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Sensitivity Analysis of the SHERPA Air Quality Model

Reliability evaluation & Key variables assessment

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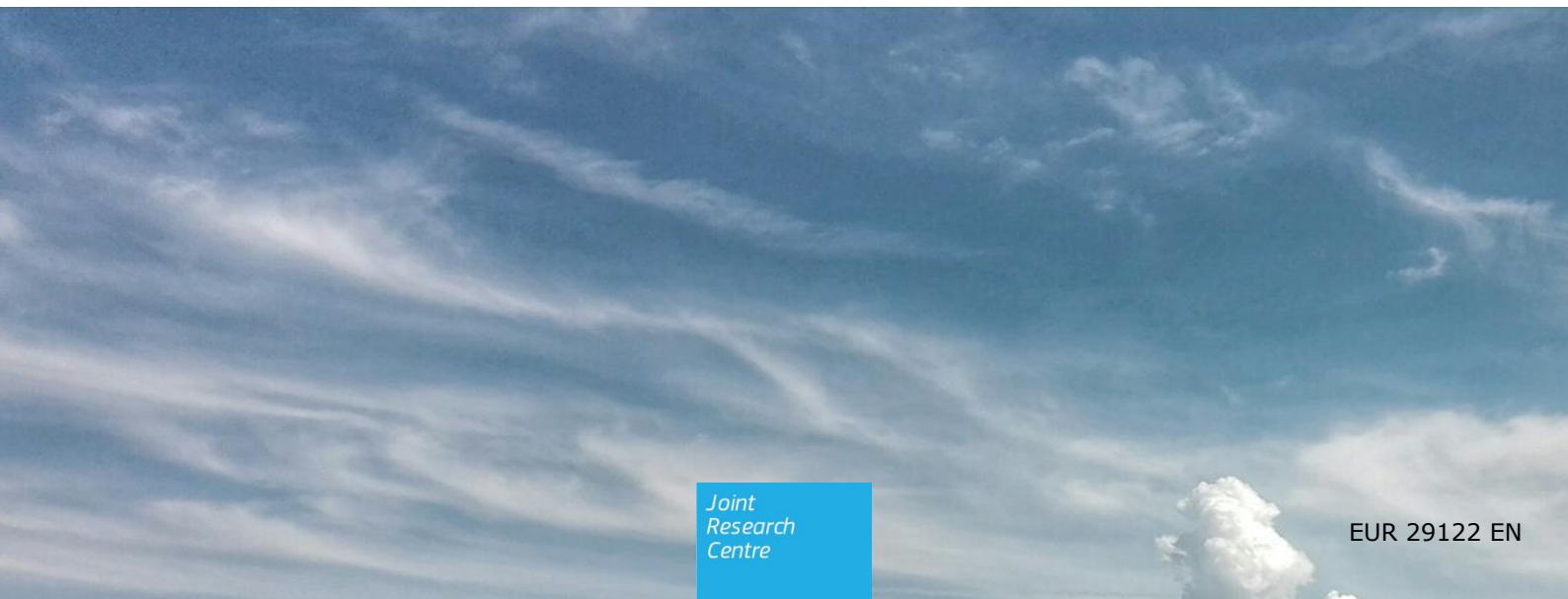

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Abstract

Uncertainty and sensitivity analysis was conducted on the SHERPA model, predicting air quality improvement linked to emission reduction scenarios. Major responsible of output uncertainty (PM2.5 concentration reductions in g/m3) stems from the uncertainty in the policy options followed by the uncertainty in the emissions (kTon/year) of PPM, NOX, and NH3.

Foreword

This deliverable was carried out under the umbrella of the European Commission Competence Centre on Modelling.

The Competence Centre on Modelling promotes a transparent, coherent and responsible use of modelling to underpin the evidence base for EU policies. It leverages the modelling capacity and competences across the Commission and beyond. Starting with the Commission-wide modelling inventory MIDAS, it supports a proper documentation, use, and reuse of models. It further helps identifying common approaches to quality and transparency of model use, and establishes a Community of Practice on Modelling.

Within the Competence Centre on Modelling, the Sensitivity Analysis of Model Output (SAMO) team has the mission to carry out uncertainty and sensitivity analyses of EC workhorse models, to conduct research in this field, to provide tools, training and ad hoc scientific support to model users in order to enhance the robustness of model-based evidences in the European Commission.
For more information on the Competence Centre please visit https://ec.europa.eu/jrc/en/modelling.

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Executive summary

In the report, an uncertainty case-study has been carried out on one of the key SHERPA (Screening for High Emission Reduction Potential on Air) model modules, forecasting air quality improvement (measured as reduction in concentrations in PM2.5 yearly average) related to emission reduction scenarios. Thirteen main sources of uncertainty in model inputs were investigated including policy options for reducing air pollution. Ten European cities (Berlin, Brussels, Bucharest, Helsinki, Constanţa, London, Madrid, Milan, Paris, and Utrecht) - representative of different meteorological and emission inventory conditions in Europe - have been chosen for the uncertainty (UA) and sensitivity analysis (SA) exercise.

Policy context

The SHERPA model has been developed as a tool to support regional/local decision makers to design air quality plans. The issue of air quality in Europe calls for novel policy approaches to support air quality management at the local level, and reinforce the EU-wide existing policies. SHERPA rapidly turned out to be a valuable instrument for evidence-based policy. Given the high stake, and the fact that uncertainty 'could change the ranking and conclusions about the policy options' (EC Better Regulation Toolbox #62 (2017))[1], an uncertainty analysis (UA) and a sensitivity analysis (SA) of a key SHERPA model module were conducted.

Key conclusions

In almost all cities, according to the model forecasts, the first action should be for the policy makers to discuss upon the best policy to implement. Afterwards the discussion could move on to how to reduce the uncertainty on the model emissions, in particular the emissions of primary particulate matter (PPM), nitrogen oxides (NO_X), and ammonia (NH_3).

Main findings

It was found that, for eight cities out of ten, the policy option uncertainty is the most responsible of the uncertainty in PM2.5 concentration reductions. Among the other inputs, the uncertainty on the emissions is by far the most influential ones, in particular the emissions of PPM, NO_X, and NH_3.

Related and future JRC work

JRC.I1 and JRC.C5 are foreseeing to extend the sensitivity analysis to the entire European space domain, so to create extended maps of uncertainty and sensitivity (in the present work, the focus was on specific cities – grid cells). In addition, as new versions of SHERPA will also include specific measures to abate emissions, one option would be to test how SHERPA uncertainties will affect the selection of abatement measures and their impact.

Quick guide

The report is structured in three main parts:

- Description of the SHERPA module;
- Description of the methodology to perform sensitivity and uncertainty analysis;
- Analysis of the results and discussion.

Annex 1 contains the profiles of the investigated cities.
Annex 2 illustrates the Web-App for sensitivity analysis developed by the JRC.I1 Unit.

[1] Brussels, 07/07/2017 - SWD(2017) 350 final

1 Introduction

In recent decades, Europe has significantly enhanced air quality (EEA, 2016). Nevertheless, alert limits are still detected for pollutants as ozone (O_3), nitrogen dioxide (NO2) and particulate matter (PM10 and PM2.5[2]). While in the past years, these exceedances were wide-spread across Europe, they now tend to concentrate mainly in hot-spots at regional and city level (Kiesewetter et al., 2015). Consequently, this new scale of the air quality issue (from "Europe-wide" to "local" exceedances) requires innovative approaches targeted to the regional air quality management, to integrate and reinforce the current EU-wide policy. In this frame, air quality models have been used, traditionally, to support the design of air quality policies. Various techniques are available for this purpose.

A first set of techniques is based on three dimensional numerical models that simulate transport, chemistry, emissions, and deposition in the atmosphere (Mailler et. al., 2016, Pernigotti et al., 2013). These models are very complex and computationally demanding (in terms of data preparation, scientific/technical knowledge and computing power) and in some cases are not fit-for-purpose (i.e. in the "science-to-policy" interface, when model should be ideally used in an interactive mode, to analyse the impact of alternative scenarios).

A second set of techniques is the so-called 'Integrated Assessment Models', which have been implemented mainly to deal with the 'science-to-policy' interface. These models are able to include various dimensions such as air quality, policy costs, benefits, etc… in a unique frame. The GAINS-EU integrated assessment model (Amann et al., 2011) has been routinely applied to select optimal country-based emission reductions, in order to achieve environmental improvements at minimum cost. In the last years, the EU integrated assessment modelling application has been complemented by regional and local approaches. This has been done with, e.g., national versions of GAINS based on finer scale modelling (as in GAINS-Italy, d'Elia et al, 2009), or with regional tools (e.g. RIAT, the Regional Integrated Assessment Tool, Carnevale et al., 2012, Pisoni et al., 2010). Unfortunately, also these tools are quite complex to be applied, mainly at regional/local scale, as they also require local data and/or a high scientific/technical know-how to be run.

To face this new challenge (i.e., addressing in a comprehensive way the air quality policy design issue at regional/local scale) the SHERPA (Screening for High Emission Reduction Potential on Air) modelling tool has been recently developed (Clappier et al., 2015, Thunis et al., 2016, Pisoni et al., 2017). Indeed, SHERPA aims at supporting regional/local decision makers in designing air quality plans, and - more in general – at contributing to the evaluation of the impact on air quality of locally-tailored policies. SHERPA is a Java/Python meta-model running on a desktop PC, able to replicate the outcomes of more complex physically-based models in a faster and resources saving way.

SHERPA is user-friendly, and does not require any preliminary complex scientific/technical tasks. Data covering the whole Europe are provided, but specific regions can be selected by the users. In addition, to decision-makers who need to plan air quality policies, SHERPA gives the possibility of implementing issues such as "source allocation" (to apportion air pollution in terms of sectors and precursors of origin); "governance" (to identify the key geographical entities contributing to the pollution in one specific area); "scenario" (to test the effect on air quality of a given sector-specific emission abatement scenario).

As the SHERPA model is used in the policy arena, it is crucial to evaluate (and guarantee) the robustness of the model responses to different sources of uncertainty. It is recommended that model output uncertainties be taken into account in the policy context - uncertainty that, as stressed in the EC Better Regulation Toolbox #62 (2017), '*could*

[2] PM: inhalable particles, with diameters that are 10 or 2.5 micrometers.

change the ranking and conclusions about the policy options'. For this purpose, uncertainty analysis (UA) and sensitivity analysis (SA) are valuable and suited techniques

Models may be considered "fit for purpose", when the uncertainty of the model output, is acceptable. In the modelling process, the uncertainty analysis aims at quantifying uncertainty in the model output, and sensitivity analysis investigates the dependency of the model output from different sources of uncertainty in the model inputs. These two types of analyses are complementary with the uncertainty analysis ideally preceding the sensitivity analysis (Saltelli et al., 2008).

Uncertainty and sensitivity analysis also assess whether alternative assumptions would lead to significantly different results.

Sensitivity analysis identifies and ranks by their influence the uncertain responsible factors (variables, assumptions, …) at play. Obviously, the most influential factors must be known with the maximum accuracy while the less influential ones can sometimes be ignored for model simplification sake.

Sensitivity analysis also reveals the possible interactions among the inputs. It can highlight unexpected relationships between inputs and outputs, and helps identifying regions of the input space that are responsible for critical values of the output.

