Implementation of a Full Air Quality Model in an Integrated Assessment Model

The Luxembourg Energy Air Quality model

L. Drouet[a], L. Aleluia Reis[b]

[a] Centro Euro-Mediterraneo sui Cambiamenti Climatici, Milan, Italy
[a] Fondazione Eni Enrico Mattei, Milan, Italy
[b] Public Research Center Tudor, Esch-sur-Alzette, Luxembourg

December 13, 2012

cmcc Centro Euro-Mediterraneo sui Cambiamenti Climatici

Fondazione Eni Enrico Mattei

Outline

- Introduction
- LEAQ model
- Methodology
- Study Case

Air Pollution

Air pollution is a major concern in

- the protection of human health,
- the protection of ecosystem,
- the climate change (GWP).

Air Pollution

High complexity phenomena

- Interaction of various pollutants (anthropogenic or biogenic)
- Interaction with local meteorology
- Non-linear relations in space and time (multiscale)

Generally described by complex physical models

- 3-D chemical transport models CTMs (Eulerian or Lagrangian)
- Topography, emissions and meteorology input data
- High resolution

Very demanding in computing time and data processing

Air Quality Regulation

International/regional/national legislation provides target values and long-term objectives.

Example: Directive on Ambient Air Quality and cleaner air for Europe(08/50/EC):

- Ozone (O_3)
- CO, NO_2, SO_2, PM_{10}
- $PM_{2,5}$

The need for an integrated tool for air pollution

- to support local/national authorities
- to assess the effects of mitigation policies
- to find **cost-efficient air quality policies**

Air Quality Integrated Models

Name	Emission model	Air quality model	Reference
Global			
Global Health Impacts	MESSAGE	TM5	Rao et al. (2012)
Regional			
MERG	MARKAL	SCA	James et al. (1985)
RAINS	PRIMES	EMEP	Alcamo and Hordijk (1990)
ASAM	EMEP/CASM	RAINS	ApSimon et al. (1994)
SAMI	EMS-95/Mobile5b	URM-1ATM,...	Odman et al. (2002)
EC4MACS	GAINS	TM5,EMEP,...	EC4MACS (2007)
SIMCA	CEP/SMOKE	CMAQ	Borge et al. (2008)
GAMES	POEM-PM	TCAM	Carnevale et al. (2008)
MINNI	RAINS-Italy	FARM	D'Elia et al. (2009)
Mexico2050	E3MG	p-TOMCAT	Barker et al. (2010)
GAINS	GAINS	EMEP	Amann et al. (2011)
RIAT	GAINS	NNET(TCAM)	Carnevale et al. (2012)
Urban			
GENEVA	MARKAL-lite	TAPOM-lite	Carlson et al. (2004)
BRUTAL	iMOVE	ADMS-Urban,...	Oxley et al. (2009)
LEAQ	ETEM	TAPOM-lite	Zachary et al. (2011)

Review of integrated models for Air pollution, including emission and AQ models (Aleluia Reis, 2012). **Models running in optimization mode**.

Objective

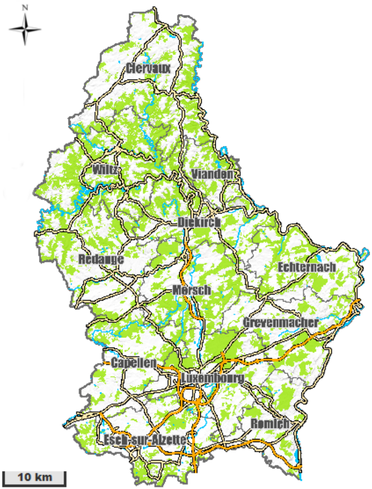
In this study, we present a framework to couple

- an energy model which computes precursors emissions (NO_x and NMVOC) and
- an fast air quality model
  - transports air pollutants
  - represents photo-chemical reaction of ozone production

Cost-effectiveness analysis:

- Minimization of the energy sector cost,
- while respecting air quality standards.

