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Modelling Spatial Uncertainties associated with Emission Disaggregation in an integrated Energy Air Quality Assessment Model

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Abstract: This paper presents a methodology to model spatial uncertainties associated to the disaggregation of sectoral emission allocation in Luxembourg. We apply it to the integrated Luxembourg Energy Air Quality assessment model for the urban and regional scale. National aggregated sectoral emissions of primary air pollutants are computed by an energy model which minimises the cost of the reference energy system. The model describes five sectors, i.e. agriculture, transport, industry, residential and commercial at five-year periods. The sectoral emissions are spatially allocated to obtain hourly to daily emission maps. The air quality model simulates the dispersion of the emitted pollutants and their chemical reactions to produce ozone for typical episodes for each five-year period. Both models are coupled by an Oracle Based Optimisation Engine (OBOE) to find the optimal energy system with a constraint on ozone concentrations. When disaggregating emissions from the national to the urban scale, small scale variation and its associated uncertainty within and across land-use boundaries have to be modelled to obtain realistic emission maps. We propose to decompose the emission value for each sector into its mean, standard deviation and spatially correlated Gaussian distributed error with zero mean and unit variance. The spatial error is modelled by spatial stochastic simulation assuming a semivariogram with local and regional scale variability to account for within-boundary and across-boundary variation. A Monte Carlo approach is used to simulate the spatially correlated error and its distribution at each grid cell of the emission map. Finally, the average disaggregated emission value and its corresponding local uncertainty can be computed for each grid cell accounting for spatial correlation at different scales and across land-use boundaries. Once uncertainties are assessed, the disaggregated emissions and its associated uncertainties can be propagated through the air-quality model for policy assessment under uncertainties.

Keywords: Spatial uncertainty; change-of-support; disaggregation; downscaling; spatial emission allocation

1 INTRODUCTION

Emissions originating from energy modelling are typically computed at the national scale to match the overall energy balance for a country including the import and export of energy supply. Attempts are currently being made to compute energy demand and sup-
ply spatially distributed to get a better idea about local emissions of air pollutants [Hat- 
zopoulou and Miller, 2010; Zachary et al., 2011]. Therefore, disaggregation methodolo- 
gies have been increasingly developed to allocate and distribute the modelled emissions 
of air pollutants in space and time. Geographic Information systems are often used to 
distribute emissions spatially. When disaggregating averaged values or sums, errors are 
often introduced due to the change of scale. These errors are usually not accounted for.

In this paper we propose a methodology to assign spatial uncertainties to emission values 
when allocating their average values in space. As a test case we use the emission 
computation for air pollutants originating from the various sources of energy. The energy 
model, ETEM, is coupled to an air quality model, AUSTAL2000-AYLTP, and computes air 
pollutant emissions for various sectors, such as residential, industrial, agricultural and 
transport at the national scale of Luxembourg (Fig. 1). The allocation of emissions is 
done by assigning an averaged value to the corresponding sector value on the map.

![Figure 1: Overview of the Luxembourg Energy Air Quality model for decision support. The data base links in the background to all LEAQ sub-models.](image)

2 METHODS

2.1 Emission allocation in the LEAQ model

National aggregated sectoral emissions of primary air pollutants are computed by the 
energy model ETEM [Drouet and Thénié, 2009] which minimises the cost of the reference 
energy system. The model describes five sectors, i.e. agriculture, transport, industry, 
residential and commercial at five-year periods. The sectoral emissions are spatially 
allocated to obtain hourly to daily emission maps. The air quality model, AUSTAL2000-
AYLTP, simulates the dispersion of the emitted pollutants and their chemical reactions to 
produce ozone for typical episodes for each five-year period [Aleluia Reis et al., 2009]. 
Both models are coupled by means of an Oracle Based Optimisation Engine (OBOE) to 
find the optimal energy system with a constraint on ozone concentrations.

1https://projects.coin-or.org/OBOE
Fig. 2 shows the different steps taken in the LEAQ model to disaggregate and allocate the emissions on the spatial grid.

![Diagram](Image)

**Figure 2: LEAQ aggregation and disaggregation.**

Figure 3 shows the different sectors in Luxembourg corresponding to the sectorial computations in ETEM. Average CO$_2$ emissions were computed with ETEM from the overall energy balance for Luxembourg and allocated to the spatial grid according to the initial ETEM allocation program. The emission values within a sector do not vary and represent averaged values.

![Maps](Image)

**Figure 3: Spatial distribution of landuse sectors in Luxembourg (left), the associated average CO$_2$ emissions [kt/y] (right).**
2.2 Spatial disaggregation accounting for uncertainty

In order to improve the spatial disaggregation and add more realistic variability, we decomposed the emission value $e(x_i)$ at each grid cell into its mean $\mu_e$, standard deviation $\sigma_e$ and spatially correlated Gaussian distributed error $\epsilon_e$ with zero mean and unit variance (see equations 1 and 2).

\begin{equation}
 e(x_i) = \mu_e + \sigma_e \epsilon_e(x_i)
\end{equation}

where $\sigma_e$ is computed from a constant fraction $\alpha \times \mu_e$ for each sector and grid cell.

\begin{equation}
 e(x_i) = \mu_e + \gamma \epsilon_e(x_i)
\end{equation}

The spatial error was modelled by spatial stochastic simulation assuming a semi-variogram with short (100m), medium (1km) and larger scale (5km) variability to account for within-boundary and across-boundary variation of the different sectors.