An important point is that sensitivity analysis only refers to the model logical consistency and not to its veracity. It is an iterative process and the modellers must constantly engage with the sensitivity analysis practitioners (the analyst), so as to better interpret the results of the UA and the SA, and link them to concrete meanings in the real world.

Both uncertainty analysis and sensitivity analysis have been applied to the SHERPA 'scenario' module (Thunis et al., 2016). This module estimates the changes in pollutant concentrations for a given pollutant emission reduction scenario, and it is the core of the SHERPA model. Therefore, testing it appeared to be of first priority. To encompass model inputs (including coefficients) spatial variation, a number of selected European cities - showing different meteorological and emission inventory conditions - have been chosen for the SA exercise.

The UA-SA analyses focus on three main issues: (1) what is the level of uncertainty associated to the SHERPA outcomes (uncertainty analysis), (2) which model inputs - parameters, precursors, and policy choices – drive the uncertainty (sensitivity analysis) (3) how SA can help the policy/decision making. Finally, the consequences of the analyses for policy/decision-making have been spotted and discussed.

In this study, global sensitivity analysis (GSA) has been carried out using the popular Sobol' sensitivity indices whose values were obtained by the variance based (VB) method and by the Polynomial Chaos Expansion (PCE) method (Sudret, 2008). For this purpose, we use the Web-App for sensitivity analysis of model output recently developed by Unit JRC.I1 and described in Appendix 2. Both methods provided similar results.

The results confirm the relevance of the policy option impact, and help identifying how and where to prioritise further model improvements and model users' actions in an effective way.

2 The SHERPA tool

SHERPA (Screening for High Emission Reduction Potentials for Air quality) is a modelling tool for studying alternative solutions to reduce the air pollution in a given region in Europe. SHERPA relies on the following steps:

- Source allocation: this step aims to assess the degree of control policymakers have on air pollution over their area. If most of the pollution is imported from outside their region, the policy makers have little control (and vice-versa). During this step, SHERPA provides information on (a) the amount of pollution originating from inside the region, detailed in terms of sectors and precursors and (b) the amount of pollution originating from outside the region.
- Governance: this step identifies the principal source areas (i.e. regions, countries) of the pollution at a location. Emissions from agriculture which require time to form secondary particulate matter will have a longer distance influence than traffic emissions that directly impact concentrations at the local scale. The SHERPA methodology is designed to identify and rank contributions (to air pollution levels) by all neighbouring and non-neighbouring regions for a specific sector of activity. This step sets the basis for fixing priorities in terms of regional collaborations that can increase the efficiency of abatement strategies.
- Scenario: the scenario analysis is the final stage in the process, once the activity sectors and their areas of origin have been identified. The policymaker then fixes the desired sector-specific emission abatements in terms of intensity and spatial coverage and tests their impacts on air quality levels.

These three steps form the core of the SHERPA methodology. They are depicted in the next figure:

Figure 1 Schematic overview of the three steps methodological approach used in SHERPA. After the "source allocation", "governance" and "scenario" steps, impacts are computed. Details are provided in the text.

This sensitivity analysis has been applied to the SHERPA 'scenario' module, which represents the core of the modelling tool, and is also a basis for the other SHERPA modules (i.e. 'source allocation' and 'governance').

2.1 The SHERPA Source/receptor relationship

2.1.1 Methodology

Air quality models are the starting point to develop the source-receptor relationships.

Air quality models use mathematical and numerical techniques to simulate the physical and chemical processes that affect air pollutants. Based on inputs of meteorological data and emissions, these models are designed to characterize both primary pollutants (that are emitted directly into the atmosphere) and secondary pollutants (that are formed as a result of complex chemical reactions within the atmosphere). In particular for emissions, these type of models use, as input, both of biogenic (generated by natural phenomena) and of anthropogenic (generated by human activities) origin emissions. Emissions are generally related to: nitrogen oxides, volatile organic compounds, ammonia, primary particulate matter, sulphur dioxide.

When the input data of these models (as said meteorology and emissions) are ready, these models can be used to design policy scenarios, which is to say to simulate pollutant concentrations deriving from emission reduction policies.

As this last type of application (scenarios) is typically a request in the 'science-to-policy' interface, the main aim of SHERPA is to mimic the behaviour of fully-fledged air quality models (AQM), so that it is able to simulate the effect on concentrations of emission changes. To do so, SHERPA assumes a linear relationship between concentration and emission changes. This has been shown by Thunis et al. (2015a,b) to be a valid assumption as long as long-term (i.e. yearly or seasonal) concentration averages are considered, as in this work.

In SHERPA the links between emission and concentration changes respectively $\Delta E_{j,k}$ and ΔC_i, are computed cell by cell without any a-priori definition of emission aggregations:

$$\Delta C_i = \sum_{j}^{N_{prec}} \sum_{k}^{N_{cell}} a_{i,j,k} \Delta E_{j,k}$$

One of the main benefits of this approach lies in its spatial flexibility. Once the coefficients "$a_{i,j,k}$" are calculated, the previous equation delivers the concentration changes resulting from emission changes applied over any geographical area, without the need to run specific additional simulations. It has been assumed that the coefficients "$a_{i,j,k}$" in the previous equation can be approximated by the following distance-function:

$$a_{i,j,k} = \alpha_{i,j} \left(1 + d_{ik}\right)^{-\omega^{i,j}}$$

where "*i*" is a grid cell within the domain in which the concentration delta is estimated, the index "*k*" runs over all grid cells within the domain and "d_{ik}" is the distance between cells "*i*" and "*k*". With only two unknowns per cell and per precursor ("*j*" see previous equation) the number of equations requested to solve the system of equation is in theory equal to twice the number of precursors. We however used slightly more simulations (between 15 and 20) to improve the robustness of the estimation of the α and ω coefficients.

This methodology permits spatial flexibility in the definition of emission abatement zones while keeping a light training phase (only a few AQM simulations are required). The cell-to-cell relationships however increases CPU time compared to other approaches but it is nevertheless manageable, taking 1–5 minutes to perform one scenario over Europe.

2.1.2 Model set-up

The SHERPA interface and tool can in theory be adapted to any region if fed with appropriate input data. By input data we mean (1) a gridded emission inventory detailed in terms of activity sectors and precursors (left to user's choice) over the area of interest; (2) a series of 15-20 simulations performed with an AQM for a series of pre-defined emission scenarios to generate the source-receptor relationships (SRR); and (3) a correspondence table matching the user-defined shape files with the emission grid cells. These shape files are then used to define the areas where emission reductions are imposed.

In this work, the CHIMERE model (AQM, Menut et al., 2014) is used to derive the SRR over the whole European territory with a spatial resolution of 7 × 7 km^2. The areas of interest (i.e. the possible control areas) are based on the European Nomenclature of territorial units for statistics (NUTS) covering the $NUTS_0$ (countries), $NUTS_2$ (regions) and $NUTS_3$ (province) levels.

2.1.3 Model baseline

In the equations ΔC_i is linked to $\Delta E_{j,k}$. Given the presence of delta values, a baseline is indispensable. The anthropogenic emissions underlying the model simulations are based on the TNO-MACC[3] emission inventory (Kuenen et al., 2014), with residential sector emissions modified to account for the enhanced wood consumption at extremely low temperatures (Terrenoire et al., 2015). The meteorological input data is based on IFS (Integrated Forecasting System from ECMWF[4]) for the year 2010.

2.1.4 Model precursors

The model has been run using as input the emissions of nitrogen oxides (NO_X), ammonia (NH_3), primary particulate matter (PPM), sulphur dioxide (SO_2). The output of the model, as considered in this study, is the yearly average PM2.5 concentrations deriving from a policy scenarios.

2.1.5 Model validation

Model validation results have been presented in literature, and can be found in Clappier et al. (2015), Pisoni et al. (2017), Thunis et al. (2016).

2.2 The case study set-up

Uncertainty analysis and sensitivity analysis were performed on the SHERPA "scenario" module in order to estimate (1) what is the level of uncertainty associated to the SHERPA outcomes (uncertainty analysis), (2) which model inputs – parameters, precursors, and policy choices- drive the uncertainty (sensitivity analysis) (3) how SA can help the policy/decision making.

Thirteen main sources of uncertainty in model inputs were investigated: the four pollutant emissions, their α and ω coefficients (different for each pollutant), and the policy option in terms of expected improvement in air quality.

[3] TNO is the Netherlands Organisation for Applied Scientific Research
[4] European Centre for Medium-Range Weather Forecasts

Being SHERPA based on spatially dependent coefficients with a huge number of grid cells, we limited the uncertainty and sensitivity analyses to ten European cities: Helsinki, Constanţa, London, Milan (Pisoni et al., *submitted*) in a first step, and successively Berlin, Brussels, Bucharest, Madrid, Paris, and Utrecht. These cities were selected to create synergies with the on-going "partnership on air quality" project, an initiative of the "Urban Agenda" for the EU (http://urbanagendaforthe.eu/partnerships/air-quality/) and to cover the different meteorological and emission inventory conditions in Europe.

As already said, in this study, we refer to the model linking emission reduction scenarios (of nitrogen oxides, ammonia, primary particulate matter, sulphur dioxide) to yearly average reduction in concentrations of PM2.5.

The delta emissions data represent the contributions from primary particulates matter (PPM) and the contributions from the secondary particulate matter from gases (NOx, NH3, SO2) that, together, form the total PM2.5 concentrations. The model output, the delta concentrations data (ΔCi), thus represents the yearly average PM2.5 concentrations, as a total of primary and secondary PM2.5 fractions.

Emission reduction scenarios were utilised for a set of CHIMERE simulations, over the entire modelling domain – the European territory - , to derive the α and ω coefficients required in the simplified SHERPA equation for each grid cell and precursor (pollutant). More details on the whole procedure can be found in Thunis et al. (2016) and Pisoni et al. (2017).

Four different policy options, that is air quality improvement at 25%, 50%, 75%, and 100% (sampled between the Current LEgislation and Maximum Feasible Reductions), were taken into account.

Global sensitivity analysis has been carried out referring to the Sobol' sensitivity indices (Sobol, 1993) whose values are obtained by both the variance based (VB) method and the spectral Polynomial Chaos Expansion (PCE) approach (Sudret, 2008).

3 Uncertainty and sensitivity analysis

Nowadays, the policy making process relies on mathematical models in many fields such as Economics, Engineering, Health, and Environment. At EU level, the policy-making process, and the policy impact assessment process strongly need mathematical model support.

Therefore, quality of models is of crucial importance in policy-making and that is where the concept of Model Quality Assurance (MQA) comes into play. MQA draws on methods and tools that offer more guarantee on the reliability of the model output(s).

Unfortunately, model outcomes are intrinsically affected by some degree of uncertainty and, in some cases, this uncertainty can be very significant.

In presence of uncertainty, model results might be no longer reliable and show low quality. The policy assessment process and thus the underlying policy decision will not be optimised and can even be wrong. Consequently, model outcomes can be effective and responsibly used only if the output uncertainties (intrinsic to any model) are acknowledged and quantified, and the relevant uncertainty sources identified.

Both model and data are subject to uncertainty, and propagate their uncertainty to the model output. Models as a tentative simplification of reality can be affected by uncertainty at different levels, namely theories, assumptions, lack of knowledge, and imperfect understanding. Input data uncertainty may have different causes such as i.e. measurement mistakes, inappropriate measurement method, poor definition of the variables, and scarcity of data. Moreover, key input knowledge is not always well known, as well as the dependency/variability linking different inputs.

