0$ [kg/number of cars/h] are coefficients related to vehicles emissions, $\sigma_{\mathbf{u}^N}$ is the corridor parametrization (3) given above, ϕ^0 represents the initial concentration of the pollutant, and $g : (x,t) \in \bar{\Omega} \times [0,T] \longrightarrow \mathbb{R}$ is the solution of the following adjoint problem with weighted forcing:

$$-\frac{\partial g}{\partial t} - \mathbf{v} \cdot \nabla g - \nabla \cdot (\nu \nabla g) + \kappa g = \sum_{k=1}^{N_Z} \frac{\omega_k}{T\,|C_k|} 1_{C_k} \quad \text{in } \Omega \times (0,T), \tag{16}$$

$$g(.,T) = 0 \quad \text{in } \Omega, \tag{17}$$

$$\mu \frac{\partial g}{\partial n} = 0 \quad \text{on } S^-, \tag{18}$$

$$\mu \frac{\partial g}{\partial n} + g\, \mathbf{v} \cdot \mathbf{n} = 0 \quad \text{on } S^+, \tag{19}$$

where:

- ν [km^2/h] and κ [h^{-1}] are, respectively, the coefficients of molecular diffusion and extinction rate of the pollutant under study, and

- $\mathbf{n}$ denotes the unit outward normal vector to the boundary $\partial\Omega = S^- \cup S^+$, with $S^- = \{(x,t) \in \partial\Omega \times (0,T)$ such that $\mathbf{v}\cdot\mathbf{n} < 0\}$ representing the inflow boundary, and $S^+ = \{(x,t) \in \partial\Omega \times (0,T)$ such that $\mathbf{v}\cdot\mathbf{n} \geq 0\}$ representing the outflow boundary.

Additionally to the ecological cost, there is also a set of restricted zones $R \subset \Omega$ that remain forbidden for the road corridor, corresponding to green areas, hospital areas, industrial areas, neighborhoods or any other prohibited zone for land use. So, in order to guarantee the inviolateness of R we define the following penalization cost functional:

$$J_P(\mathbf{u}^N) = p_R \int_0^{L_{\mathbf{u}^N}} \chi_R(\sigma_{\mathbf{u}^N}(\lambda))\, d\lambda, \tag{20}$$

being p_R the penalization weight, and χ_R a characteristic function of set R (taking high values in R and zero values in $\Omega \setminus R$).

Finally, the economic sustainability and viability of the corridor depends on the policy of forecasting carried out by the public authorities (the municipality, local government or other decision-maker) that supports the construction of the road. This forecast can be understood as an average cost $\bar{E}$ per built kilometer which encompasses construction expenses, fuel consumption, drivers' travel time and others related costs. So, the economic cost associated with the road corridor will be proportional to its length $L_{\mathbf{u}^N}$ and can be written as:

$$J_L(\mathbf{u}^N) = \bar{E} L_{\mathbf{u}^N} = \bar{E} \sum_{j=1}^{N+1} L_j(\Delta s_j, \Delta r_j) \tag{21}$$

where L_j is the length of each corridor segment (cf. expression (2)) generated by the polygonal lengths $\Delta s_j, \Delta r_j$.

Within this context, the economic cost (21) presents necessarily a strong *a priori* restriction: the total length $L_{\mathbf{u}^N}$ of the road corridor cannot be larger than a quantity ϵ_L that the decision-maker is able to maintain with its budget. Thus, we will incorporate the economic cost into our optimal control problem as an ϵ_L-constraint (see, for instance, [33, 34] for further details).

2.2.5. The mixed integer nonlinear problem

According to all the above exposed issues, the optimal design of the ecological corridor is formulated as the following mixed integer nonlinear problem (MINLP)

$$\begin{aligned} \min_{\mathbf{u}^N \in \mathbb{N}\times\mathbb{R}^{2N}} \; & J(\mathbf{u}^N) = J_E(\mathbf{u}^N) + J_P(\mathbf{u}^N) \\ \text{subject to} \quad & (4) - (7), \\ & L_{\mathbf{u}^N} \leq \epsilon_L, \end{aligned} \tag{22}$$

where objective functionals $J_E(\mathbf{u}^N)$ and $J_P(\mathbf{u}^N)$ are given respectively by (15) and (20).