Luxembourg context



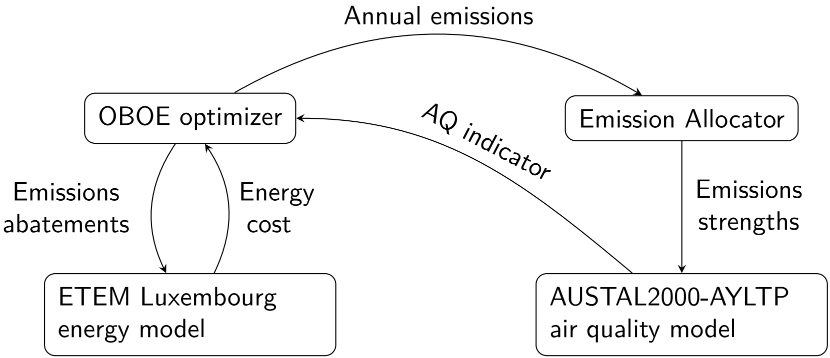
Source: ACT, Luxembourg

- Domain: $\approx$ 50km $\times$ 80km
- Urban/National scale

- Population: 500'000
- Commuters: 150'000
- Highest GDP per capita in EU
- Low excise tax for oil (tank tourism)

- Moderate levels of NO_x and Ozone concentration.

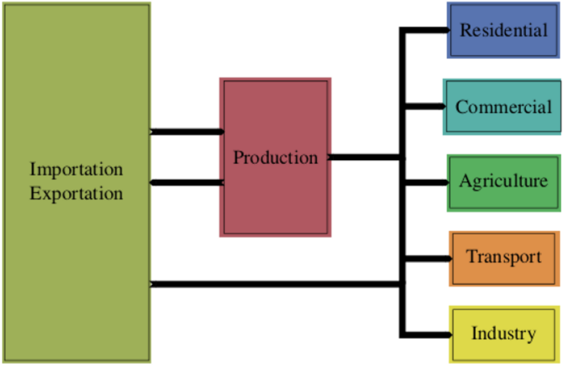
The LEAQ framework



The Luxembourg Energy Air Quality LEAQ model

ETEM Luxembourg

ETEM Luxembourg (Drouet, 2011) is a bottom-up energy model.



Refererence Energy System of Luxembourg

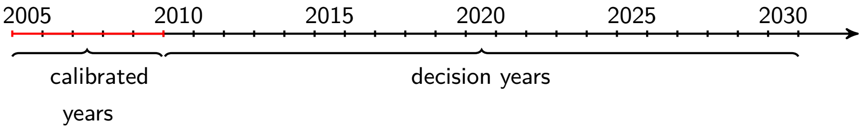
ETEM characteristics

The *Energy Techno-Economic Model* ETEM (Drouet and Thénié, 2008) has been developed to assess urban sustainable policies.

- Dynamic linear optimization model;
- Partial equilibrium;
- Driven by the demands in energy services (exogenous);
- Perfect foresight & perfect information on the time-horizon;
- Bottom-up approach (technology rich);
- Detailed description of the energy system: supply, conversion, transformation, final demands;
- Similar to the MARKAL/TIMES family of models;
- Open-source, written in GNU MathProg.

ETEM Luxembourg

- Time Horizon: 2005–2030
- Base years: 2005–2010
- Period duration: 1 year



- Existing and future generation of technologies (700)
- Energy carriers (Fossil fuels, electricity and renewables)
- GHG (CO_2, CH_4, N_2O)
- Air pollutants (NO_x, VOC)

Energy services

Sector	Energy services	Unit
Agriculture	Energy services in Agriculture	PJ
Commercial	Commercial, Institutional buildings	PJ
Industry	Chemicals	PJ
	Iron and Steel	PJ
	Non metal mineral products	PJ
	Other industries	PJ
Residential	residential cooking	PJ
	residential lighting	PJ
	residential other energy services	PJ
	residential space heating	PJ
	residential water heating	PJ
Transport	Air Transport - Energy use	PJ
	Water Navigation	PJ
	Road Transport - Buses	Mpkm
	Road Transport - Cars	Mpkm
	Road Transport - Commuters	Mpkm
	Road Transport - Light commercial trucks	Mtkm
	Road Transport - Motorcycles	Mpkm
	Road Transport - Tank tourism	Mvkm
	Road Transport - Trucks	Mtkm
	Rail transport - Goods	Mtkm
	Rail transport - Persons	Mpkm
	Road transport - Consumption abroad	PJ