Uncertainty analysis and sensitivity analysis methods contribute to the necessary MQA scheme, in a prominent and unique way, by quantifying how model output, and thus policy options impacts, would change w.r.t. the alternative assumptions or different (even slight) input amplitudes, i.e. different input uncertainty characteristics.

Box 1. The Monte Carlo method

Monte Carlo is a popular computational method to simulate random events. It can be used to propagate the input uncertainty through the computer model and quantify the uncertainty in model output(s). The Monte Carlo approach relies on three steps:

1. Generate for each of the k input(s), N sampled values from their respective probability distribution or better their probability density function (p.d.f.),
2. Generate a Monte Carlo sample associating randomly the N sets of the k sampled values ,
3. For each of the N sets of sampled input values, run the model and save the response(s) of interest,
3. Perform the uncertainty and sensitivity analysis by examining the input and output values.

Specifically, uncertainty analysis (UA) techniques aim at characterising model outcome uncertainty given the model input uncertainties, while sensitivity analysis (SA) methods explore the dependency of quantified model output uncertainty on the different sources of uncertainty in the model inputs. Therefore, they should be considered as inseparable and complementary parts of the model assessment, with the uncertainty analysis notionally carried out before the sensitivity analysis (Saltelli et al., 2008).

UA-SA can reveal unexpected relationship(s), identify crucial input factors (data, variables, assumptions…) and how their influence would shape different policy options and policy impacts.

Yet, sensitivity analysis refers to the model logical reliability (model consistency), and not the correctness of the model *per se* (model veracity). Therefore, an active (and continuous) collaboration between modellers (including model expert-users) and

sensitivity analysis practitioners (analysts) is strongly recommended to better interpret findings and evaluate their meanings in the real world.

A UA and a SA popular technique were used to evaluate the SHERPA ”scenario” module (Thunis et al., 2016) developed to forecast, air quality improvement linked to emission reduction scenarios. Additionally, both the Sobol’ main indices and total indices were computed again employing the recent polynomial chaos expansions method (PCE).

The UA and SA exercises will first focus on two main concerns: (1) the resilience of the SHERPA model in terms of outcomes uncertainty (uncertainty analysis), (2) the dependency of the model output(s) from the uncertainty in the model inputs – parameters, precursors, and policy choices – and consequently, the better assessment of the variable roles (sensitivity analysis).

3.1 Methodology

Uncertainty analysis assesses the model output uncertainty on the basis of the known uncertainties in the model inputs. Conversely, sensitivity analysis aims at apportioning total output variability to the different input factors. UA and SA are different but complementary analyses. Historically, uncertainty analysis and sensitivity analysis were firstly carried out using local approaches, where inputs (or model parameters) are changed One at a Time (OAT) while the others are maintained fixed. In this way, calculations (or estimations) of indices are possible only around a specific (given) point in the input space, whose exploration is thus reduced. Local sensitivity analyses are computationally cheap, but they do not account for possible interactions between model inputs or can be poorly informative for non-linear models, and models with high dimensional input spaces.

Global sensitivity analysis overcomes the drawbacks of local analysis, allowing the simultaneous and full range exploration of all uncertain inputs and capturing nonlinearities and interactions among model inputs, whatever the dimension. The drawback is that GSA is much more expensive to carry out than a local analysis because many model executions are often necessary. Consequently, GSA is strongly recommended when models are not linear or not merely additive (Campolongo & Saltelli, 1997, Saltelli & Annoni, 2010). Moreover, with respect to local derivative-based SA, GSA better assures against the risk of declaring non important an input which is actually important (type II errors[5]).

The global approach takes its origin in the early nineties, with the screening methods (Morris, 1991), the non-parametric or regression-based approaches (Saltelli & Marivoet, 1990; Helton, 1993), the variance-based methods (Sobol’, 1993; Iman & Hora, 1990; Sacks et al., 1989), and density-based studies (Park & Ahn, 1994). Since then, GSA has been successfully carried out in a huge number of domains (i.e. Environment, Engineering, Medicine, Chemistry …) showing itself vital and providing a crucial contribution to modelling.

[5] From “Global Sensitivity – The Primer”, page 15: we refer to type I error when erroneously defining as important a non-influential factor. Type II error occurs when we classify an important factor as non-influential

3.1.1 Uncertainty analysis

As previously mentioned, both the uncertainty analysis and the sensitivity analysis of the SHERPA model have been carried out, with the sensitivity analysis following the uncertainty analysis. For the uncertainty analysis we used the Monte Carlo (MC) simulations. This method implies the propagation of the input uncertainty throughout the model using a comprehensive set of random value inputs.

The simulation thus needs a prior clear identification and characterization, in terms of probability density function, of each uncertain model input (inputs included in the analysis), to be able to create a set of random value inputs. The relevant distribution functions can be known by the modeller (i.e. input collected data, literature review, laboratory measurements…), or must be indirectly appraised (i.e. Bayesian inference, expert judgement, belief…). On this basis, the set of random input values is generated and then passed through the model. The model output is quantitatively estimated, and analysed, deriving for example the output mean and variance or spread, in other words the sought output uncertainty.

It is important to stress that the model structure (internal model function) per se may be ignored by the uncertainty practitioner, who is primarily interested in recorded model output values to estimate the model output uncertainty.

Uncertainty analysis has been applied to the SHERPA "scenario" module in order to evaluate the range of variability of the output depending on the different uncertainties in the model inputs. The function form of the model (non-linear additive) and the prominent model inputs to be investigated were already well-known to the modellers. Consequently, the first step of the process was a short check of the identified input variables and the quantification of their level of uncertainties (see Box 2).

Box 2. Input of the UA-SA analysis

Model coefficients:	α and ω are spatially dependent coefficients. They define the link between emissions and concentrations (one for each emission input),
Emission inputs:	Pollutant elements - nitrogen oxides (NO_X,), ammonia (NH_3), primary particulate matter (PPM), sulphur dioxide (SO_2),
Selected policy:	level of ambition in air quality improvement (in terms of emission reductions) - four policies have been investigated as in the Air Quality Package Review (Amann et al., 2014).

The SHERPA model utilises spatially dependent coefficients (α and ω), and obviously their values vary from city to city. Consequently, the analysis was firstly restricted to four cities: Helsinki, Constanţa, London, and Milan were selected to create synergies with the "partnership on air quality" project (http://urbanagendaforthe.eu/partnerships/air-quality/), an initiative of the "Urban Agenda" for the European Union. Later, it was extended to six additional cities: Berlin, Brussels, Bucharest, Madrid, Paris, and Utrecht, to encompass different conditions in Europe. We report in the following the main input data for the city of Milan (see Annex I for the other cities):

	variable	acronym	Distribution[1]	Type[2]	Accuracy[3]
Coefficient*	X_1	ω_NO_X	N(1.97, $4.88x10^{-4}$)	C	H
	X_2	ω_NH_3	N(1.60, $4.08x10^{-4}$)	C	H
	X_3	ω_PPM	N(2.33, $3.00x10^{-4}$)	C	H
	X_4	ω_SO_2	N(1.34, $8.34x10^{-5}$)	C	H
	X_5	α_NO_X	N(0.05, $2.55x10^{-5}$)	C	H
	X_6	α_NH_3	N(0.07, $1.76x10^{-4}$)	C	H
	X_7	α_PPM	N(1.97, $1.78x10^{-3}$)	C	H
	X_8	α_SO_2	N(0.01, $2.27x10^{-5}$)	C	H
Precursor Emissions	X_9	NO_X	U(-0.30 - 0.30)	C	L
	X_{10}	NH_3	U(-0.50 - 0.50)	C	L
	X_{11}	PPM	U(-0.50 - 0.50)	C	L
	X_{12}	SO_2	U(-0.10- 0.10)	C	L
	X_{13}	Policy	U[1-2-3-4]	D	M

*Values for Milan

Table 1: Model input values and ranges

([1]) U: Uniform distribution, N: Normal distribution
([2]) C: Continuous variable, D: Discrete variable
([3]) The modellers belief regarding the assigned prior uncertainty: L=Low, M=Medium and H=High.

Mean (central value) and standard deviation of α and ω coefficients were known to the modeller for each grid cell as well as their Gaussian/Normal distribution characteristics. Mean and standard deviation together with the relevant probability density function (p.d.f.) were used for the random generation of the data in the MC simulations.
Greater 'ignorance' concerned the distributions of the emissions inputs (NO_X, NH_3, PPM and SO_2)[6]. Thus, their probability density functions were assumed to be uniform around their respective nominal value, obtained from the SHERPA emission inventory, while the ranges of variability were derived from scientific literature (Nielsen et al., 2014; Kuenen et al., 2014). These assumptions were kept constant for all the examined cities. In Table 1, the ranges are reported: i.e. NH_3 shows a variation of $\pm$50% around its nominal value.

Finally, four policy options, that is four different levels of ambition in trying to improve air quality, were considered as discriminant variables, choosing the values between the CLE-Current LEgislation and the MFR-Maximum Feasible Reductions (the two extreme policies). Specifically, air quality improvement at 25% (between CLE and MFR), 50%, 75% and 100% were defined as possible policy options.

[6] The issue of emission uncertainties in air quality modelling has been recently cited in Trombetti et al., 2018. The authors analysed the six main emission inventories available in Europe, and showed that substantial differences in terms of total emissions, sectorial emission shares and spatial distribution exist between these datasets.

3.1.2 Sensitivity Analysis - Variance-based sensitivity indices

Variance–based sensitivity analysis notion moved from the possibility of decomposing the total variance of the model output into terms of increasing dimensionality, as suggested by the Russian mathematician I.M. Sobol' in the early nineties (Sobol', 1993). When the output function f(X)=Y is square-integrable and the inputs $X=(X_1,\ldots,X_d)$ are independent, the total variance of the output can be split into the sum of different terms (partial variance) over the input space Ω^d (the so-called ANOVA decomposition):

$$V(Y)=\sum_{i=1}^{d} V_i + \sum_{j>i}^{d} V_{i,j} + \cdots + V_{1,\ldots,d}$$

where the first term of this sum V_i represents the partial contribution to the variance of the input solely considered (1st order effect):

$$V_i = V(E(Y|X_i))$$

and V_{ij} measures the interaction effect of the pair (X_i, X_j) on Y (2nd order effect):

$$V_{i,j} = V_{i,j}(E(Y|X_i, X_j)) - V_i(E(Y|X_i)) - V_j(E(Y|X_j))$$

while the following $V_{1,2,\ldots d}$ terms of the sum show the higher order interactions.

Finally, dividing the variance (de)composition by V(Y), gives the sensitivity indices:

$$1 = \sum_{i=1}^{d} S_i + \sum_{j>i}^{d} S_{i,j} + \cdots + S_{1,\ldots,d}$$

The first-order effect of model input X_i, that is the conditional variance, is defined by $V(E(Y|X_i))$, that divided by the total variance V(Y) of the model output gives the first order sensitivity index S_i, also called main effect of the model input X_i:

$$S_i = \frac{V(E(Y|X_i))}{V(Y)}$$

The first-order sensitivity index S_i is thus normalized between 0 and 1. The same is done for the higher order indices ($S_{i,j}$, $S_{i,j,k}$, …).

A high value of S_i denotes a prominent quantitative influence of the X_i uncertainty on the model output (Y) uncertainty, while low values of the index mean a negligible influence of the X_i variable alone.