3. Numerical solution of the MINLP

To solve above mixed integer nonlinear problem, we need to follow two equally important steps. The first one is concerned with the full discretization of the continuous problem in order to rewrite it in a manageable formulation from the finite-dimensional optimization viewpoint. The second step is related to the choice of a suitable minimization algorithm for solving efficiently the fully discretized optimization problem. We describe both points in a detailed manner in bellow subsections.

3.1. Discretization of cost functionals J_E and J_P

In this subsection, the discretization of both functionals J_E and J_P are presented. For the former, the authors have already formulated an efficient discretization in [30, 32], meanwhile classical techniques will be used for the latter.

Let us consider a polygonal approximation Ω_h of Ω with an admissible triangulation τ_h such that its N_v vertices z_k, $k = 1, \ldots, N_v$, lie on Ω or on its boundary $\partial\Omega$. With respect to time, the step $\Delta t = T/M$ is used to compute the discrete time instants $t^m = m\Delta t$, $m = 0, \ldots, M$. With this space-time discretization, the adjoint problem (16)-(19) can be solved with the Algorithm 3 of [32], computing the discrete adjoint values $\{\{g_{h,k}^m\}_{k=0}^{N_v}\}_{m=0}^{M}$, where $g_{h,k}^m$ represents the finite element approximation of $g(z_k, t^m)$.

In order to solve the LWR model (8)-(11), the interval $I = [0, L_{\mathbf{u}^N}]$ is divided into N_C cells $I_j = [\lambda_{j-1/2}, \lambda_{j+1/2}]$, $j = 1, \ldots, N_C$, of length $\Delta\lambda > 0$, where $\lambda_j = (\lambda_{j-1/2} + \lambda_{j+1/2})/2$ denotes the midpoint of each cell. Then, using the finite volume method and above time discretization, the discrete densities $\{\{\rho_j^m\}_{j=1}^{N_C}\}_{m=0}^{M}$ at cell midpoints can be computed (with ρ_j^m representing the finite volume approximation of $\rho_c(\lambda_j, t^m)$), and the discrete flows $\{\{f_{j\pm1/2}^m\}_{j=1}^{N_C}\}_{m=0}^{M}$ at cell ends can be estimated by using the supply-demand rule [32, 30] (where $f_{j\pm1/2}^m$ stands for the approximation of $f_c(\rho_c(\lambda_{j\pm1/2}, t^m))$). Therefore, the continuous functional cost J_E can be approximated by the following quadrature rule:

$$J_E^{\Delta}(\mathbf{u}^N) = \Delta t \sum_{m=1}^{M} \Delta\lambda \sum_{j=1}^{N_C} \{\gamma f_c(\rho_j^m) + \eta \rho_j^m\}\, g_h^m(\sigma_{\mathbf{u}^N}(\lambda_j))\, \|\sigma'_{\mathbf{u}^N}(\lambda_j)\| + \frac{1}{3} \sum_{\mathcal{T}\in\tau_h} |\mathcal{T}| \sum_{z_k\in\mathcal{T}} \Phi^0(z_k) g_{h,k}^0 \tag{23}$$

On the other hand, given a corridor $\sigma_{\mathbf{u}^N}(I) \subset \Omega$, and once the forbidden zones R are fixed, the penalty functional J_P can be discretized in the straightforward form:

$$J_P^{\Delta}(\mathbf{u}^N) = \Delta\lambda \sum_{j=1}^{N_C} \chi_R(\sigma_{\mathbf{u}^N}(\lambda_j)), \tag{24}$$

In agreement with the points above exposed, the discrete MINLP can be now reformulated as follows:

$$\begin{aligned} \min_{\mathbf{u}^N \in \mathbb{N}\times\mathbb{R}^{2N}} \; & J^{\Delta}(\mathbf{u}^N) = J_E^{\Delta}(\mathbf{u}^N) + J_P^{\Delta}(\mathbf{u}^N) \\ \text{subject to} \quad & (4) - (7), \\ & L_{\mathbf{u}^N} \leq \epsilon_L. \end{aligned} \tag{25}$$

It is worthwhile remarking here that whichever is the numerical optimization method chosen to solve the MINLP problem, it will require a great number of evaluations of both the nonlinear constraints and the discrete functionals J_E^{Δ} and J_P^{Δ}. In particular, in the case of J_E^{Δ}, each evaluation will need the resolution of the LWR traffic model and a previously computed adjoint state.

