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

The Luxembourg Energy Air Quality model

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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

<table>
<thead>
<tr>
<th>Name</th>
<th>Emission model</th>
<th>Air quality model</th>
<th>Reference</th>
</tr>
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<tbody>
<tr>
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<td>RAINS</td>
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<td><strong>GENEVA</strong></td>
<td>MARKAL-lite</td>
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<td>Oxley et al. (2009)</td>
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<td><strong>LEAQ</strong></td>
<td>ETEM</td>
<td>TAPOM-lite</td>
<td>Zachary et al. (2011)</td>
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</tbody>
</table>

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 ($\text{NO}_x$ 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

- Domain: \( \approx 50\text{km} \times 80\text{km} \)
- 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.

Source: ACT, Luxembourg
The Luxembourg Energy Air Quality (LEAQ) model

The LEAQ framework

Annual emissions

OBOE optimizer

Emission Allocator

Emissions abatements

Energy cost

ETEM Luxembourg energy model

AUSTAL2000-AYLTP air quality model

AQ indicator

Emissions strengths

The Luxembourg Energy Air Quality LEAQ model
ETEM Luxembourg (Drouet, 2011) is a bottom-up energy model.
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

2005 2010 2015 2020 2025 2030

- calibrated years
- decision years

- Existing and future generation of technologies (700)
- Energy carriers (Fossil fuels, electricity and renewables)
- GHG (CO$_2$, CH$_4$, N$_2$O)
- Air pollutants (NO$_x$, VOC)
### Energy services

<table>
<thead>
<tr>
<th>Sector</th>
<th>Energy services</th>
<th>Unit</th>
</tr>
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<tbody>
<tr>
<td>Agriculture</td>
<td>Energy services in Agriculture</td>
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<tr>
<td>Commercial</td>
<td>Commercial, Institutional buildings</td>
<td>PJ</td>
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<td>Chemicals</td>
<td>PJ</td>
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<td>Iron and Steel</td>
<td>PJ</td>
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<td></td>
<td>Non metal mineral products</td>
<td>PJ</td>
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<tr>
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<td>Other industries</td>
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<td>PJ</td>
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<td></td>
<td>residential lighting</td>
<td>PJ</td>
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<td></td>
<td>residential other energy services</td>
<td>PJ</td>
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<td>PJ</td>
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<td></td>
<td>residential water heating</td>
<td>PJ</td>
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<td><strong>Road transport - Consumption abroad</strong></td>
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<td>Category (Source)</td>
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<td>NO&lt;sub&gt;x&lt;/sub&gt; [t]</td>
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<td>Agriculture</td>
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</tbody>
</table>

NO<sub>x</sub> and VOC emissions above Luxembourg in 2006
ETEM formulation

\[
\min_{x} \{ c'x \mid Ax = b, x \geq 0 \}
\]

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

ETEM as a function of emission limits.

$$\gamma(\hat{e}) = \min_x \{ r'x \mid Ax = b, m'x = e, e \leq \hat{e}, x \geq 0 \}$$

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

We ensure, by construction,

- the minimization has an optimal solution,
- at least one of the constraints $e \leq \hat{e}$ 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

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

Normalizing conditions:

\[ \int_s f_\mu(s)ds = 1, \forall \mu \in \xi, \]

\[ \int_0^T h_\mu(t)dt = 1, \forall \mu \in \xi. \]
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).
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

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

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

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

\[U[AOT_i]\] is 95% upper limit of the confidence interval
Value of the Air Quality Indicator as a function of annual NO$_{x}$ and NMVOC emissions.
min \{ \gamma(\hat{e}) : p(\hat{e}) - \hat{p} \leq 0 \}, \quad (2)

where

- \hat{e}: pollutant’s annual emission bounds,
- \gamma(\hat{e}): energy system cost,
- p(\hat{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*
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

\[ \gamma(\hat{e}) = \min_x \{ r'x \mid Ax = b, m'x \leq \hat{e}, x \geq 0 \}, \]

Function value \( c \)

The optimal cost value \( \gamma(\hat{e}) \).

Gradient values \( a \)

The optimal dual values associated with the constraints \( m'x \leq \hat{e} \).
Feasibility cuts

Emission allocation + AUSTAL2000-AYLTP

\[ p(\hat{e}) \leq \hat{p} \]

Function value \( c \)

The gap = \( p(\hat{e}) - \hat{p} \)

Gradient values \( a \)

Approximate by finite difference:

\[ \nabla p(\hat{e}) = \left( \frac{\partial p(\hat{e})}{\partial \hat{e}_q, \mu} \right) \approx \frac{p(\hat{e} + \epsilon) - p(\hat{e})}{\epsilon} \]
OBOE algorithm

optimal

start

OBOE

proposes

Pollutant’s emissions

+ \epsilon

Air quality indicator \leq\text{ threshold}?

no

Total Energy Cost

yes

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AOT-indicator response surface with stable meteo:

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

- NO\textsubscript{X} and VOC emissions are interdependent in the energy model.
- The Domain is rather NO\textsubscript{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

<table>
<thead>
<tr>
<th>Coupling var.</th>
<th>AQI</th>
<th>Domain</th>
</tr>
</thead>
<tbody>
<tr>
<td>Test 1 National NO\textsubscript{X}</td>
<td>AOT\textsubscript{1}</td>
<td>Luxembourg</td>
</tr>
<tr>
<td>Test 2 Sectoral NO\textsubscript{X}</td>
<td>AOT\textsubscript{1}</td>
<td>Luxembourg</td>
</tr>
<tr>
<td>Test 3 National NO\textsubscript{X}</td>
<td>DAVG, AOT\textsubscript{40}, AOT\textsubscript{80}</td>
<td>Greater Region</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Run</th>
<th>Mean # iter. (Max)</th>
<th>Mean Resolution time</th>
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</thead>
<tbody>
<tr>
<td>Test 1</td>
<td>15.75 (27)</td>
<td>2h20</td>
</tr>
<tr>
<td>Test 2</td>
<td>23 (44)</td>
<td>3h30</td>
</tr>
<tr>
<td>Test 3</td>
<td>16 (51)</td>
<td>4h00</td>
</tr>
</tbody>
</table>
Results — Test 1

Annual NO\textsubscript{x} emissions

Optimal emissions vs AOT\textsubscript{1}-indicator

Relative cost vs AOT\textsubscript{1}-indicator
Results - Test 2

Sector NO\textsubscript{x} emissions

![Graph showing expected and upper AOT\textsubscript{1} for different air quality thresholds for different sectors.]

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Implementation of a Full Air Quality Model in an Integrated Assessment Model
Results — Test 3

Daily average

AOT$_{40}$
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!

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