The total sensitivity effect of an input (Homma and Saltelli, 1996) is expressed by the sum of all the effects of any order involving that same input ($S_{Ti} = S_1 + S_{1,2} + S_{1,3} + \ldots + S_{1,2,3} + \ldots$). The sum of all possible sensitivity terms should be equal to 1. Consequently

the difference between 1 and the normalized value of $V(E(Y|X_{\sim i}))$ - that is all terms of any order that do not include input X_i (*~i* indicates all terms but i) - gives The total effect of input X_i. It is given by the following expression:

$$S_{Ti} = 1 - \frac{V(E(Y|X_{\sim i}))}{V(Y)} \qquad \text{with index } {}_{\sim i} \text{ meaning all terms but } X_i$$

Therefore, given that: $V(Y) = E\left(V\left(Y \middle| X_i\right)\right) + V\left(E\left(Y \middle| X_i\right)\right)$

the total sensitivity index of X_i can also be calculated with:

$$S_{Ti} = \frac{E(V(Y|X_{\sim i}))}{V(Y)}$$

Third-order and higher sensitivity indices have analogous definitions.

Box 3. Variance-based Sensitivity index properties

Main properties of variance-based sensitivity indices:

— Are model free,

— Provide an X-ray of the input-output relationship:

$1 \geq S_{Ti} \geq S_i \geq 0$	Always (unless inputs are dependent)
$\sum_{i=1}^{d} S_i \leq 1$	Always (unless inputs are dependent)
$\sum_{i=1}^{d} S_i = 1$	Additive model (no interactions)
$1 - \sum_{i=1}^{d} S_i \gg 0$	Indicator of the presence of interactions

An overall set of 2^{d-1} indices can be computed that reflect the structure of the input-output relationship.

Sensitivity indices can be computed with many different methods (Sobol', 2001; Kucherenko et al., 2012, Borgonovo, 2007, Liu & Homma, 2009, Plischke et al., 2013, Saltelli et al., 2010, Mara & Tarantola, 2012), and among the most powerful and popular ones, we have: meta-modelling based approaches (Oakley & O'Hagan, 2004; Buzzard & Xiu, 2011), spectral techniques (Saltelli et al, 1999; Sudret, 2008; Shao et al., 2017), and sampling-based Monte-Carlo evaluations (Saltelli, 2012, Sobol', 1933, Saltelli et al., 2010).

On top of the GSA VB technique, the GSA spectral Polynomial Chaos Expansion (PCE) technique (Sudret, 2008) was also successfully used in this study and both techniques showed very similar results.

3.1.3 Sensitivity Analysis - Polynomial chaos expansions (PCE)

An advanced SA method

A quite recent computational method to assess the Sobol' indices is the polynomial chaos expansion technique (Sudret, 2008). While the Monte-Carlo approach, applied to the previous phase of the research (Pisoni et al., *submitted*), aims at directly estimating the individual terms of the sum into which the total variance is decomposed, PCE gives an estimation of the output function (Y). The intuition of the method is that the assessment of each term of the variance of the estimated output function is easily possible starting from the multi-dimensional orthonormal polynomial approximating the characteristics of the function f(x)=Y.

Under the same assumptions as the ANOVA decomposition, the function can be (re)written as:

$$Y = \sum_{\boldsymbol{\alpha} \in N^k} a_{\boldsymbol{\alpha}} \psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$$

where $\psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$ is the so-called multivariate orthonormal polynomial chaos:

$$\psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) = \psi_{\alpha_1}(x_1) \times \ldots \times \psi_{\alpha_d}(x_d)$$

and $\boldsymbol{\alpha} = \alpha_1 \ldots \alpha_d$, with $\alpha_i \in \mathbb{N}$, is a multi-index and $a_{\boldsymbol{\alpha}}$ the polynomial coefficient indicating the dependency of Y on $\psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$[7]. The polynomial $\psi_{\alpha_i}(x_i)$ is of degree $\alpha_{\boldsymbol{i}}$.

Therefore, $\psi_{\boldsymbol{\alpha}}(\boldsymbol{x})$ is a multidimensional polynomial of degree $(\alpha_1 + \alpha_2 \ldots + \alpha_d)$. Notably, we always have $\psi_0(x_i) = 1$.

The appropriate form of the univariate polynomial $\psi_{\alpha_i}(x_i)$ is derivable from the probabilistic distribution of the input variables (Xiu & Karniadakis, 2002). Such univariate orthonormal polynomials are, for instance, the normalised Legendre polynomials when x_i is uniformly distributed. Therefore, given the orthonormality property of polynomial elements ($E\left(\psi_{\boldsymbol{\alpha}}(\boldsymbol{x}) \times \psi_{\boldsymbol{\beta}}(\boldsymbol{x})\right) = \delta_{\boldsymbol{\alpha\beta}}$)[8] the total variance is:

$$V(Y) = \sum_{\boldsymbol{\alpha} \in N^d} a_{\boldsymbol{\alpha}}^2 - a_{0\ldots0}^2$$

and consequently, the Sobol' indices can be estimated from the PCE coefficients as follows:

$$S_i = \frac{V[E(Y|X_i)]}{V(Y)} = \frac{\sum_{\alpha_{i_1} \in N} a_{0\ldots0\alpha_{i_1}0\ldots0}^2}{\sum_{\boldsymbol{\alpha} \in N^d} a_{\boldsymbol{\alpha}}^2 - a_{0\ldots0}^2}$$

[7] From this representation any statistical moment of Y=f(X) can be computed:
$\mathrm{E}[Y] = a_{0\ldots0}$; $\mathrm{E}[Y^2] = \sum_{\boldsymbol{\alpha} \in N^d} a_{\boldsymbol{\alpha}}^2$; $\mathrm{V}(Y) = \mathrm{E}[Y^2] - \mathrm{E}[Y]^2 = \sum_{\boldsymbol{\alpha} \in N^d} a_{\boldsymbol{\alpha}}^2 - a_{0\ldots0}^2$

[8] $\mathrm{E}[f_\alpha(X) f_\beta(X)] = V_\alpha \delta_{\alpha\beta}$ where δ is the symbol of Kronecker

$$S_{Ti} = \frac{E[V(Y|X_{\sim i})]}{V(Y)} = \frac{\sum_{\boldsymbol{\alpha}\in\mathcal{N}^d:\alpha_{i_1}>0} a_{\boldsymbol{\alpha}}^2}{\sum_{\boldsymbol{\alpha}\in\mathcal{N}^d} a_{\boldsymbol{\alpha}}^2 - a_{0\ldots0}^2}$$

The challenge with the PCE method for variance-based sensitivity analysis is the estimation of the coefficient $a_{\boldsymbol{\alpha}}$ (polynomial chaos expansion). When this estimation is obtained, the following step of the index computation is quite immediate and (very!) cheap. In fact, all indices are calculated from the same polynomial expansion. The elaboration cost (number of model runs) is an imperative element to be considered when the SA of a model response is undertaken, and PCE is generally a very cost-effective technique.
The rate of convergence of the polynomial series depends on the smoothness of the model response. When the output function is not regular (i.e. binary/discrete values), the PCE might encounter some difficulties and fail at estimating with the needed precision. In this case, other SA methods should be preferred.

The regular responses of the SHERPA model shown by prior SA make this model a suitable case-study for the application of the PCE technique. In this work, we used the Bayesian sparse PCE approach as proposed by Shao et al. (2017). This method provides the variance decomposition from one single Monte Carlo sample of size N with N typically less than a thousand.

4 Results and Discussion

As said in section 2.2, the model output, the delta concentrations data ($\square C_i$), thus represents the yearly average PM2.5 concentrations, as a total of the primary and secondary PM2.5 fractions.
The preliminary uncertainty analysis of the SHERPA model, aiming at the quantification of the uncertainty in the model output, identifies different ranges depending on the city.
For example the concentration reduction range (uncertainty) for Helsinki is around 3 $\mu g/m^3$ while Milan shows more than 40 $\mu g/m^3$ uncertainty. Nevertheless, the predominant influence of the assumptions linked to the chosen policy (four air quality improvement at 25%, 50%, 75%, and 100%) is constantly confirmed.
Hence, it was decided to study the effect of the four main policies, namely the air quality improvement at 25%, 50%, 75%, and 100%.

The global sensitivity analysis provided a rank for the 13 uncertain inputs, namely the four coefficients α and ω, the four emissions (NO_X, NH_3, PPM, and SO_2), and the policy options. It still confirms the latter to be a very relevant input.
On the contrary, the study shows the α and ω coefficient inputs to be quite negligible, that is their variabilities do not bring about a consistent uncertainty in the model output. Note that the four pollutants (NO_X, NH_3, PPM, and SO_2) show variant SA indices, with an eventual importance of PPM uncertainty in many cities.

Another remark is that all the first order sensitivity indices (S_i) and their corresponding total sensitivity indices (S_{Ti}) present very little difference, which is a sign of absence of interactions among the inputs in the model. As a result, we only consider only total indices (S_{Ti}) in the following.

Results for the city of Helsinki, London, and Milan are shown in the following section. Results for all the investigated cities are reported in Annex-1.

4.1 Uncertainty Analysis

As already mentioned (section 3.1.1), the model coefficients α and ω are defined at regional level and their distribution functions are specific for each city (spatially dependent), consequently also UA results are specific for each city. For all cities, increased ambitions in terms of pollutant concentration reduction (higher ΔC) are associated to a larger range in model outcomes, as expected, while the associated probability density function (pdf) is smoother. Results are showed for the city of Helsinki (figure 2), London (figure 3), and Milan (figure 4). The x-axis represents the pollutant concentration reduction (ΔC) in concentrations in PM2.5 yearly average (in relation to the baseline case), and the y-axis represents the probability of the linked occurrence[9].

For the case of Helsinki, UA shows values between 1 $\mu g/m^3$ and 4.5 $\mu g/m^3$ (figure 2a), giving a range of about 3 $\mu g/m^3$. When the four policies are distinctly considered (figure 2b), ranges associated to each case are different. When the ambition level grows (from 25% to 100%) also the uncertainty on the results grows. The black line shows that the pdf of the most ambitious policy (100%) is clearly much larger (range of uncertainty)

[9] The pdf have been estimated on the basis of the results of the MC perturbation of the nominal values of inputs and model coefficients

than in the other three cases. For the intermediate policy (at 50%), the most frequent result is around 2.1 μg/m^3.