3.2. Resolution of the discretized MINLP

The hybridized algorithm using to solve the discretized MINLP is described in this subsection.

The discretized mixed integer nonlinear problem presents two very different types of variables: the integer variable $N \in \mathbb{N}$, and the continuous variables $(\Delta s_1, \Delta r_1, \ldots, \Delta s_N, \Delta r_N) \in \mathbb{R}^{2N}$.

Regarding the value of N, the following precisions are necessary: the magnitude of the integer variable (and, consequently, the associated computational cost) is bounded by technological constraints (6) and (7), that is, the total number of mean tangents in the baseline must be very limited. Therefore, we can consider N as a small number, allowing us to find it by means of an exhaustive search process, after fixing a maximal value N_{max}. However, in the unusual case when this number becomes larger, we would need to employ a more specific method like, for instance, Branch and Bound or Generalized Benders Decomposition.

Then, in order to deal with the continuous variables related to section lengths, for each value of N the corresponding nonlinear problem will be solved by means of a hybridized method which combines a genetic algorithm with an interior-point method, both included in the solvers `ga` and `fmincon` of the Optimization Toolbox of Matlab R2017a. The solver `ga` is a free-gradient method, that can be executed in parallel, and uses the three basic probabilistic rules of the natural selection: elite, crossover and mutation to generate the next generation. On the other part, the solver `fmincon` can approximate the cost functional gradient in case of not availability (as happens in our case) and can be also executed in parallel. The hybridization between both is allowed by the option `hybrid` of the solver `ga`, combining it with the solver `fmincon` (or any other Matlab optimization solver).

The main aim of this hybridized algorithm centers on using the solver `ga` to achieve a "good" initial guess for the design of the road corridor, so that the conjugate-gradient algorithm of `fmincon` can arrive in an easy way to a high-quality solution of the MINLP.

4. Numerical experiences

Although we have developed a large number of numerical experiences in order to test our methodology, we will only present here a few raised in the Guadalajara Metropolitan Area (Mexico), which is the second largest metropolis in the country, with a total surface area of about 2800 km^2 and a population of almost 5 million inhabitants.

4.1. Domain, data and space-time discretization

This subsection is devoted to describes the urban domain, road network, forbidden zones, pollution sensible zones, and other elements taking account in numerical tests in subsections (4.2) and (4.3).

The complex area of the city of Guadalajara is approximated by a polygonal domain $\Omega \subset \mathbb{R}^2$, and a dominant north-west wind is considered as its current field (see figure 3(a)). Taking as only pollution tracer the NO_x concentration (with zero initial concentration for the sake of simplicity), we will search for a road corridor beginning at junction 1 -with two convergent avenues A_1 and A_2- and ending at a point close enough to the border -final end of avenue 14- so that the corridor allows vehicles to leave the city.

The polygonal domain Ω has been represented by a mesh of 898 triangles, with $N_v = 491$ vertices, satisfying standard regularity hypotheses, in order to guarantee the numerical method convergence. With respect to forbidden zone R and pollution sensitive areas C_k, $k = 1, \ldots, N_Z$, we assume the presence of four restricted urban zones associated with residential, commercial, industrial and green areas. We also consider the existence of $N_Z = 5$ pollution sensitive areas located in the most contaminated areas of the city (south, south-east, and center) [35], where we expect a drop-down of pollution levels in agreement with a priority order characterized by the suitable use of weight parameters (see figure 3(b)).

For solving the LWR model, we set the parameters $\beta_{1c} = 0.5$, $\beta_{2c} = 0.5$, indicating that only the 50% of drivers from avenues A_1 and A_2 will be able to take the corridor. Moreover, with the purpose of simplifying the boundary conditions, an arbitrarily large potential flow at corridor end $S_l(\rho_l(a_l, .)) = \infty$, for $a_l \in \partial\Omega$ with $l \in \mathcal{I}^{out}$, is imposed -in fact, this implies a free outlet flow at boundary, $f_c(\rho_c(L_{\mathbf{u}^N}, .)) = \sum_{l \in \mathcal{I}^{out}} \alpha_{lc} D_c(\rho_c(L_{\mathbf{u}^N}, .))$. With respect to time discretization we choose a time step of $\Delta t = 4.0\ 10^{-3}$ (measured in hours) and the interval $I = [0, L_{\mathbf{u}^N}]$ is divided into cells large enough to guarantee the standard CFL condition.