ETEM Luxembourg

Category (Source)	Sector	NO_x [t]	VOC [t]
Energy Sector (ETEM)	Energy production	1 435	36
	Road Transport	10 260	1 408
	Rail Transport	278	26
	Residential Buildings	748	368
	Comm./Instit. Buildings	390	145
	Industry	2 263	24
Biogenic (AUTH)	Biogenic	—	9 053
Non-energy (EMEP)	Production processes	200	1 148
	Extraction/distribution	—	339
	Solvent use	1	3 761
	Agriculture	258	505

NO_x and VOC emissions above Luxembourg in 2006

ETEM formulation

$$\min_{\mathbf{x}}\{\mathbf{c}'\mathbf{x} \mid \mathbf{A}\mathbf{x} = \mathbf{b}, \mathbf{x} \geq 0\}$$

- Minimization of the total discounted energy cost while satisfying the demands in energy services and the structural constraints;
- Decision variables $\mathbf{x}$:
  - Activity of technologies,
  - Investments in new technology capacities,
  - Import/exports of commodities (fuels, electricity);

ETEM formulation

ETEM as a function of emission limits.

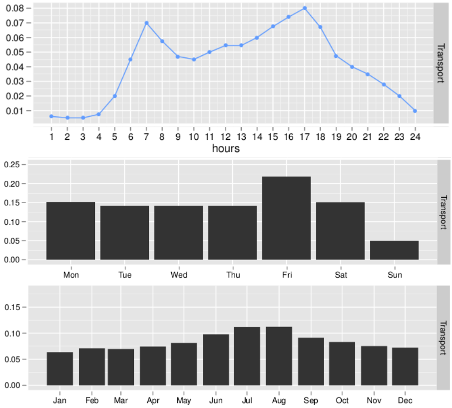
$$\gamma(\widehat{\mathbf{e}}) = \min_{\mathbf{x}}\{\mathbf{r}'\mathbf{x} \mid \mathbf{A}\mathbf{x} = \mathbf{b}, \mathbf{m}'\mathbf{x} = \mathbf{e}, \mathbf{e} \leq \widehat{\mathbf{e}}, \mathbf{x} \geq 0\}$$

- Emission levels are obtained from the technology activities and emission coefficients.
- $\widehat{\mathbf{e}}$ are annual sector emissions.

We ensure, by construction,

- the minimization has an optimal solution,
- at least one of the constraints $\mathbf{e} \leq \widehat{\mathbf{e}}$ is binding at the optimal solution.

Emission Allocation



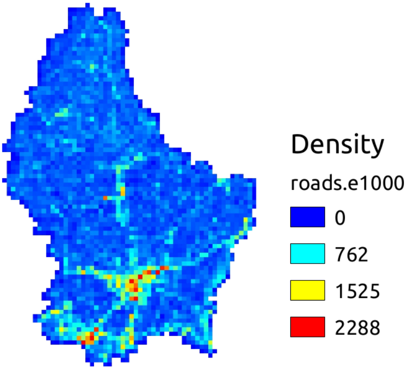
Time scheduling

Time profile functions $h_\mu(t)$

- Residential
- Transport
- Service
- Industry
- Production
- Biogenic

Main source: GENEMIS database

Emission Allocation



Downscaling

Spatial allocation functions $f_\mu(s)$

- Roads
- Rails
- Buildings residential
- Buildings services
- Industry
- Non-energy
- Biogenic

Sources: OBS land-cover, EMEP

Emission Allocation

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

where

- $\widehat{\mathbf{e}} = \hat{e}_{q,\mu}$: annual sectoral emissions ($\mathrm{t} \cdot \mathrm{yr}^{-1}$).
- $e_q(t, s)$: emissions strengths ($\mathrm{g} \cdot \mathrm{s}^{-1}$).