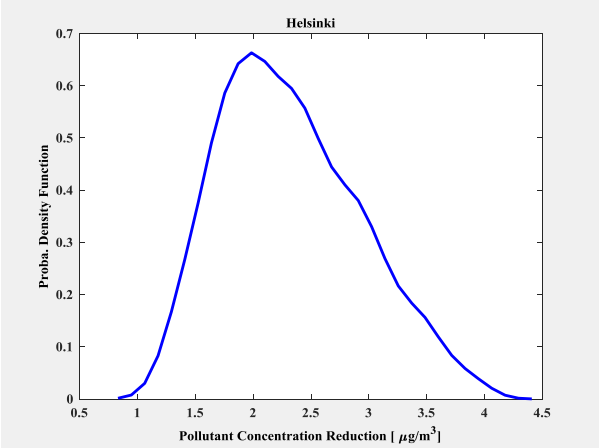


Figure 2a: Probability Density Function of the estimated concentration reduction

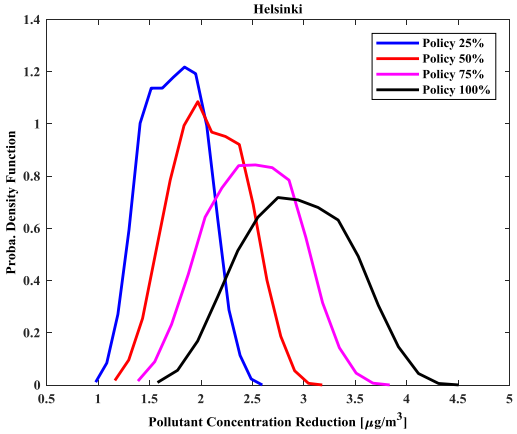


Figure 2b: Probability Density Function of concentration reduction grouped into the four analysed policies

A similar uncertainty is shown for London (figure 3a). For this city, the uncertainty ranges from 2 μg/m^3 to 6 μg/m^3, being quite similar to the prior case (4 μg/m^3 while 3 μg/m^3 for Helsinki). The *Policy 50%* (figure 3b – red line) has as 'most frequent' value around 3.4 μg/m^3. Again, moving to the cases of *Policy 75%* and *Policy 100%* the uncertainty widens (figure 3b –purple and black line respectively).

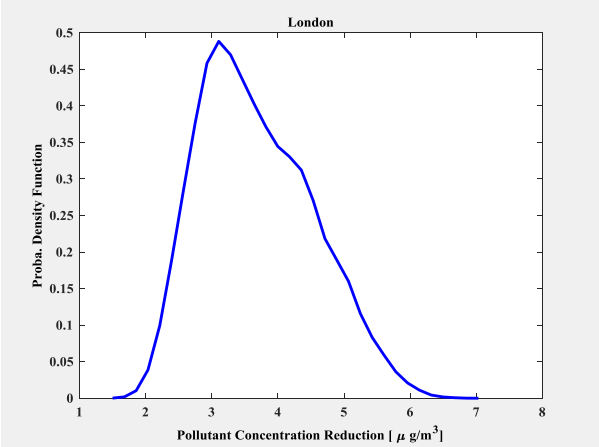


Figure 3a: Probability Density Function of the estimated concentration reduction

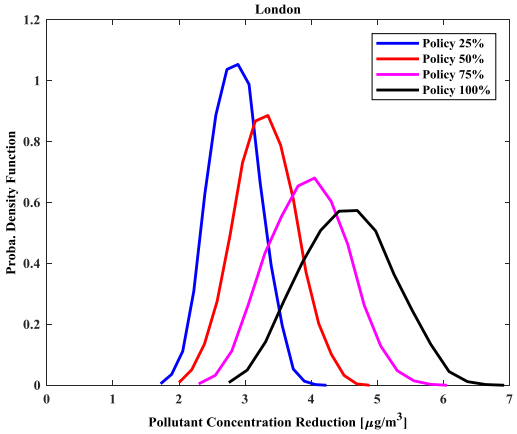


Figure 3b: Probability Density Function of concentration reduction grouped into the four analysed policies

The case of Milan is the most uncertain one. Pollutant concentration reduction varies between 10 μg/m^3 - 52 μg/m^3, with a range of uncertainty of more than 40μg/m^3. Considering the individual policies, even the case of *Policy 25%* shows a higher uncertainty range (about 25μg/m^3) than the other investigated cities (see also Annex 1). Thus, for the Milan case, policy decision-making might be less effective due to the greater uncertainty in the model outcomes.

The above results stress how the model appears more robust, in terms of reduced variability, when working in "less extreme" scenarios, as i.e. the one close to *Policy* - 25/50% air quality improvement. In fact, this case shows a smaller range of uncertainty (see blue curves compared to the others one in figure 4b). However, the most remarkable result of the UA study is the constant overlapping of the four areas representing the different policies. This means that due to the hypothesized uncertainty in the inputs, the derived uncertainty in the output gives no possibility to distinguish between the policy options. The investment in the most costly option *Policy 100%* does not guarantee a better result in absolute terms.

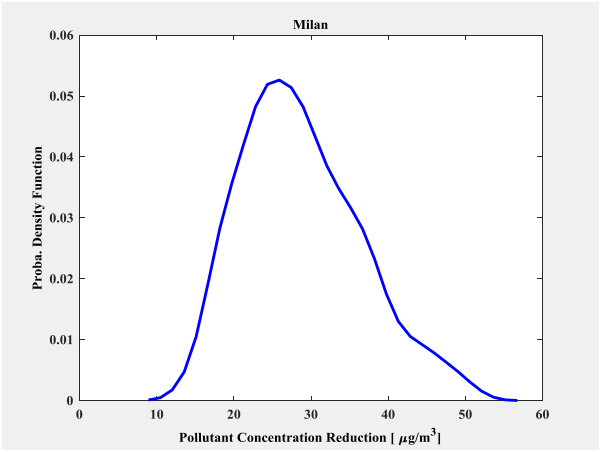


Figure 4a: Probability Density Function of the estimated concentration reduction

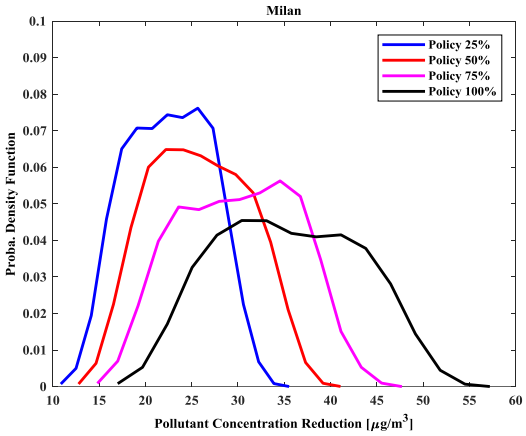


Figure 4b: Probability Density Function of concentration reduction *grouped into the four analysed policies*

In similar case, the decision 'impasse' is solved devoting more efforts to the study of the sources of uncertainty, identified by SA to reduce the overlapping of the outcomes, namely an attempt to have distinct policy effects, and thus a more effective decision (see section 4.3).

4.2 Sensitivity Analysis

As for uncertainty analysis, sensitivity analysis of SHERPA model has been carried out with respect to the different city profiles/characteristics. Therefore, the SA results might be different from one city to another, being not unique the distributions of the associated coefficients α_s and ω_s and pollutant emission levels.

The analysis took account of thirteen uncertain inputs, namely the four α_s and ω_s, the four emissions (NO_X, NH_3, PPM, and SO_2), and the policy option (ambition in air quality improvement). For almost all cities, the SA results show the policy option to be the main input. In fact, the total SA indices for the policy variable are in the range between 0.39 (Madrid) and 0.64 (London). This means that a significant part (~40%) of the uncertainty in the outcome can be apportioned to the uncertainty in the policy choice. On the other hand, the global sensitivity study reveals that the coefficient α and ω values are quite negligible. In most cases the SA indices are lower than 0.005having thus very little impact on the uncertainty in the model output. The four pollutants emissions (NO_X, NH_3, PPM, and SO_2) show variant SA indices, with some noticeable importance for the PPM uncertainty in many cities (the highest one equals 0.38 for Milan).

In a next step, sensitivity analyses were conducted assuming a given policy (i.e. 25% air quality improvement) taking thus into account 12 uncertain inputs. The SA results show which inputs, among the remaining 12 (the policy is fixed), mainly contribute to the uncertainty in the concentrations reduction. The different outcomes, achieved with this additional analysis, confirm a diverse behaviour of the evaluated cities. Nevertheless again the coefficients α_s and ω_s have little effect on the uncertainty of the model output (concentration reduction).

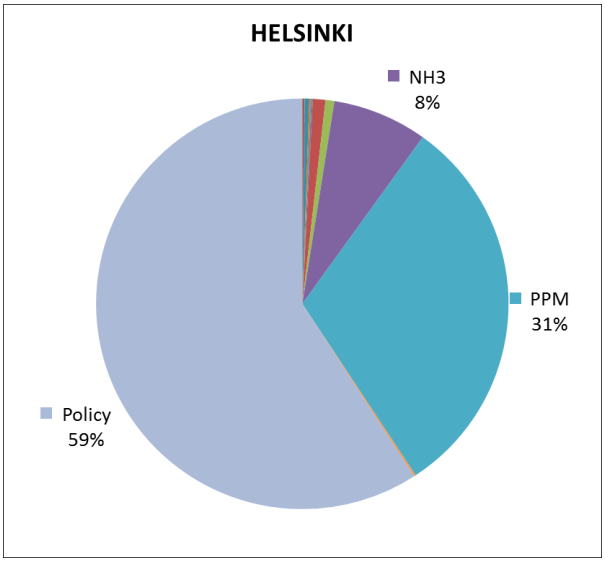


Figure 5: Sensitivity Analysis results for Helsinki (13 inputs)

In the case of Helsinki (figure 5), SA indicates that the 'policy option' (total index S_{Ti} = 0.59) and the emission PPMs (S_{Ti} = 0.31) are the most important inputs, explaining together about 80% of the variability of the outcomes. The NH3 follows with a total SA index of around 8%, while all other inputs have a very low influence on the concentration reductions. This means that time and efforts should not be focused on reducing the uncertainty of such inputs because the pollutant reduction values are not 'sensitive' to their improvement in terms of accuracy.

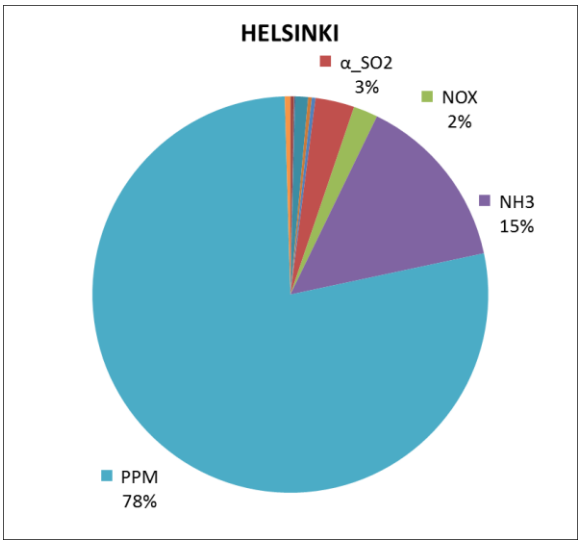
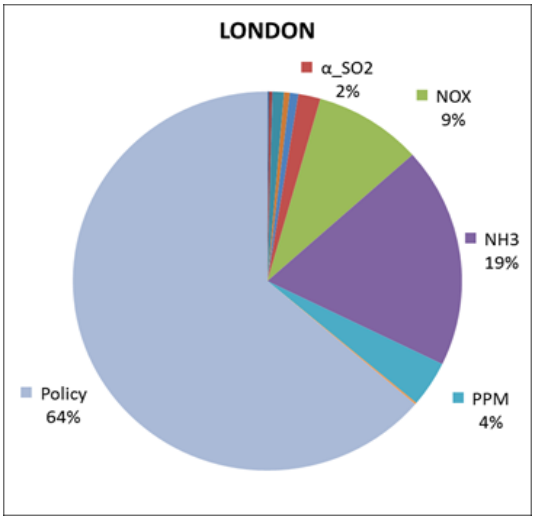


Figure 6: Sensitivity analysis results for Helsinki (12 inputs)

Once the policy is fixed, the PPMs emission becomes the main contributor to model uncertainty. The S_{Ti} for PPM input reaches 0.78 and the NH3 S_{Ti} index increases up to 0.15. These two emissions explain about 83% of the variability in the model. The uncertainties associated to the coefficients α_s and ω_s continue to be not influential.