On the other part, the 2D characteristic function χ_R related to the set of forbidden zones is defined as a set of paraboloids with a circle as its projection on Ω. So, χ_R takes its higher values in the circles' centers and presents its minimal values ($\chi_R = 0$) on its border and outside them. In figure 3(c) χ_R is displayed using a L_2-projection over a triangular mesh of Ω, showing values of χ_R proportional to the diameter of each restricted zone.

Regarding to the ecological cost (15) and the adjoint state model (16)-(19), they are linked to the pollutant chosen, which is characterized by the parameters

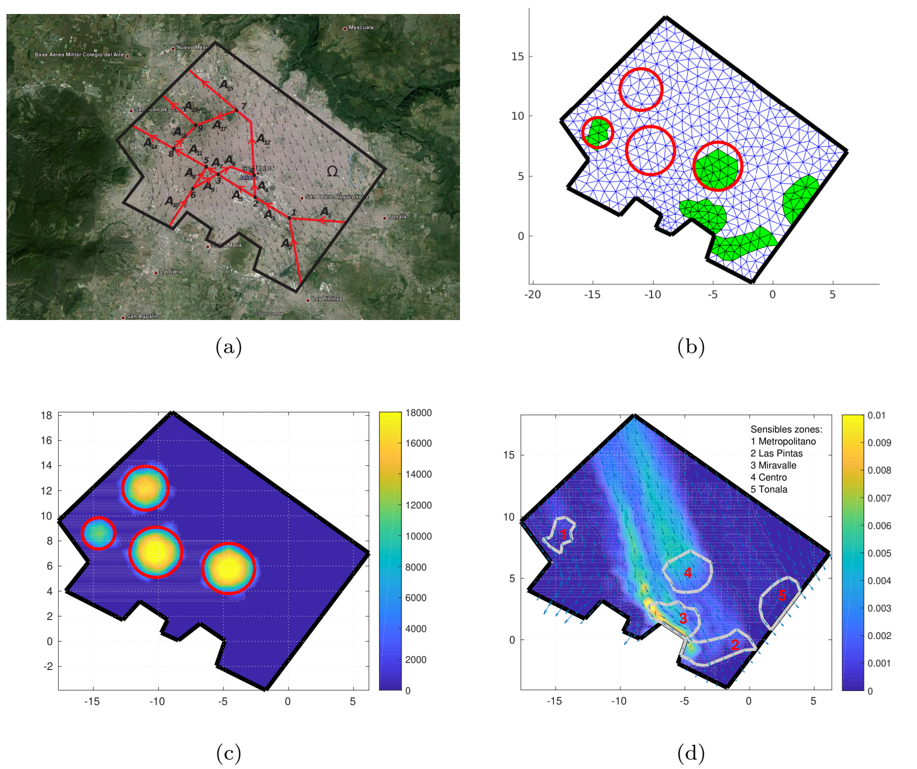

Figure 3 Graphical representation of different elements in the numerical resolution of the MINLP: (a) polygonal domain Ω and road network showing the number labels for avenues and junctions, (b) restricted zones (inside of red-lined circles) and pollution sensitive areas (coloured in green) represented over the triangular mesh considered for Ω, (c) values for the characteristic function χ_R corresponding to forbidden zone R, and (d) isolines for the mean values of the adjoint g and number labels for the sensitive zones, highlighting the adjoint trails from the priority zones: Las Pintas (2), Miravalle (3) and Centro (4).

Zone	Tonalá	Las Pintas	Miravalle	Centro	Metropolitano
Value	0.0061	0.0329	0.0170	0.0297	0.0113

Table 1 Mean NO_x pollution levels for sensitive areas in the absence of road corridor (i.e., considering only the original road network).