A Monte Carlo approach implemented in the Gstat software Pebesma and Wesseling, 1998 was used to simulate the spatially correlated error and its distribution at each grid cell of the emission map. Finally, the average disaggregated emission value and its corresponding “local” uncertainty was computed for each grid cell to account for spatial correlation at different scales and across land-use boundaries.

The results were retrieved following the steps below to model the uncertainty associated to the emission disaggregation:

1. Compute the global emission value for each sector using ETEM.
2. Distribute the global mean emission value across sector grid.
3. Compute the global standard deviation by determining the variation coefficient $\alpha$ per sector and allocate to each grid cell.
4. Infer the spatial variogram model from expert knowledge to model spatial correlated error. National count statistics from measuring stations across Luxembourg were analysed as well as the spatial distribution of land use sectors (3) inferred to estimate the parameters shape, nugget, range and the partial sills.
5. Generate realisations for local error using unconditional sequential Gaussian block simulation based on the assumed mean and semivariogram model.
6. Compute local standard deviation from local error and global standard deviation.
7. Compute local emissions from global mean and local standard deviation.
8. Compute statistics, i.e. mean, standard deviation, confidence intervals.

3 RESULTS AND DISCUSSION

The first important parameter to infer was the variation coefficient $\alpha$ from eq. 1. Table 1 shows the values determined for $\alpha$. These values were based on expert knowledge and national statistics. The most influential sectors are traffic with short (0.5) and medium
Table 1: Variation coefficients for $\alpha$ derived from expert knowledge and national statistics.

<table>
<thead>
<tr>
<th>Sector</th>
<th>$\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Residential</td>
<td>0.6</td>
</tr>
<tr>
<td>Industrial</td>
<td>0.5</td>
</tr>
<tr>
<td>Agriculture</td>
<td>0.1</td>
</tr>
<tr>
<td>Forest</td>
<td>0.1</td>
</tr>
<tr>
<td>Motorways</td>
<td>0.1</td>
</tr>
<tr>
<td>National roads</td>
<td>0.3</td>
</tr>
<tr>
<td>Municipal roads</td>
<td>0.5</td>
</tr>
</tbody>
</table>

(0.3) scale variation as well as industry (0.5) and residential (0.6) with a larger scale variation.

The final nested semivariogram model to compute the spatially correlated error had the following structures and parameters:

$$
\gamma_c(h) = \gamma_{c1} + \gamma_{c2} + \gamma_{c3} \tag{3}
$$

$$
\gamma_{c1} := \{n = 0.1, s_1 = 0.3, r_1 = 100, m = \text{Exp}\} \tag{4}
$$

$$
\gamma_{c2} := \{s_2 = 0.3, r_2 = 1000, m = \text{Sph}\} \tag{5}
$$

$$
\gamma_{c3} := \{s_3 = 0.2, r_3 = 5000, m = \text{Sph}\} \tag{6}
$$

where $\gamma$ is the semivariance, $n$ the nugget, $s$ the partial sill, $r$ the range and $\text{Exp}$ and $\text{Sph}$ the exponential and the spherical shape of the semivariogram model. All parameters were derived from expert knowledge and spatial analysis of the land use patterns across the Luxembourg map.

The distribution of the spatially correlated error using the above semivariogram and stochastic Gaussian simulation is shown in Fig.4. It is shown for simulation number 1 (top left). We can clearly see the different spatial patterns reproduced from the semivariogram.

The spatially correlated error was used to derive the total emission map for simulation 1 and 4 by adding the spatially correlated error to the average emission map from Fig. 3. Both maps are also shown in Fig. 4. The map at the bottom right shows the difference between simulation 1 and 4 and shows slight differences in the spatial allocation but respecting the overall spatial patterns.

The presented methodology enables us to model spatial uncertainties. Due to the unconditional simulation we are not able to reproduce areas with high emissions and hot spots always accurately and at the locations where they occur, such as urban areas with high population density. The incorporation of a trend surface derived from population density into a universal Gaussian simulation approach, such as used in universal kriging, could improve areas with typically high emissions [Leopold et al., 2006].

Assumptions for variation coefficient $\alpha$ and semivariogram model $\gamma$ obviously strongly influence results and would need further investigation to verify whether the assumed structures are correct and where they might be improved. The semivariogram model is very uncertain and could be improved by further analysis of the different land use patterns for each of the different sectors. A validation with emission observations, experts and further analysis of land use/sector patterns would help to improve the semivariogram.
model.

In order to account also for occurring hot spots when disaggregating emission values population and other land use related information could as be incorporated as a trend.
This would enable us to improve the variation at e.g. dense populated or industrial areas.

4 Conclusion

The underlying assumptions, influence the results of the disaggregation approach and associated uncertainties. Incorporating the population density and more accurate information on heavy industries in the dis-aggregation approach could help to better locate hot spots and areas of high primary emissions. Nevertheless, this approach takes the modelling of primary pollutants a step further and allows accounting for uncertainties locally. These uncertainties are important when applied to spatial planning and health impact studies. Once the uncertainties are assessed, the disaggregated emissions and its associated uncertainties can be incorporated in an uncertainty propagation analysis of the air-quality model or a stochastic version of the energy optimisation algorithm.

Further work on semivariogram inference is needed. Maybe a Bayesian approach to estimate and include uncertainty of semivariogram parameters would be appropriate. Furthermore, other distributions for the spatially correlated error could be tested: 1) Explore land use/sector semivariance to determine the ranges; 2) Incorporate population or other explanatory variables as trend. 1) Extend the approach to a spatial-temporal correlated error to model hourly and daily uncertainties.

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References


