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Implementing the Oracle-Based Optimisation for an Integrated Assessment Model for Air Pollution: the Luxembourg Energy Air Quality model

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Abstract In this paper, we present the implementation of an advanced convex optimisation method in the framework of integrated assessment modelling. The integrated assessment of optimal policies requires a flexible and modular optimisation framework to exchange information between models while providing a consistent response in a reasonable time. In the Luxembourg Energy Air Quality model, the NO_x and VOC emissions are computed by an energy model and the dispersion of air pollutants, including produced ozone, are simulated by an air quality model. Here we implement an oracle-based optimisation technique to couple the energy model and the air quality model in cost-effectiveness mode. Each model is queried by a program, the so-called "oracle", which supplies the model output and sensitivity information to a main program. The convergence of procedure is ensured given sufficient assumptions on the convexity by the cutting plane method Proximal-ACCPM. Encouraging results show the capability of the method to handle the non-convex behaviour of the ozone production, but also to find an optimal solution within a reasonable timeframe of a few hours.

Keywords: Integrated assessment; Air quality policy; AUSTAL2000; LEAQ; Proximal-ACCPM

1 INTRODUCTION

The integrated assessment (IA) models combine the knowledge coming from different scientific fields to bring a better understanding of a problem which cannot be attain with a single discipline approach. These models explore the possible states of the human and natural systems in order to analyse the key environmental issues [IPCC, 2007]. The coupling of models from different disciplines requires advanced framework, especially when the aim of the IA model is to find an optimal strategy. The IA framework exchanges information between the models and is required to be flexible enough to work with existing tools, to capture the different feedbacks and to keep an overall good level of consistency.

This paper presents the implementation of such an optimisation framework to the Luxembourg Energy Air Quality model (LEAQ) [Zachary et al., 2011], which attempts to find the air pollution optimal strategies for the Grand Duchy of Luxembourg. The LEAQ model contains the two sub-models: ETEM, an energy techno-economic model [Drouet and Thénié, 2008] and AUSTAL2000-AYLTP, an air quality model [Janicke, 2000]. The energy model computes the emissions of NO_x and non-methane VOC, and the air quality model simulates the air pollutant dispersion and the photochemistry to produce ozone.

The two models are coupled through an optimisation model solved by an advanced convex optimisation method, the so-called "oracle-based optimisation" [Babonneau et al., 2006].

The first section presents the coupling methodology. The second section describes the implementation of the oracle-based optimisation method. And finally, the first results of the coupling are shown.

2 COUPLING METHODOLOGY

2.1 Energy techno-economic model

The ETEM model has been developed to assess urban sustainable development policies [Drouet and Thénié, 2008]. It is a dynamic linear optimisation model and belongs to the techno-economic MARKAL/TIMES family of models [Seebregts et al., 2001]. The optimal value of its objective function can be defined as the result of a minimisation:

$$\gamma(\hat{\mathbf{e}}) = \min_{\mathbf{x}}\{\mathbf{r}'\mathbf{x} \mid \mathbf{A}\mathbf{x} = \mathbf{b}, \mathbf{m}'\mathbf{x} = \mathbf{e} \leq \hat{\mathbf{e}}, \mathbf{x} \geq 0\}, \tag{1}$$

where $\mathbf{x} \in \mathbb{R}^n$ is the vector of the decision variables (technology investments and activities), $\mathbf{r} \in \mathbb{R}^n$ is the cost vector and the constraint $\mathbf{A}\mathbf{x} = \mathbf{b}$ describes the structure of the reference energy system, the characteristics of the technologies and of the energy resources.

The model also calculates the annual emissions $\mathbf{e} = e_{q,\mu}$ of the air pollutants $q \in \{NO_x, VOC\}$ for each sector $\mu \in \xi$, using stoichiometric coefficients $\mathbf{m}$. The emissions are constrained by upper bounds $\hat{\mathbf{e}}$ representing the yearly maximum sectoral emissions.