ν, κ, γ and η. In our particular case, typical values for NO_x [36] ($\nu = 3.5\ 10^{-8}$ km^2/h, $\kappa = 0.6\ 10^{-2}$ h^{-1}, $\gamma = 10^6$ kg/number of cars/km, $\eta = 3.16\ 10^{-5}$ kg/number of cars/h) have been taken. Evidently, the achieved results will depend on the choice of the pollutant (through their characteristic parameters). So, for each study case we must choose that pollutant whose effects are more harmful for the region under study (NO_x in our case, since is directly related to the predominant use of gasoline vehicles in this metropolitan area). Regarding to the wind velocity, we have considered a constant-time field, with a mean magnitude $\|\mathbf{v}\| = 1.5\,km/h$ and blowing SE, as it is usual in this area [35]. To guarantee that the incompressibility hypothesis of Theorem 3.1 of [30] is satisfied, this wind field (see Figure 3(a)) has been obtained by the numerical solution of a Navier-Stokes type model with suitable boundary conditions [37]. In Figure 3(d) the mean values of the discrete adjoint function are displayed. It can be clearly noted as the higher adjoint values lie on the pollution sensitive areas and their trails extend to the upper part of Ω conducted by the wind direction.

Finally, with respect to our objective of dropping down the NO_x levels on the sensitive areas, as a first step, we identify those zones with highest levels running the model without ecological road corridor added -or, in other words, with equal priority to all areas- (see table 1). The output indicates that the priority zones must be in, higher-to-lower priority order, Las Pintas, Centro and Miravalle; the rest -Metropolitano and Tonalá- presents notably less pollution and, consequently, less priority. Therefore, we fix for all the numerical tests the following vector of weight parameters $\omega = (0.05, 0.3, 0.2, 0.4, 0.05)$, and the results of table 1 will be used as a benchmark for comparison in the design of the optimal road corridors.

4.2. Numerical experiences with $\epsilon_L = \infty$

This first set of numerical tests aims to understand how the layout of the optimal corridor changes to its traffic load. Therefore in this subsection, an infinitely large corridor was treated with different traffic loads.

We will assume that the road corridor could be infinitely large, that is, we will take $\epsilon_L = \infty$. However, the corridor length will remain bounded, since it will be kept inside the urban domain because of the others constraints of the minimization. Moreover, in the following numerical tests we will impose (for the sake of simplicity) equal drivers' preferences, $\alpha_{c1} = \alpha_{c2}$, giving the rate of vehicles from A_1 and A_2 that are going to take the ecological road corridor. One of the aims of this block of experiences is understanding the effects of different vehicular densities on corridors' lengths and locations and, subsequently, on the pollution levels at prioritized sensitive areas.

	Tonalá	Pintas	Miravalle	Centro	Metropol.	J_E	$L_{\mathbf{u}^N}$
N	0.0003	0.0099	0.0034	0.0119	0.0006	0.0261	-
N+C: 50%	0.0011	0.0094	0.0034	0.0121	0.0007	0.0267	27.38
N+C: 60%	0.0009	0.0086	0.0030	0.0106	0.0008	0.0239	25.11
N+C: 70%	0.0009	0.0079	0.0026	0.0097	0.0008	0.0219	26.60
N+C: 90%	0.0010	0.0063	0.0022	0.0061	0.0007	0.0163	26.19

Table 2 Normalized mean pollution levels for sensitive areas corresponding to the road network only (N), and to the network with the road corridor added (N+C: α%) for drivers' preferences of percentage α when taking the corridor. For this second block we also show the total length of the optimal road corridor.

The results of this numerical experience are shown in table 2, where the normalized mean NO_x pollution concentration for each interest zone is displayed. It can be observed that the corridor-efficiency concerning the pollution is higher when the percentage of drivers is also higher, reaching better pollution levels for all the interest zones. (For instance, we can reduce to almost the half the pollution level at Centro zone with a drivers' preference of 90%). In contrast, as drivers' preference percentage is reduced, the pollution levels tend to those for the network-only case. (Within this scenario, the 50% seems to be a turning point, worsening up to a 2% pollution level in the Centro zone, so it can be expected that for minor percentages the situation becomes less satisfactory). In all these tests, the penalization cost function J_P has always remained null (that is, restricted areas are respected), and the ecological cost function J_E has achieved the values shown in table 2.