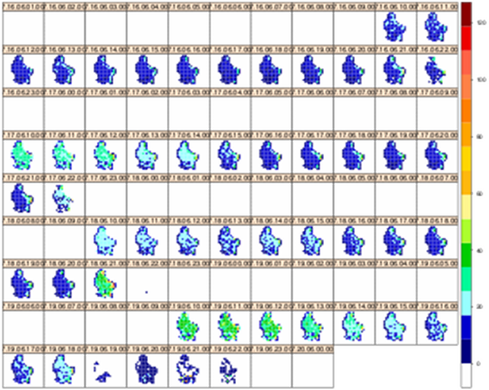
Normalizing conditions:

$$\int_s f_\mu(s) \mathrm{d}s = 1, \; \forall \mu \in \xi,$$

$$\int_0^T h_\mu(t) \mathrm{d}t = 1, \; \forall \mu \in \xi.$$

AUSTAL2000-AYLTP

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).



Ozone concentration ($\mu g/m^3$)

AUSTAL2000-AYLTP

- Lagrangian model (Markovian "random-walk")
- Advection and diffusion of pollutants
- Fast photo-chemical module (AYLTP)
- Look-up table of reaction rates
- outputs: O_3, NO_x and VOC concentrations

$$e_q(t, s) \rightarrow (c(s, t), \sigma_s(s, t)) \tag{1}$$

Air Quality Indicators

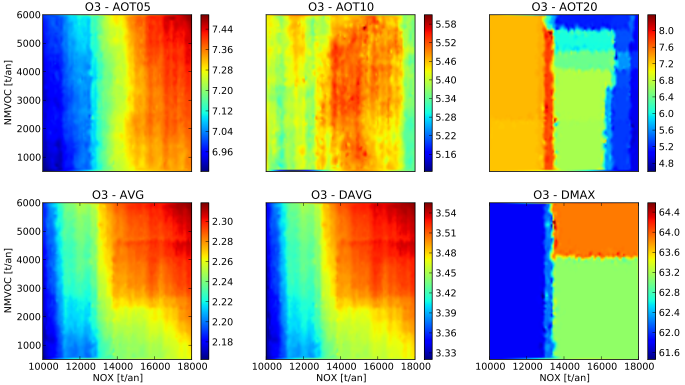
Accumulated Ozone exposure over a Threshold (AOT):
a measure of the ozone concentration exceedances over a certain threshold measured during the day (from 8:00 to 20:00)

$$E[AOT_i] = \frac{1}{|S| \cdot |t_2 - t_1|} \int_S \int_{t_1}^{t_2} \max(0, (c(s,t) - i)) \, \mathrm{d}t \mathrm{d}s,$$

$$U[AOT_i] = \frac{1}{|S| \cdot |t_2 - t_1|} \int_S \int_{t_1}^{t_2} \max(0, (c(s,t) + 1.96\sigma_c(s,t) - i)) \, \mathrm{d}t \mathrm{d}s.$$

$U[AOT_i]$ is 95% upper limit of the confidence interval

Air Quality Indicators



Value of the Air Quality Indicator as a function of annual NO_x and NMVOC emissions.

LEAQ meta-model

$$\min_{\widehat{\mathbf{e}}} \left\{ \gamma(\widehat{\mathbf{e}}) : p(\widehat{\mathbf{e}}) - \hat{p} \leq 0 \right\}, \qquad (2)$$

where

- $\hat{e}$: pollutant's annual emission bounds,
- $\gamma(\widehat{\mathbf{e}})$: energy system cost,
- $p(\widehat{\mathbf{e}})$: air quality indicator on ozone,
- $\hat{p}$: air quality indicator target,

Oracle-Based Optimization

The oracle based optimization engine OBOE is a cutting plane method which solves problem of the form:

$$\min_x \{f(x) | x \in U\},$$

where

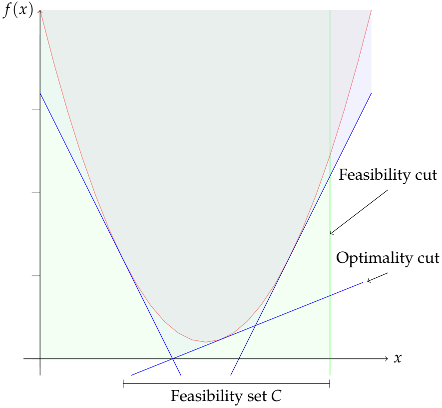
- f is a convex function,
- U is a convex set.