By construction, we ensure that Eq. (1) has an optimal solution and that the constraint $\mathbf{e} \leq \bar{\mathbf{e}}$ on sectoral emissions is an equality at optimality (e.g. when an optimal solution $\mathbf{x}^\star$ is found, we have $\mathbf{e} = \hat{\mathbf{e}}$). As a result, $\gamma(\hat{\mathbf{e}})$ is a convex function.

2.2 Spatial Emission Allocation

The aggregated annual emissions $\hat{\mathbf{e}} = \hat{e}_{q,\mu}$ are distributed per sector according to the spatial allocation functions $f_\mu(s)$, $s \in$ the region S and the time profile functions $h_\mu(t)$, $t \in [0, T]$ to obtain the allocated emissions

$$e_q(t, s) = \lambda \sum_{\mu \in \xi} h_\mu(t) \times f_\mu(s) \times \hat{e}_{q,\mu}. \tag{2}$$

λ is a conversion factor which transforms emissions from tonnes per year ($\mathrm{t} \cdot \mathrm{yr}^{-1}$) to gramme per second per square meter ($\mathrm{g} \cdot \mathrm{s}^{-1} \cdot \mathrm{m}^{-2}$) .

2.3 Air quality model

The air quality model is based on AUSTAL2000, an atmospheric dispersion model for simulating the dispersion of air pollutants in the ambient atmosphere [Janicke, 2000]. It is called AUSTAL2000-AYLTP and is an augmented version which also integrates a fast photochemical calculator to simulate the ozone production [Aleluia Reis et al., 2009].

From the emission strengths $e_q(t, s)$, AUSTAL2000-AYLTP computes the concentrations of pollutants at every time step t over the region S. Capturing the errors in the dispersion modelling, it provides the expected values of the concentrations $\bar{c}(s,t)$ and their standard errors with $\sigma_c(s,t)$.

An air quality indicator is calculated as the Accumulated Ozone exposure over a Threshold (AOT). As defined in the Directive 2008/50/EC, the AOT is a measure of the ozone concentration exceedances over a certain threshold measured during the day (from 8:00 to 20:00), e.g. AOT_{40} corresponds to the accumulated ozone exposure over a threshold of 40 ppb [EU, 2008]. In this study, the indicator AOT_1 is used, as a measure of the average ozone concentration, where ozone concentration includes both transport and species generation.

The expected value of AOT_i is defined as:

$$E[AOT_i] = \alpha \int_S \int_{t_1}^{t_2} \max(0, (\bar{c}(s,t) - i))\,\mathrm{d}t\mathrm{d}s, \tag{3}$$

where $\alpha = (|S| \cdot |t_2 - t_1|)^{-1}$. t_1 and t_2 are respectively 8:00 and 20:00 of the last day of the episode, and $|S|$ is the surface of the region S.

Taking into account the air quality model sampling error σ_c, using the 95% upper limit of the confidence interval of the concentrations levels, an upper limit of the AOT can be calculated as follows:

$$U[AOT_i] = \alpha \int_S \int_{t_1}^{t_2} \max(0, (\bar{c}(s,t) + 1.96\sigma_c(s,t) - i))\,\mathrm{d}t\mathrm{d}s. \tag{4}$$

The AQ indicator can be generalised as a function dependent on ê, which is the input of the emission allocation transformation and, consequentially, the input of the air quality model. We then denote the air quality indicator as $p(\hat{\mathbf{e}}) = E[AOT_i]$ or $U[AOT_i]$.

2.4 General problem definition

In a cost-efficient analysis, the optimisation problem minimises the discounted total energy system cost while respecting an air quality restriction is the following:

$$\min_{\hat{\mathbf{e}}} \left\{ \gamma(\hat{\mathbf{e}}) : p(\hat{\mathbf{e}}) - \hat{p} \leq 0 \right\}, \tag{5}$$

where $\hat{p}$ is the air quality indicator target. $\gamma(\hat{\mathbf{e}})$ is issued from Eq. (1) and $p(\hat{\mathbf{e}})$ is the chosen air quality indicator, calculated from Eq. (3) or Eq. (4).