Similarly to Helsinki, the results for London (figure 7) show that the policy input is predominant (S_{Ti} = 0.64) with respect to the other uncertain inputs. Still, this confirms that it is important to devote efforts to better know the uncertainty on the policy choice. However, contrarily to the prior case, the PPMs emission sensitivity index is only 0.04. In fact, the uncertainty is mainly attributed to the NH_3 and NOx inputs, which have a total index (S_{Ti}) equal to 0.19 and 0.09 respectively. This pattern is replicated when the policy is fixed (figure 8). Therefore, when the policy option is certain and when we want to improve the accuracy of the concentrations reductions, we should make efforts to better know the uncertainty on the emissions of NH_3 and NO_X. The indices related to α_s and ω_s are still negligible.

Figure 8: Sensitivity results for London (12 inputs)



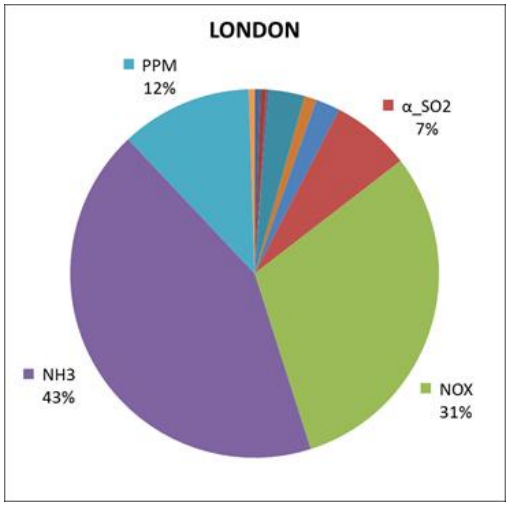
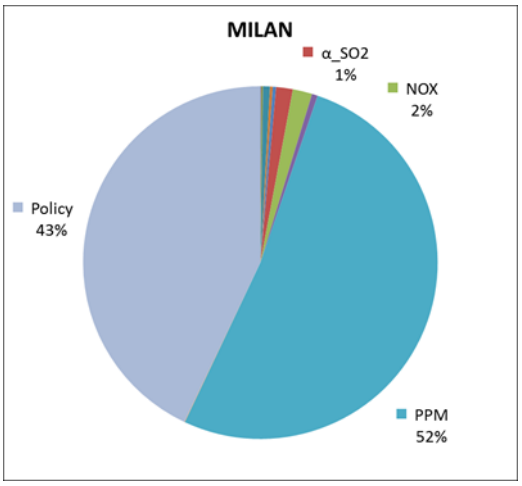


Figure 7: Sensitivity results for London (13 inputs)

Finally, we present the results for the city of Milan (for an extensive discussion of this case see the following paragraph). The study with the 13 input variables indicates that the policy option and the PPM emissions are the only relevant factors.

Their SA indices are S_{Ti} = 0.43 for policy and S_{Ti} = 0.52 for PPMs, thus only a residual 5% of model) outcome uncertainty is not explained by these two inputs. If the policy uncertainty is eliminated, PPMs variability is able to give total account of almost the totality of the model output uncertainty. Its S_{Ti} is equal to 0.90 (figure 10). All other inputs are individually little relevant.

Figure 10: Sensitivity results for Milan (12 inputs)



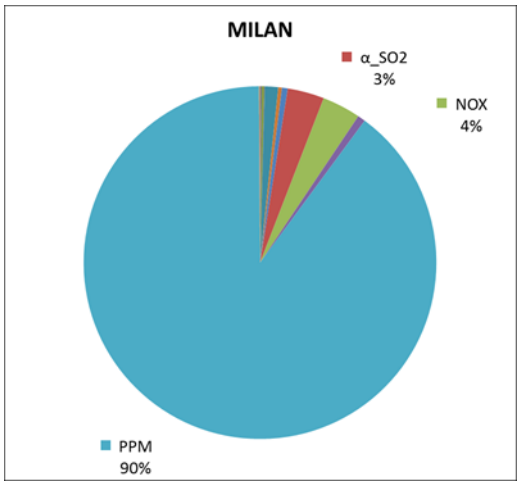


Figure 9: Sensitivity results for Milan (13 inputs

4.3 UA-SA for decision-making: The case of Milan

4.3.1 The problem setting

We have shown that, among the studied cities, Milan was the case with the highest potential of pollutant concentration reduction. Indeed, the uncertainty analysis has shown that the possible reduction that one could achieve lies within the range [10, 45] $\mu g/m^3$.

We now undertake a more insightful analysis aiming at pointing out the best policy choice. The question asked is: « Given that *Policy 100%* is more expensive to implement than *Policy 25%*, is it worth to choose it? ».

To answer the question, an analysis must be carried out by making a clear distinction between the two policy options. Instead of re-executing the SHERPA model with a new sample set for the two different policies, we filter the sample at hand by only keeping the input/output draws that only concern *Policy 25%* and *Policy 100%* respectively. This provides two subsamples of modest sizes (around 512 draws) that we subsequently analyse with the Polynomial Chaos Expansion method (see section 3.1.3).

4.3.2 Decision-making under uncertainty

Computer models can be valuable tools for decision-making in a policy context. Modellers usually provide model-based evidences after executing their model by assuming that the model input values are known and correct, and that their models are error-free. They tend to overlook the inevitable issue of uncertainty. Good modelling practice should acknowledge the presence of uncertainties in the model and the data. This is the prerequisite for robust decision-making.

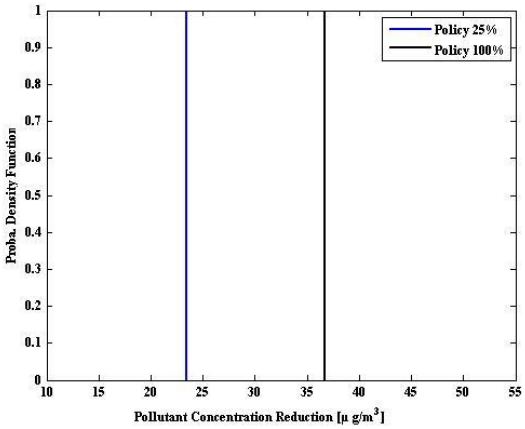


Figure 11: SHERPA result assuming known the model inputs

Although uncertainty due to model error is not easy to handle, accounting for model input uncertainty (data) is straightforward and should at least be of current practice. As an illustration of how classical approaches can go wrong, let us consider the problem defined in the previous section. We computed the expected reduction of pollutant concentration with SHERPA if *Policy 25%* and *Policy 100%* are respectively applied to the city of Milan. In this exercise, the input parameters are set to their nominal value.

The results are depicted in figure 11. We note that, by doing so, the results lead to the conclusion that by applying *Policy 25%,* a reduction of the pollutant of about 24 µg/m^3 could be achieved while applying *Policy 100%* a reduction of about 37 µg/m^3 could be expected. Therefore, a further improvement of 13 µg/m^3 could be achieved with *Policy 100%*. This inference is of course misleading because it is not clear whether this improvement is significant or not. This is a crucial issue as *Policy 100%* might be more difficult and/or expensive to implement than *Policy 25%.*. Hence, it is important to assess whether the policy-makers will get their money worth. One way to assure that is to rely on the modeller's best knowledge about the model input values. As discussed in section 3.1.1, uncertainties in the model inputs were quantified by the modeller and a rough estimation of the model input distributions was undertaken on the basis of a good literature review (see Table 1).

SHERPA was executed/run with a quasi Monte Carlo sample in order to account for model inputs uncertainties. For each policy, a subsample of the predicted pollutant concentration reduction was obtained as described in section 4.1. The resulting uncertainties in the model responses for the two policy scenarios are depicted in figure 12. We can see that the predicted pollutant concentration reduction ranges from 12 μg/m^3 to 35 μg/m^3 for *Policy 25%* while it ranges within [17, 55] μg/m^3 for *Policy 100%*. We also note that the predicted probabilities overlap. Therefore, it is not clear whether *Policy 100%* would effectively be more efficient than *Policy-25%.* In such a situation, it is difficult to make a choice between the two policies.

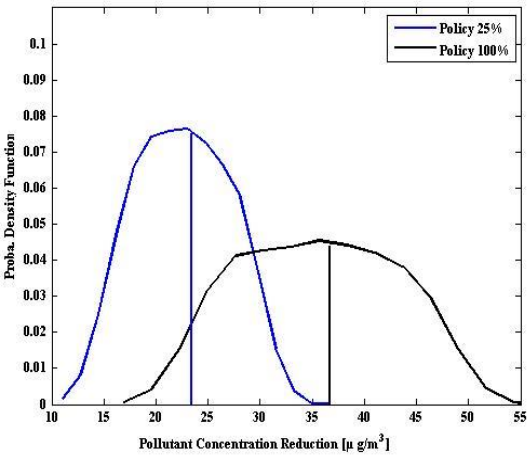


Figure 12: SHERPA response uncertainty when uncertainties in the inputs are accounted for.

It is then recommended to identify the inputs responsible for such an overlapping. This is the role of sensitivity analysis.

4.3.3 Sensitivity analysis for guiding future works

Reducing the uncertainty in the model responses is the key to clearly assess the benefit of applying/implement one policy instead of the other one. Therefore, we carry out a study to compare the effect of two different policies.

To this aim, the sensitivity analysis of the difference between the pollutant concentration reductions obtained with the two policies has been performed. The model was run with the two policies separately but with the same sets of input values. This exploratory step was based on the polynomial chaos expansions identified in the previous analysis (i.e. the PCEs are used as surrogate models).

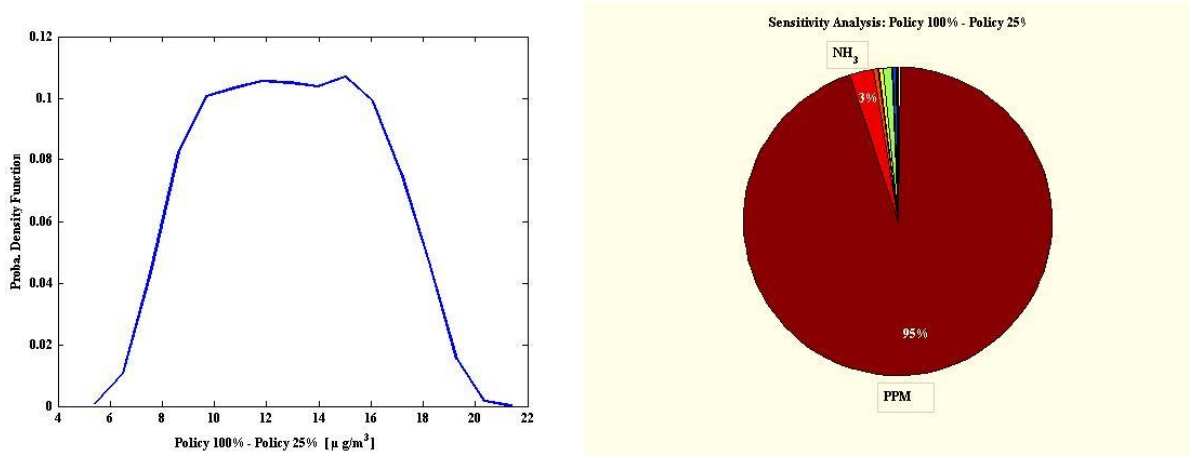


Figure 13: On the left, probability density of the difference between the reduction in concentration of pollutant due to the two policies (25%, 10%). On the right, variance decomposition of the difference between the two policies. The latter highlights the importance of emission of primary particulate matter.