Babonneau et al. (2006), Proximal-ACCPM: a versatile oracle based optimization method, *Computational and Management Science*

OBOE

At each iteration, OBOE draws the problem using

- either an optimality cut to define a linear support of f, or
- or feasibility cut(s) to define an outer space of U.



OBOE definitions

Oracle

Definition 1. *A first-order oracle for problem (1) is a black box procedure with the following property. When queried at u, the oracle returns 1 or 2.*

1. *$u \notin U$ and (a, c) is such that $a^T u' - c \leq 0, \forall u' \in U$ (feasibility cut). In that case, we set $f_1(u) = +\infty$.*
2. *$u \in U$ and (a, c) is such that $a^T u' - c \leq f_1(u'), \forall u' \in U$ (optimality cut). In general, $a \in \partial f_1(u)$, $c = a^T u - f_1(u)$, but this is not necessarily so. The cut may have no intersection with the epigraph set (i.e., may be situated strictly below that set).*

(Babonneau, 2006)

Localization set

The generated cuts define a Localization set $\mathcal{L}$. The analytic center of $\mathcal{L}$ is **the next query point**.

Optimality cut

ETEM energy model

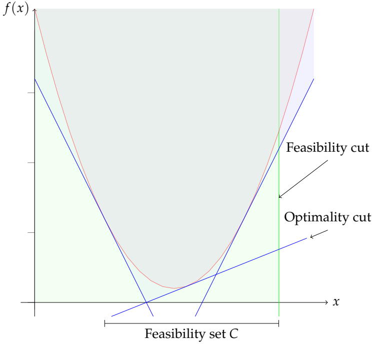
$$\gamma(\widehat{\mathbf{e}}) = \min_{\mathbf{x}} \{\mathbf{r}'\mathbf{x} \mid \mathbf{A}\mathbf{x} = \mathbf{b}, \mathbf{m}'\mathbf{x} \leq \widehat{\mathbf{e}}, \mathbf{x} \geq 0\},$$

Function value c

The optimal cost value $\gamma(\widehat{\mathbf{e}})$.

Gradient values a

The optimal dual values associated with the constraints $\mathbf{m}'\mathbf{x} \leq \widehat{\mathbf{e}}$.



Feasibility cuts

Emission allocation + AUSTAL2000-AYLTP

$$p(\widehat{\mathbf{e}}) \leq \hat{p}$$

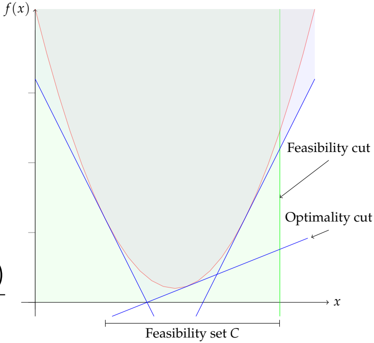
Function value c

The gap $= \mathbf{p}(\widehat{\mathbf{e}}) - \widehat{\mathbf{p}}$

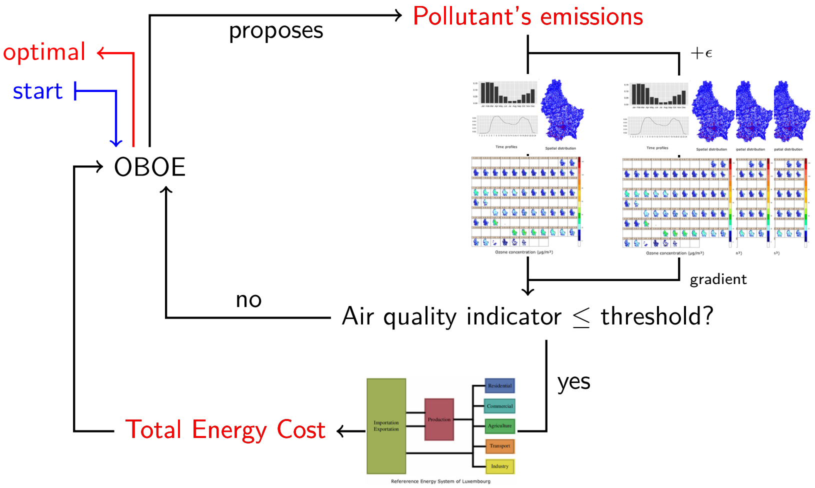
Gradient values a

Approximate by finite difference:

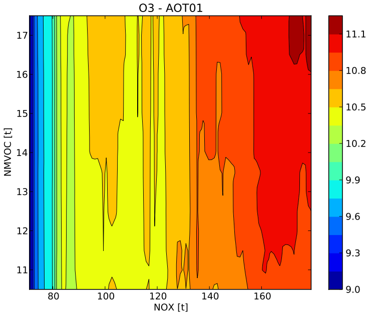
$$\nabla p(\widehat{\mathbf{e}}) = \left(\frac{\partial p(\widehat{\mathbf{e}})}{\partial \hat{e}_{q,\mu}}\right) \approx \frac{p(\widehat{\mathbf{e}} + \epsilon) - p(\widehat{\mathbf{e}})}{\epsilon}$$



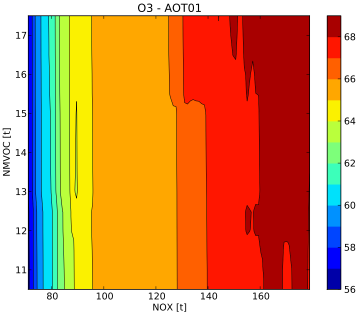
OBOE algorithm



Meteorology



observed meteorology

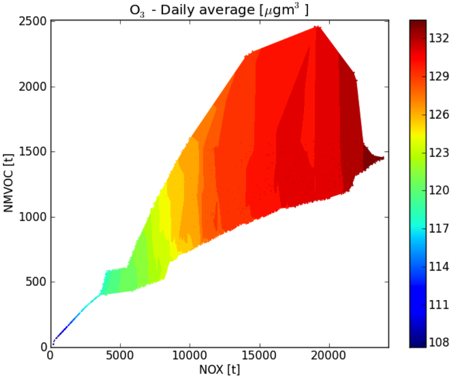


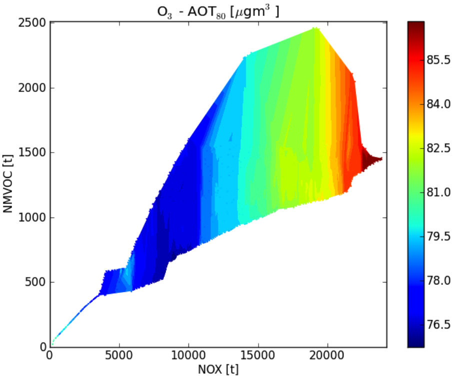
stable meteorology

AOT-indicator response surface with stable meteo:

- Low wind speed, constant wind, high air temperature.
- Smoother and closer to convexity.

Air quality policy





- NO_x and VOC emissions are interdependent in the energy model.
- The Domain is rather NO_x sensitive than VOC sensitive.

Study Case

To find optimal air pollution emission levels from Luxembourg

- to comply with drastic air quality limits after 2020
- by simulating a three-day episode (16th to 19th of July)
- with unfavorable meteorological conditions

	Coupling var.	AQI	Domain
Test 1	National NO_x	AOT_1	Luxembourg
Test 2	Sectoral NO_x	AOT_1	Luxembourg
Test 3	National NO_x	DAVG, AOT_{40}, AOT_{80}	Greater Region

Results — Performance

Time performance

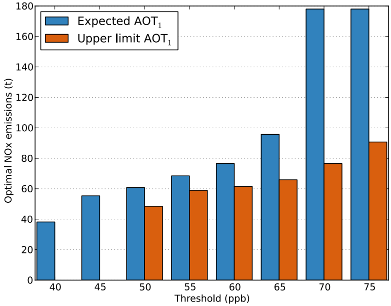
- ETEM (GAMS version): 3 min
- AQ model: 5 min to 10 min
- One iteration: 9 min to 15 min