3 IMPLEMENTATION

3.1 Oracle-based optimisation

The optimisation problem, Eq. (5), is non-differentiable, and can be solved by a cutting-plane method, such as the Proximal Analytic Center Cutting Plane Method [Goffin and Vial, 1993]. The oracle-based optimisation engine implements such a method and provides a convenient framework introducing the concept of “oracle” [Babonneau et al., 2006]. An oracle is a “black-box” program which computes the information required by the optimiser and gives a reply under the form of an inequality, called “cut”. The oracle returns either an optimality cut, to support the objective function, or a feasibility cut, to define an outer space of the feasible set.

At a query point, the optimality cuts (O) and the feasibility cuts (F) are defined by:

- the objective function value (when an optimality cut occurs) or the left-hand side of the constraint (in the case of a feasibility cut),
- the sub-gradients, as defined hereafter,
- an indicator index: 0 (O) or 1 (F).

The gradient values of the objective function $\delta\gamma$ at the query point $\hat{\mathrm{e}}$ are equal to the optimal dual values of the constraints $\mathbf{e} \leq \hat{\mathrm{e}}$, in Eq. (1). The linear program solver provides these values as a result of the minimization contained in the equation.

The sub-gradient values, required by the feasibility cut, cannot be obtained analytically because $p(\hat{\mathrm{e}})$ results from a call to AUSTAL2000-AYLTP. An estimation of the sub-gradient can be calculated by finite differences:

$$\delta p(\hat{\mathbf{e}}) \approx \frac{p(\hat{\mathbf{e}} + \epsilon) - p(\hat{\mathbf{e}})}{\epsilon}, \tag{6}$$

where $p(\hat{\mathrm{e}} + \epsilon)$ is a vector of the values of the perturbed air quality indicator.

At each iteration, the optimiser proposes a new query point chosen as the analytic center of a localisation set, built from the generated optimality and feasibility cuts and containing all admissible solutions. This localisation set is shrinking as the iterations proceed, and when the stopping criterion is attained, the optimal solution is found as the last query point.

The resolution algorithm is the following:

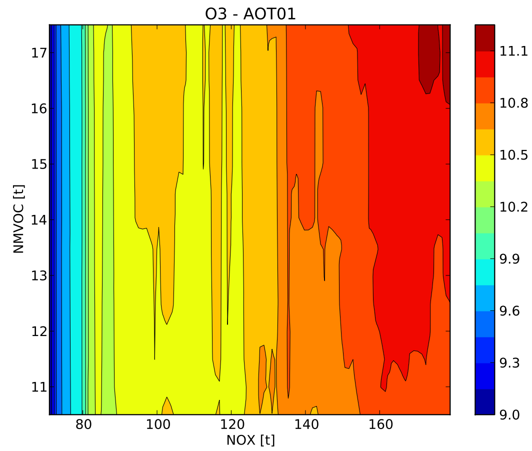
1. Define a starting query point $\hat{\mathrm{e}}_{n=0}$;
2. Evaluate the air quality indicator $p(\hat{\mathbf{e}}_n)$:
   (a) Allocate $\hat{\mathrm{e}}_n$ during the episode and over Luxembourg,
   (b) Run AUSTAL2000-AYLTP,
   (c) Compute $p(\hat{\mathbf{e}}_n)$;
3. If $p(\hat{\mathbf{e}}_n) > \hat{p}$ then generate of a feasibility cut:
   (a) Evaluate each component of $\delta\mathbf{p}(\hat{\mathbf{e}}_n + \epsilon)$,
   (b) Calculate $\delta\mathbf{p}(\hat{\mathbf{e}}_n)$,
   (c) Define the cut as $[p(\hat{\mathbf{e}}_n) - \hat{p}, \delta p(\hat{\mathbf{e}}), 0]$

   else generate of an optimality cut:
   (a) Run ETEM with bounds on emissions=$\hat{\mathbf{e}}_n$,
   (b) Get the optimal objective value and the dual values of bounds,
   (c) Define the cut as $[\gamma(\hat{\mathbf{e}}_n), \delta\gamma(\hat{\mathbf{e}}_n), 1]$
4. Send the generated cut to the optimiser;
5. Get the next query point $\hat{\mathrm{e}}_{n+1}$ from the optimiser;
6. If the stopping criterion is met then stop else $n = n + 1$ and go to 2.