For a better understanding of these results, corresponding to a maximal value $N_{max} = 5$, in figure 4 we show the mean pollution isolines for the road network only, and for the network with the ecologically optimized corridor for different drivers' preferences (50%, 70% and 90%). It can be easily noted there that all of these optimal corridors correspond essentially to the same design, with $N+1 = 5$ sections in all cases (that is, $N = 4$). Indeed, all of them present a layout that goes to the upper part of the city, avoiding the forbidden zones, and then descends close to the urban zone border to reach the road corridor end. However, this performance is only possible for very large corridor lengths, that could be unfortunately associated to unwanted side effects as, for instance, long travel times, expensive construction costs or high fuel consumptions. Definitely, this result is due to the lack of constraints on the corridor length ($\epsilon_L = \infty$), and strongly suggests the need for a comparative analysis with experiments including this kind of constraints ($\epsilon_L < \infty$).

4.3. Numerical experiences with $\epsilon_L < \infty$

In this subsection, a fixed traffic load and different restrictions on its maximum length are considered for the corridor in this second set of numerical tests. This to evaluate the effect of a less and less large corridor in the sensible pollutant zones.

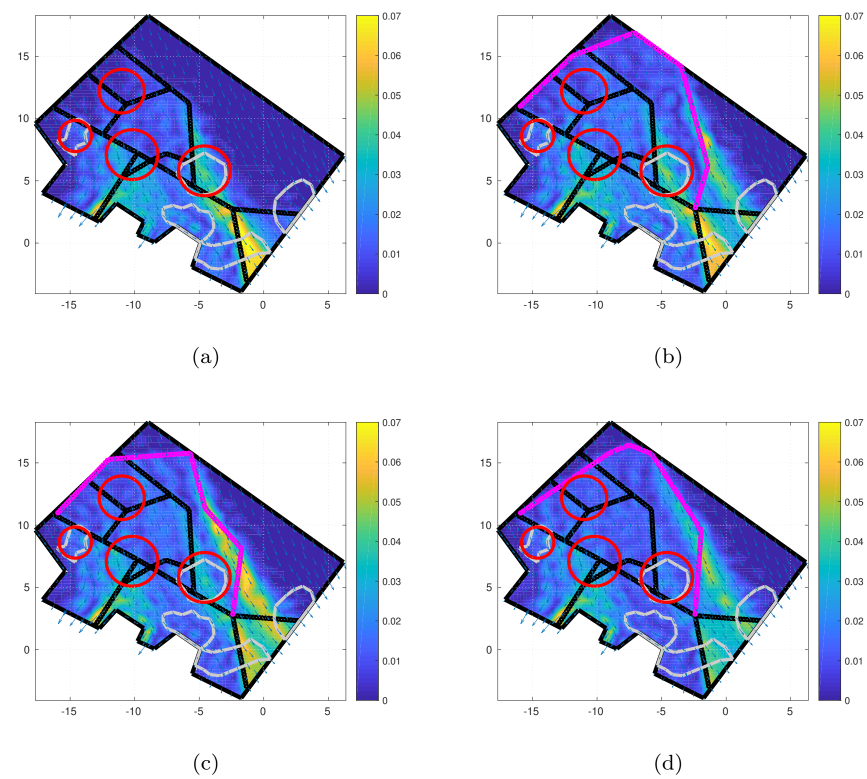

Figure 4 Mean pollution concentrationn on Ω for unlimited corridor lengths, with forbidden zones in red, sensitive areas in grey, road network in black and optimal road corridor in magenta: (a) the network only case, for comparison purposes; (b), (c) and (d) network with optimal corridor for drivers' preferences of 50%, 70% and 90%, respectively.

	Tonalá	Pintas	Miravalle	Centro	Metropol.	J_E	$L_{\mathbf{u}^N}$
N	0.0003	0.0099	0.0034	0.0119	0.0006	0.0261	-
$w_L = \infty$	0.0009	0.0079	0.0026	0.0097	0.0008	0.0219	26.60
$w_L = 9/10$	0.0006	0.0083	0.0032	0.0100	0.0008	0.0229	21.16
$w_L = 4/5$	0.0007	0.0083	0.0032	0.0102	0.0008	0.0232	20.44
$w_L = 3/4$	0.0004	0.0086	0.0033	0.0107	0.0008	0.0238	19.44
$w_L = 2/3$	0.0003	0.0098	0.0054	0.0074	0.0008	0.0237	17.61

Table 3 Normalized mean pollution levels for sensitive areas corresponding to the road network only (N), to the network with the road corridor added but no length limitation ($w_L = \infty$), and to the network with the road corridor added for different length constraints ($w_L = 9/10$, $4/5$, $3/4$, $2/3$). For the second and third blocks we also show the total length of the optimal road corridor.