Number of iterations

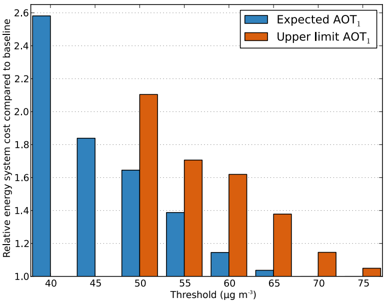
Run	Mean # iter. (Max)	Mean Resolution time
Test 1	15.75 (27)	2h20
Test 2	23 (44)	3h30
Test 3	16 (51)	4h00

Results — Test 1

Annual NO_x emissions



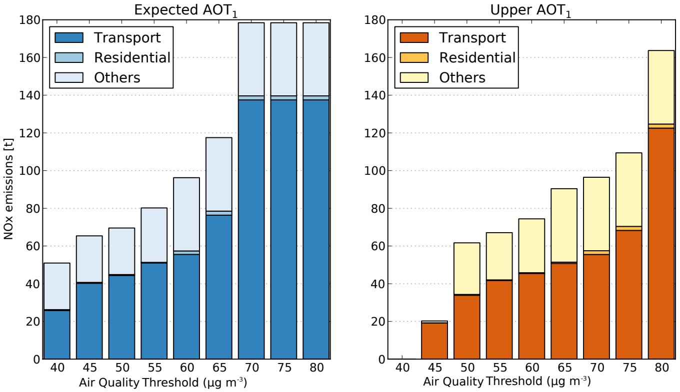
Optimal emissions vs AOT_1-indicator



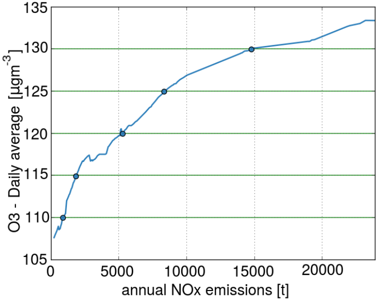
Relative cost vs AOT_1-indicator

Results - Test 2

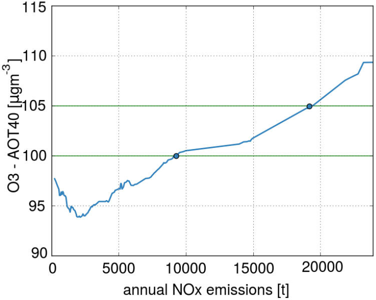
Sector NO_x emissions



Results — Test 3

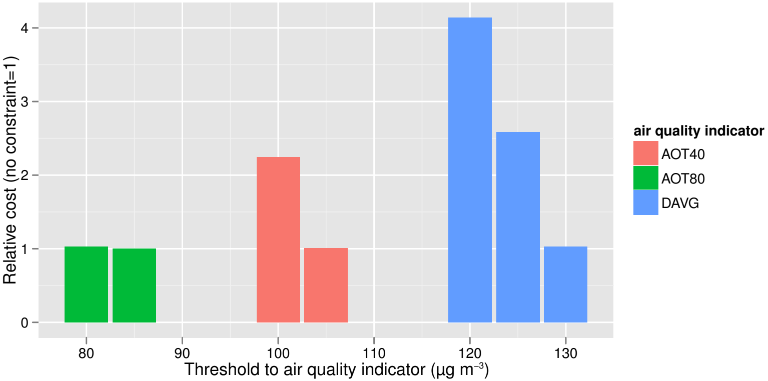


Daily average



AOT_{40}

Results — Test 3



Conclusions

- We have implemented an air quality model in the LEAQ model, in an optimization framework,
- The convexity requirement imposes non realistic meteorological scenario,
- Luxembourg energy policies are limited to control air quality
  - Dependent on neighborhood countries policies,
  - Transport sector is more responsive than others energy sectors,
  - End of pipe measures rather than cleaner technologies,
  - Non-energy sectors have an high influence on ozone level.

- Perspectives in other contexts:
  - Other city (Thessaloniki)
  - Annual AQ indicator: SOMO, PM concentrations
  - Regional, Global scale

Thank you for your attention !