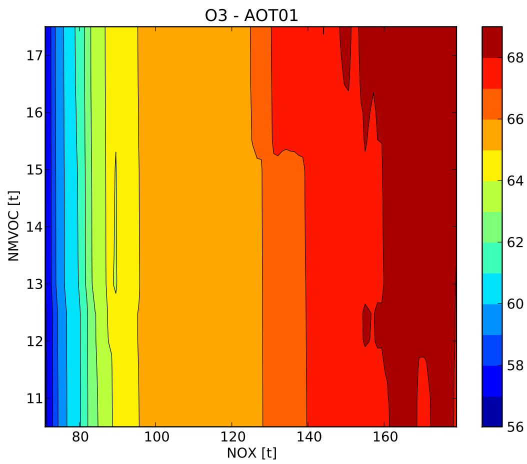
3.2 Convexity

One major requirement of the oracle-based optimisation is the convexity of the optimisation problem. Here, the objective function, assimilated to ETEM Luxembourg, is convex by construction: when the emissions bounds $\hat{\mathrm{e}}$ decrease, the total energy cost increases and vice versa.

The convexity of the feasible set, where lies the solution, is more difficult to established because the response of the air quality is not convex: an increase in NO_x emissions could result in the production or in the destruction of ozone, depending on the NO_x/VOC ratio. Nevertheless, in practice, a pseudo-convex response can be obtained by restricting the search domain of the coupling variables.



(a) Real meteorological conditions



(b) Unfavourable meteorological conditions

Figure 1: The air quality indicator E[AOT_1] surface (in ppb) as a function of the total NO_x and VOC emissions (in t) during a three-day episode, using AUSTAL2000-AYLTP with two setups: (a) real meteorological conditions and (b) unfavourable meteorological conditions.

Figure 1 shows two surfaces of AOT_1 in function of the total emission of NO_x and VOC during a three-day episode. They compare the air quality model outputs when using two setups : using real meteorological conditions, and using stable meteorological conditions, e.g. low constant wind speed, constant wind direction, constant high temperature, constant relative humidity. The surface functions shows that the domain of interest is rather NO_x-sensitive than VOC-sensitive. Consequently, the coupling variables are NO_x emissions.

3.3 Study case

A study case has been simulated to determine the optimal NO_x emission levels from Luxembourg to comply with drastic air quality limits after 2020, by simulating a typical three-day episode in unfavourable meteorological case scenario. If the energy strategy complies with the worse meteorological scenario, then it will comply for the whole year. We have performed two tests. In the first test (Test 1), the coupling variable is the total Luxembourg NO_x emission in tonne per episode. In the second test (Test 2), the coupling variable is a vector containing the NO_x emissions from the transport sector (the biggest emitter), the residential sector and the other sectors instead of the total. In this study case, only the impacts from the energy policy implemented in Luxembourg are considered. We then exclude the impacts on the ozone concentrations in the surrounding countries, but also the impacts in Luxembourg induced by the energy policies implemented in the surrounding countries.

ETEM Luxembourg describes the Luxembourg energy sector from 2005 to 2030. The years 2005–2010 are calibrated with the national energy balances, according to the National Institute for Statistics and Economic Studies of the Grand Duchy of Luxembourg. The model is driven by a total of 24 end-use demands (energy demands in agriculture, chemicals, iron and steel, non metallous mineral products and other industries, energy demands in commercial/institutional buildings, energy services in transport and in residential). The energy model takes into account 22 different energy carriers (including the fossil fuels and renewable) and includes a database of more than 700 technologies (existing and future generation). The coupling variables limit the yearly NO_x emissions during the period 2020–2030.