We choose $\alpha_{c1} = \alpha_{c2} = 0.7$ fixed drivers' preferences as a reference value, due to the low sensibility of the optimal solution to these parameters, as shown in subsection (4.2). We must recall that, in this case, the road corridor length is $\epsilon_L = 26.60$ km, achieving a decrease in the NO_x pollution level for the three priority zones of 20%, 24%, and 18% (see table 2). So, with the main aim of evaluating the impact of a reduction in the corridor length in its design, a weight parameter w_L, with $0 \leq w_L \leq 1$, is introduced in the ϵ_L-constraint of MINLP, rewriting it as:

$$L_{\mathbf{u}^N} \leq w_L \, \epsilon_L, \tag{26}$$

enforcing the optimal road corridor to have a shorter length as the weight parameter w_L decreases. (We must also keep in mind that the total length of the road corridor will always remain lower-bounded by the distance between the two ends of the corridor).

Taking the optimal design corresponding to the unbounded case (i.e., $w_L = \infty$) as our reference for comparison, we have chosen the weight parameters $w_L = 9/10, 4/5, 3/4, 2/3$ in order to solve the MINLP. The outputs for each weight choice is displayed in table 3. Analyzing the results in this table, it can be clearly seen that the more we reduce the length of the road corridor, the more difficult it is to maintain levels of pollution lower than those in the reference case, being $w_L = 2/3$ a turning point with a worse NO_x level at Miravalle zone. Again, in all tests, penalization cost function $J_P = 0$, and ecological cost function J_E reaches the values given in table 3.

As in previous case, in figure (5) the optimal corridor location corresponding to the different weights is displayed with the mean pollution concentration isolines and the whole road network. In these figures we can note as the corridor gets closer to the road network when w_L decreases, and also how its pollution trail becomes increasingly close to the sensitive areas.

Finally, it is worthwhile remarking here that all the computational tests presented in this section have been executed in parallel in an AMD Threadripped 2970WX CPU at 3.2 GHz with 28 cores and 48 threads desktop, 32 GB RAM, and Linux Mint 18.4 OS.