We performed 1024 runs of the two surrogate models (PCE expansion) and computed, for each run, the difference between the predicted pollutant concentration reductions provided by *Policy 25%* and *Policy 100%.* The uncertainty of the computed response is shown in figure 13 (left-hand side). We can infer that the difference between the two policies in terms of pollution reduction varies from 6 $\mu g/m^3$ and 20 $\mu g/m^3$. The difference is positive which means that *Policy 100%* will always perform better than *Policy 25%*. However, the improvement can be significant (close to 20 $\mu g/m^3$) or not (~6 $\mu g/m^3$).

After, another iteration of the sensitivity analysis was necessary to know which input - **if better characterized** - would allow reducing the uncertainty in the model prediction so that the stakeholder could take an easier decision.

This is achieved with the Web-App for sensitivity analysis of model output developed by Unit JRC.I1 and described in Annex 2.

The results are represented in figure 13 (right-hand side) in the form of a pie chart. The latter is the variance decomposition of the difference in pollution reduction between the two policies. The sensitivity analysis clearly pointed out the importance of the value assigned to the Emission of PM2.5 (KTons/year) in the surroundings of Milan. We recall that this input varied between +/- 50% with respect to the reference value. As a conclusion, future effort should be dedicated to the characterization of the emission of PM2.5 in the area of Milan if one wants to infer if one policy is significantly better than the other one.

5 Conclusions

In the report, we addressed the use of 'uncertainty and sensitivity analysis techniques' to check the robustness of air quality models. As in Europe, we are moving to a situation in which exceedances of air quality legislation thresholds are mainly measured in specific regions or cities, the focus has been on the application of uncertainty and sensitivity analysis to the SHERPA model, which has been specifically designed for supporting regional/local decision makers.

A case-study has been conducted on one of the key SHERPA modules used to forecast air quality improvement linked to emission reduction scenarios. Given that SHERPA is based on coefficients and spatially varying inputs, a number of selected European cities[10] - representative of different meteorological and emission inventory conditions - have been chosen for the UA-SA exercise.

Firstly, the uncertainty of the SHERPA outcomes (yearly concentrations of PM2.5 in $\mu g/m^3$) has been quantified by uncertainty analysis (UA). This has been done considering the SHERPA inputs variability (in terms of emissions of precursors of PM2.5 concentrations), the SHERPA model coefficients uncertainty (considering perturbation of coefficients α_S and ω_S nominal values), and the policy option variable. The results helped identifying how and where to prioritise further model improvement and policy makers' actions.

Moreover, the uncertainty analysis was followed by a sensitivity analysis to identify the most influential inputs and their possible interactions. It was found that, for eight cities out of ten, the policy option, that is the level of desired reduction considered by the air quality plan, is the most influential input. This means that the choice of the policy, namely, the policy option variability is more important than the other model input and coefficient variabilities. In the two remaining cases (Milan and Madrid), the sensitivity index of the policy choice is the second relevant one.

This means that according to the model forecasts, the first action should be for the policy makers to discuss upon what is the best policy to implement. After, once the policy has been agreed upon, the discussion could move on to how to reduce the other sources of uncertainty. Among the other inputs, the pollutant emissions (KTons/year) are by far the most influential ones, in particular the emissions of PPM, NO_X, and NH_3. The SHERPA model coefficients (α and ω) are quite unimportant inputs, even if the α coefficients are slightly more relevant than the ω ones.

In the Milan and Madrid cases, the uncertainty on the emissions of PM2.5 is the main contributor to the inaccuracy of the model output (total sensitivity indices are S_{Ti}=0.52 for Milan and S_{Ti}=0.59 for Madrid). For these cities, it would be advisable also to spend resources to get a better knowledge of the PPMs emission quantities.

As shown in a recent work (Trombetti et al., 2018), EU cities show substantial differences in terms of total emissions, sectorial emission shares and spatial distribution. These differences determine different model output uncertainty. Therefore, a specific UA-SA is necessary for each city.

Finally, the case of Milan has been exhaustively discussed. The authors used the Web-App for sensitivity analysis developed within the Competence Center on Modelling (CC-MOD) to carry out a forecasting analysis. This last step confirmed that the knowledge (and possible control) of the level of uncertainty affecting the model inputs is determinant for the policy-decision process, and the key-role played by SA in this regard.

[10] Berlin, Bruxelles, Bucuresti, Helsinki, Constanţa, London, Madrid, Milan, Paris, and Utrecht.

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List of abbreviations and definitions

AQM	Air Quality Model
CC-MOD	Competence Centre on Modelling
ECMWF	European Centre for Medium-Range Weather Forecasts
IA	Impact Assessment
INERIS	Institut National de l'Environnement Industriel et des Risques
GSA	Global Sensitivity Analysis
MACC	Monitoring Atmospheric Composition and Climate
MC	Monte Carlo
MQA	Model Quality Assurance
NH_3	Ammonia
NO_x	Nitrogen oxides
OAT	One at A Time
PCE	Polynomial Chaos Expansion
PPM	Primary Particulate Matter
SA	Sensitivity Analysis
SAMO	Sensitivity Analysis of Model Output
SHERPA	Screening for High Emission Reduction Potential on Air
SO_2	Sulphur dioxides
SRR	Source-Receptor Relationships
S_i	Sensitivity First Effect Index
S_{Ti}	Sensitivity Total Effect Index
UA	Uncertainty Analysis

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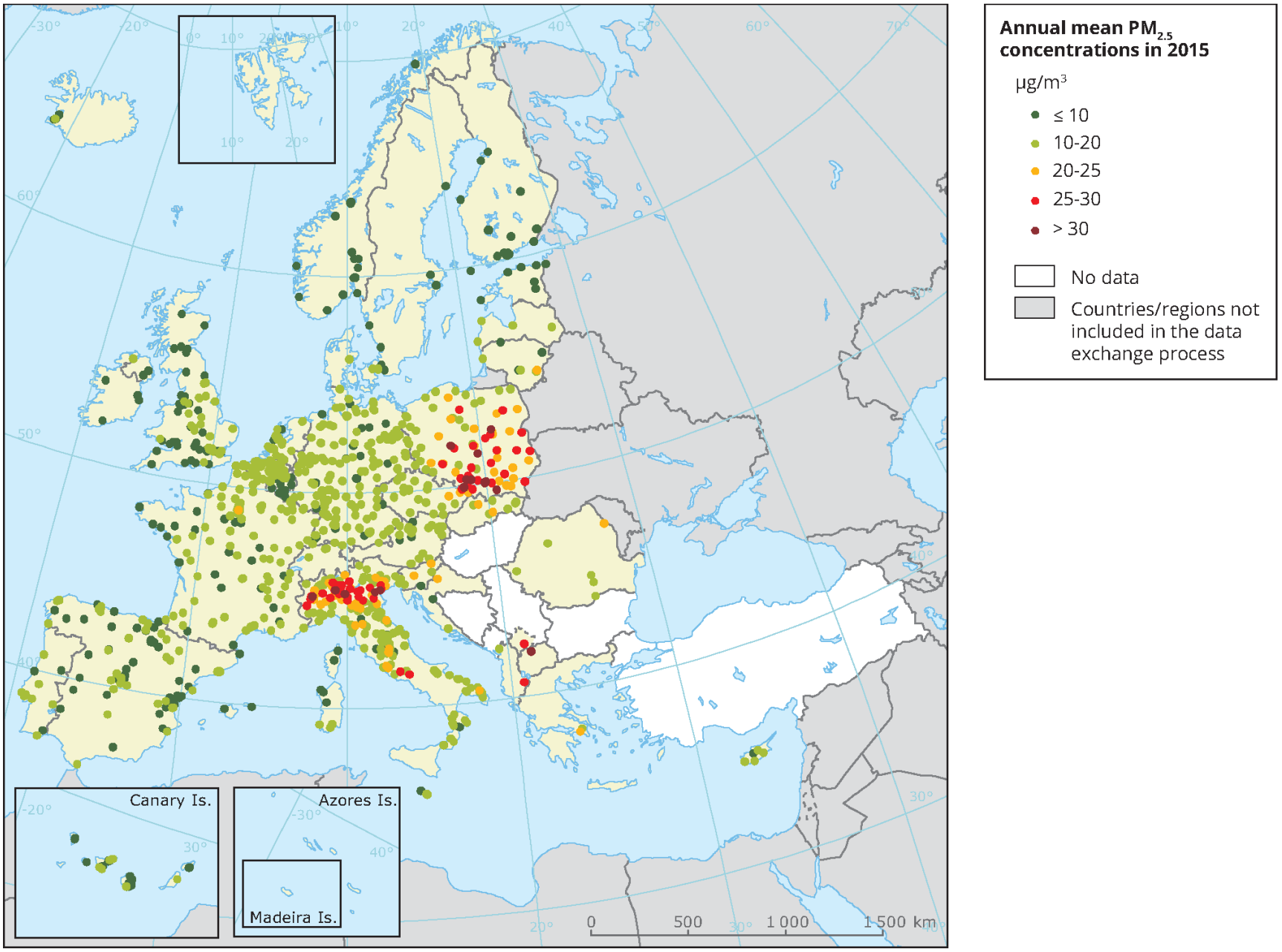
Annual mean PM2.5 concentrations in 2015
µg/m3
≤ 10
10-20
20-25
25-30
> 30
No data
Countries/regions not included in the data exchange process
Canary Is.
Azores Is.
Madeira Is.
0
500
1 000
1 500 km