Yearly emissions are distributed in space according to a land-use vector map of Luxembourg subsequently aggregated to a 1 km grid raster map. Temporal emissions loads per sector have been provided by the GENEMIS database from the University of Stuttgart, Germany [Friedrich, 1997]. AUSTAL2000-AYLTP simulates a three-day episode in the summer, from the 16th to the 19th of July. Additionally to the energy-related emissions, the background biogenic VOC emissions are also taken into account, using data from the Aristotle University of Thessaloniki. The spatial domain is a 20×24×1 grid with an horizontal resolution of 5km and a vertical layer of 20m. The time step is set to 1h. The air quality indicators, expected and upper AOT_1, are calculated for the last day of the episode from 8:00 to 20:00 over Luxembourg as defined in the Section 2.

4 Results

For each test, the optimisation problem (Eq. 5) is solved for different values of the threshold $\hat{p} \in \{40, 45, 50, 55, 60, 65, 70, 75, 80\}$. An iteration took nearly 9 minutes to be completed on our computer (4×quad-core AMD 800 MHz CPU), given that the sensitivity of the air quality model is calculated in parallel. The number of iterations varies depending on the values of the starting point and the stopping criterion. In our tests, the starting point is fixed as the middle point in the interval of the possible values for NO_x and the stopping criterion is equal to 10^{-5}. The number of iterations doesn't vary with the air quality indicator, but increases with the number of coupling variables. In Test 1, the average number of iterations is 15.75 (i.e. 2h20), while, in Test 2, the average number of iterations is 23 (i.e. 3h30). For 4 runs, the number of iterations exceeds 40 iterations (i.e. 6h).

4.1 Test 1 - National NO_x emissions

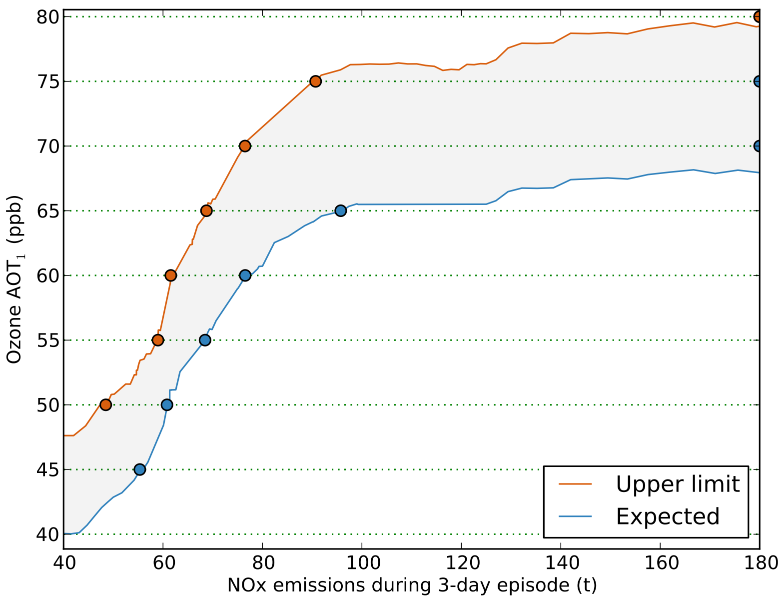


Figure 2: Test 1 — The curves are the expected and upper limit of AOT_1 as a function of NO_x emissions. The points mark the optimal solutions, e.g. the optimal NO_x emissions, at each threshold denoted on the y-axis.

Figure 2 plots the values of the expected and upper limit of AOT_1 (ppb) for each encountered query point, i.e. the national NO_x emissions. The optimal solutions can be retrieved easily from this graph, where they lie at the intersection between the function curve and the vertical line at the threshold level. The figure highlights the optimal emissions for each runs. The shapes of the functions are almost monotonous increasing, and have a very flat part between 100 and 180 tonnes. For values of threshold equal to {70, 75, 80} for the expected AOT_1 and {80} for the upper limit, the solution is the maximum NO_x emission level 180t.