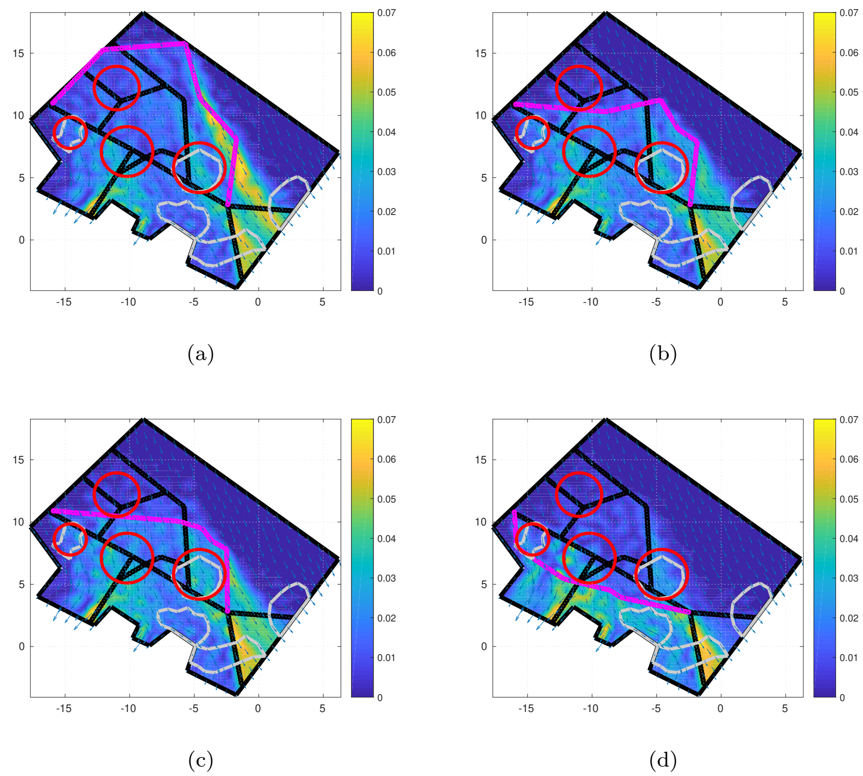

Figure 5 Mean pollution concentrationn on Ω for upper-bounded corridor lengths, with forbidden zones in red, sensitive areas in grey, road network in black and optimal road corridor in magenta: (a) the unbounded case, for comparison purposes; (b), (c) and (d) network with optimal corridor for drivers' preferences of 70%, for weight parameters $w_L = 9/10$, $3/4$ and $2/3$, respectively.

5. Conclusions

In this work we have introduced a novel methodology in order to obtain the optimal design (length and location) for a road corridor to be connected to an already existing urban road network, avoiding a set of restricted zones, and reducing the undesirable effects of air pollution at some sensitive areas that need to be protected.

After a rigorous mathematical formulation of the environmental problem, we propose a full algorithm for computing the ecologically optimized design of the road corridor. The efficiency of our methodology has been assessed through several computational experiences for a real-world case study. By a direct analysis of the numerical results obtained here, we can deduce that some issues in the model present a low sensitivity when computing the optimal design (as could be, for instance, the volume of traffic expected for the road corridor), but other ones show a much higher sensitivity (mainly, the total length of the corridor).

The achieved results also indicate a simple (expected) fact: if the decision-maker does not have enough resources to maintain a sufficiently large road corridor (with the negative consequences exposed above), it will be very hard to hold the objective of dropping down the pollution levels in those sensitive areas.

The numerical examples presented in this work correspond to the case of a time-constant wind field for the sake of simplicity -with the obvious limitations on the results associated to this simplification. Nevertheless, our methodology remains fully valid for the case of a general wind field varying in time.

Last but not least, we should also mention that, although our study focuses on the optimal design of an urban road corridor, the novel methodology presented here can be used in many other different scenarios, for example, the construction of a road through protected forest reserves (not necessarily within a city), or even the design of a trainway.

Acknowledgements

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Declaration of interest: none

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Letter to reviewer #1 (List of changes):

We thank the reviewer for the new careful reading of the manuscript and its interesting comments, which have helped us improve its readability.

As the referee comments, this is only a preliminary attempt to include traffic-related air pollution into the optimal design of a road corridor. So, this has been made very general, not trying to incorporate all the particular issues.

Following your kind remarks, we have addressed all of your recommendations on below modifications and/or corrections:

- We agree with the referee in the fact that the domain where the wind field **v** is defined is missing. Thus, on page 9 we have included these details for the first time that the wind field appears (**v** : (x,t) \in \bar\Omega \times [0,T] \to R^2). Also, **v** was eliminated from the list of parameters on page 10 to not look repetitive.

- On page 15 -and in References section- we have included a new reference about the numerical computation of the wind field, in order to assure its incompressibility, by a Navier-Stokes type model with suitable boundary conditions.

- With respect to the limitations of a time-constant wind field in our numerical example, we have added in the Conclusions section a new paragraph, where we note that we use a time-constant wind for the sake of simplicity -suffering from above mentioned limitations-, but that our methodology is fully applicable for any general wind field depending on time.

We feel confident that with this new redaction, all the weaknesses and deficiencies of the manuscript have been overcome.

For an easier review, these changes have been highlighted in blue.

Letter to reviewer #2 (List of changes):

We are very grateful for the previous suggestions on the paper, which have greatly helped us to improve the manuscript. We also thank you for your comments on the interest in the work.

Highlights

- The design of highways regarding forbidden zones and air pollution is analyzed.
- A novel nonlinear problem for the optimal design of highways' layout is formulated.
- A full numerical methodology is presented to solve the problem.
- Numerical results for a real-world case are given to illustrate the methodology.

Author contributions

N. García-Chan: Software, Methodology, Writing - Original Draft, **L.J. Alvarez-Vázquez**: Writing - Original Draft, Formal analysis, **A. Martínez**: Formal analysis, Writing - Review & Editing
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