Contact:

- `laurent.drouet@cmcc.it`

References I

J. Alcamo and L. Hordijk, editors. *The RAINS model of acidification: science and strategies in Europe*. Dordrecht, The Netherlands: Kluwer Academic Publishers, 1990.

M. Amann, I. Bertok, J. Borken-Kleefeld, J. Cofala, C. Heyes, L. Höglund-Isaksson, Z. Klimont, B. Nguyen, M. Posch, P. Rafaj, R. Sandler, W. Schöpp, F. Wagner, and W. Winiwarter. Cost-effective control of air quality and greenhouse gases in europe: Modeling and policy applications. *Environmental Modelling & Software*, 26(12):1489–1501, 2011.

H. ApSimon, R. Warren, and J. Wilson. The abatement strategies assessment model: Applications to reductions of SO_2 emissions in europe. *Atmospheric Environment*, 24(4):649–663, 1994.

T. Barker, A. Anger, O. Dessens, H. Pollitt, H. Rogers, S. Scrieciu, R. Jones, and J. Pyle. Integrated modelling of climate control and air pollution: Methodology and results from one-way coupling of an energy–environment–economy (e3mg) and atmospheric chemistry model (p-tomcat) in decarbonising scenarios for mexico to 2050. *Environmental Science & Policy*, 13(8):661–670, December 2010.

References II

R. Borge, V. Alexandrov, J. J. del Vas, J. Lumbreras, and E. Rodriguez. A comprehensive sensitivity analysis of the wrf model for air quality applications over the iberian peninsula. *Atmospheric Environment*, 42(37): 8560–5874, December 2008.

D. A. Carlson, A. Haurie, J. P. Vial, and D. S. Zachary. Large scale convex optimizationmethods forair quality policy assessment. *Automatica*, 40(3): 385–395, March 2004.

C. Carnevale, E. Pisoni, and M. Volta. A multi-objective nonlinear optimization approach to designing effective air quality control policies. *Automatica*, 44: 1632—1641, 2008.

C. Carnevale, G. Finzi, E. Pisoni, M. Volta, et al. An integrated assessment tool to define effective air quality policies at regional scales. *Environmental Modelling & Software*, 38:306—3015, 2012.

I. D'Elia, M. Bencardino, L. Ciancarella, M. Contaldi, and G. Vialetto. Technical and non-technical measures for air pollution emission reduction: The integrated assessment of the regional air quality management plans through the italian national model. *Atmospheric Environment*, 43: 6182–6189, 2009.

References III

EC4MACS. Life iii ec4macs european consortium for modelling of air pollution and climate strategies. Technical report, International Institute for and Applied Systems Analysis, June 2007.

D. E. James, J. A. Chambers, J. D. Kalma, and H. A. Bridgman. Air quality prediction in urban and semi-urban regions with generalised input-output analysis: The hunter region, australia. *Urban Ecology*, 9:25–44, 1985.

M. T. Odman, J. W. Boylan, J. G. Wilkinson, A. G. Russell, Mueller S. F., R. E. Imhoff, K. G. Doty, W. B. Norris, and R. T. McNider. SAMI air quality modeling, final report. Technical report, School of Civil and Environmental Engineering Georgia Institute of Technology, 2002.

T. Oxley, A. Valiantis, M.and Elshkaki, and H. M. ApSimon. Background, road and urban transport modelling of air quality limit values (the BRUTAL model). *Environmental Modelling & Software*, 24(9):1036–1050, September 2009.

S. Rao, V. Chirkov, F. Dentener, R. Van Dingenen, S. Pachauri, Purohit. P., M. Amann, C. Heyes, P. Kinney, P. Kolp, Z. Klimont, K. Riahi, and W. Schoepp. Environmental modeling and methods for estimation of the global health impacts of air pollution. *Environ Model Assess*, 2012. on-line.

D. S. Zachary, L. Drouet, U. Leopold, and L. Aleluia Reis. Trade-offs between energy cost and health impact in a regional coupled energy-air quality model: the LEAQ model. *Environmental Research Letters*, 6(2):024021, 2011.