4.2 Test 2 - Sectoral NO_x emissions

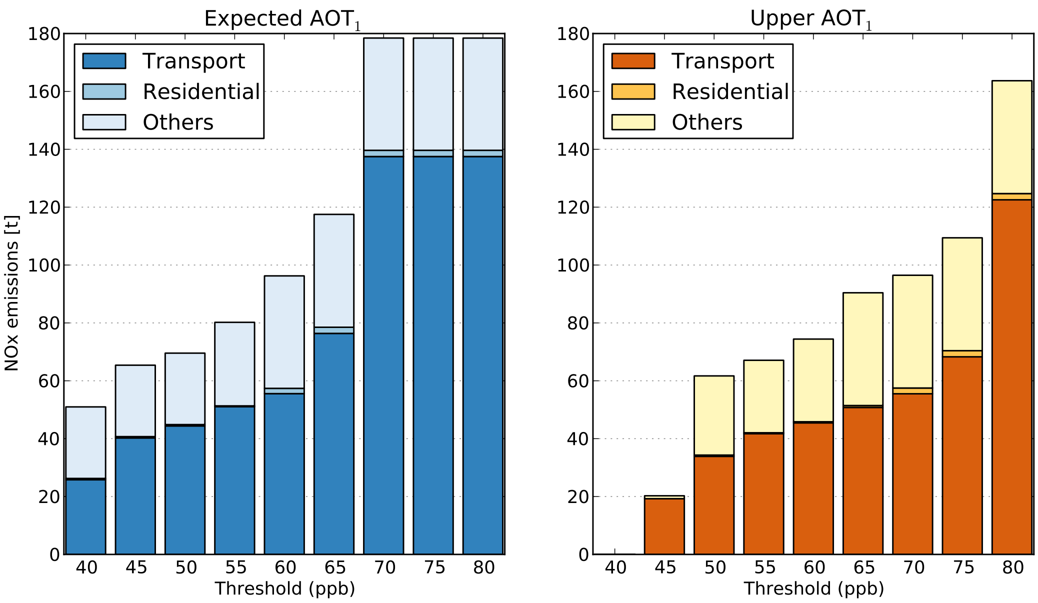


Figure 3: Test 2 — Optimal NO_x emissions for the sectors transport, residential and others, at each threshold.

Figure 3 plots the optimal solutions for each threshold and for the two AQ thresholds with and without uncertainty. Results are detailed per sectors. The most impacted sector is the transport sector where the emission reductions are more easy to implement, and are also the cheapest. Then, comes the residential sector and finally the others sectors, where industry is the biggest emitter. The energy model contains backstop technologies, i.e non pollutant technologies which can substitute any others technologies but with a very high price. This allows the solver to find a solution with a limit of 20 tonnes as it is the case for the threshold “45” and the upper limit AOT_1.

5 Conclusion

We have implemented the Luxembourg Energy Air Quality model with the help of the oracle-based optimisation engine. The framework has been tested in cost-effectiveness analysis, for different levels of air quality indicators. The quality of the response of the air quality model is very important, and it should have provide an AOT functionality which is convex.This can be achieved by defining worst case meteorological conditions in the air quality model.

This work can be seen as a follow-up of the work of Zachary et al. [2011], where the energy description represents the Grand Duchy of Luxembourg from 2005 to 2030. The representation has been greatly refined and updated, and the air quality model is more realistic and finer in the representation of the air pollutant dispersion and photochemistry. We have shown that, a fast air quality model can be implemented in an optimisation IA framework, delivering results in a reasonable time frame. We also demonstrate how to take into account the transport model uncertainty and then find the robust solutions to air quality limits. A further step would be the introduction of others type of uncertainties, such as the meteorological inputs and the ones coming from the desegregation in time and in space of the annual emissions.

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