Annexes

Annex 1. Investigated city profiles

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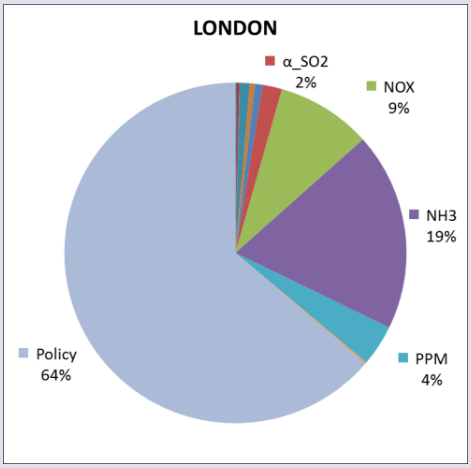
<tr><td rowspan="8"> 
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<tr><td>ω_NH₃</td><td>1.62</td><td>0.01</td></tr>
<tr><td>ω_PPM</td><td>2.51</td><td>0.66×10^{-2}</td></tr>
<tr><td>ω_SO₂</td><td>1.38</td><td>0.01</td></tr>
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<tr><td>α_PPM</td><td>0.28</td><td>0.03</td></tr>
<tr><td>α_SO₂</td><td>0.23×10^{-2}</td><td>0.05×10^{-2}</td></tr>
<tr><td>LONDON</td><td>The U.K.</td><td colspan="2">Inhabitants: 8,787,892</td></tr>
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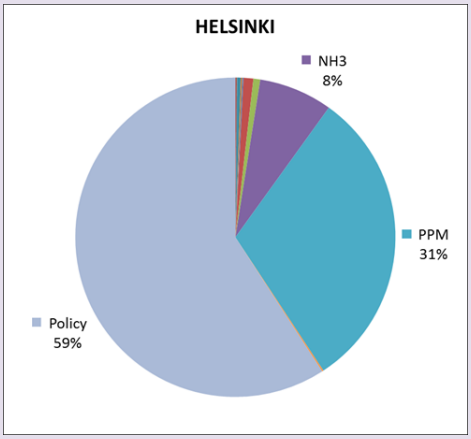
<tr><td rowspan="8"> 
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<tr><td>α_PPM</td><td>0.50</td><td>0.87×10^{-2}</td></tr>
<tr><td>α_SO₂</td><td>0.26×10^{-2}</td><td>0.04×10^{-2}</td></tr>
<tr><td>HELSINKI</td><td>Finland</td><td colspan="2">Inhabitants: 629,512</td></tr>
<tr><td colspan="4"></td></tr>
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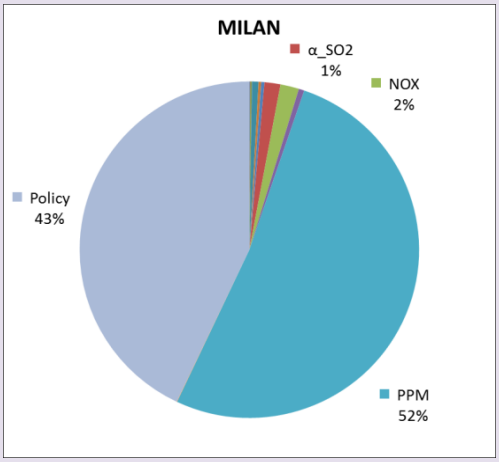
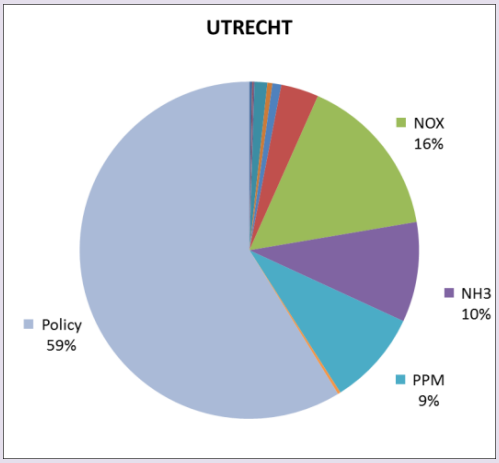
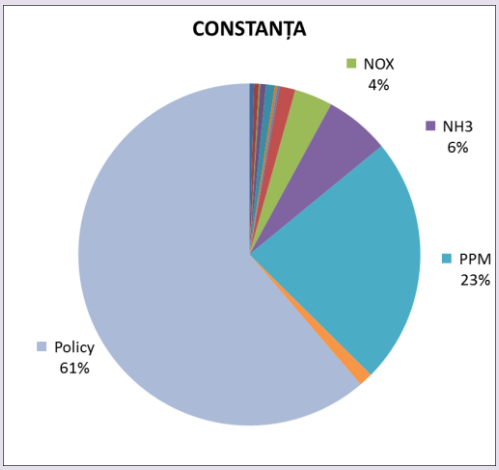
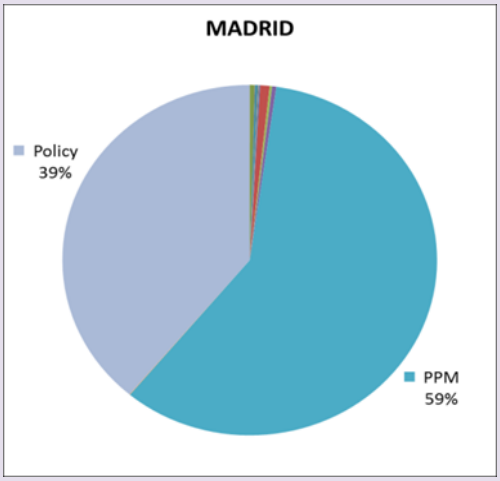
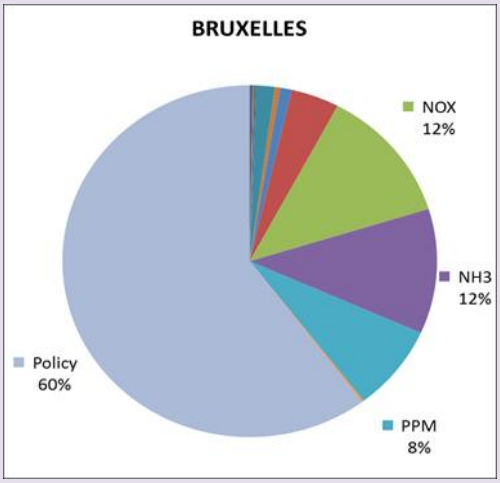
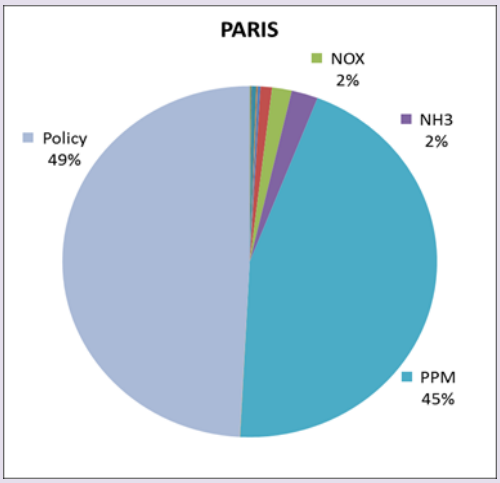
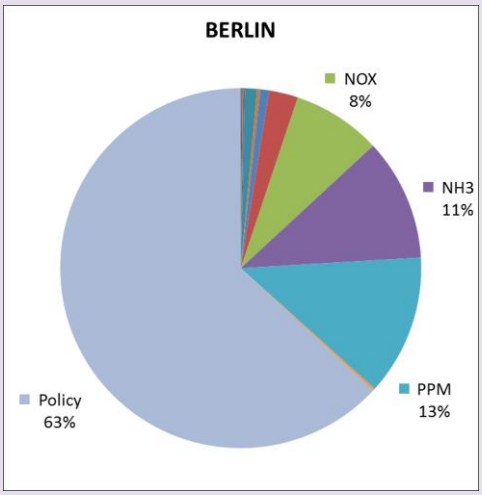
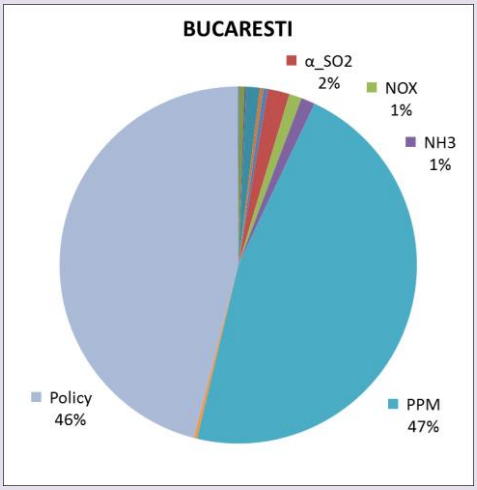
	ω_NO_x	1.97	0.02
	ω_NH_3	1.60	0.02
	ω_PPM	2.33	0.02
	ω_SO_2	1.34	0.91×10^{-2}
	α_NO_x	0.05	0.50×10^{-2}
	α_NH_3	0.07	0.01
	α_PPM	1.97	0.04
	α_SO_2	0.01	0.48×10^{-2}
MILAN	**Italy**	Inhabitants: 1,368,590	
	ω_NO_x	1.87	0.01
	ω_NH_3	1.62	0.01
	ω_PPM	2.51	0.66×10^{-2}
	ω_SO_2	1.38	0.01
	α_NO_x	0.02	0.10×10^{-2}
	α_NH_3	0.04	0.24×10^{-2}
	α_PPM	0.56	0.05
	α_SO_2	0.55×10^{-2}	0.12×10^{-2}
UTRECHT	**The Netherlands**	Inhabitants: 338,000	
	ω_NO_x	1.97	0.02
	ω_NH_3	1.60	0.02
	ω_PPM	2.33	0.02
	ω_SO_2	1.34	0.91×10^{-2}
	α_NO_x	0.05	0.41×10^{-2}
	α_NH_3	0.07	0.39×10^{-2}
	α_PPM	0.53	1.33×10^{-2}
	α_SO_2	0.65×10^{-2}	0.04×10^{-2}
CONSTANȚA	**Romania**	Inhabitants: 300,000	

	ω_NO_x	1.97	0.02
	ω_NH_3	1.60	0.02
	ω_PPM	2.33	0.02
	ω_SO_2	1.34	$0.91x10^{-2}$
	α_NO_x	0.0078	0.0013
	α_NH_3	0.0320	0.0060
	α_PPM	1.5938	0.0198
	α_SO_2	0.0084	0.0021
MADRID	**Spain**	Inhabitants: 3,141,991	
	ω_NO_x	1.87	0.01
	ω_NH_3	1.62	0.01
	ω_PPM	2.51	$0.66x10^{-2}$
	ω_SO_2	1.38	0.01
	α_NO_x	0.0180	0.0011
	α_NH_3	0.0506	0.0031
	α_PPM	0.4518	0.0407
	α_SO_2	0.0036	0.0011
BRUSSELS	**Belgium**	Inhabitants: 1,175,173	
	ω_NO_x	1.87	0.01
	ω_NH_3	1.62	0.01
	ω_PPM	2.51	$0.66x10^{-2}$
	ω_SO_2	1.38	0.01
	α_NO_x	0.01	$0.08x10^{-2}$
	α_NH_3	0.06	$0.47x10^{-2}$
	α_PPM	0.92	$1.69x10^{-2}$
	α_SO_2	$0.35x10^{-2}$	$0.13x10^{-2}$
PARIS	**France**	Inhabitants: 2,229,621	

	**ω_NO_x**	1.87	0.01
	ω_NH_3	1.62	0.01
	ω_PPM	2.51	$0.66x10^{-2}$
	ω_SO_2	1.38	0.01
	α_NO_x	0.02	$0.11x10^{-2}$
	α_NH_3	0.08	$0.40x10^{-2}$
	α_PPM	0.57	$3.50x10^{-2}$
	α_SO_2	$0.39x10^{-2}$	$0.08x10^{-2}$
BERLIN	**Germany**	Inhabitants: 3,670,622	
	**ω_NO_x**	1.97	0.02
	ω_NH_3	1.60	0.02
	ω_PPM	2.33	0.02
	ω_SO_2	1.34	$0.91x10^{-2}$
	α_NO_x	0.04	$0.69x10^{-2}$
	α_NH_3	0.06	0.01
	α_PPM	0.95	0.02
	α_SO_2	$0.76x10^{-2}$	$0.11x10^{-2}$
BUCURESTI	**Romania**	Inhabitants: 1,883,425	

Annex 2. An on-line EC Application for Sensitivity Indices Estimate

Introduction

In order to assist the European commission in their daily work, the Sensitivity Analysis of Model Output (SAMO) team of the Competence Center in Modelling (CC-MOD) in Directorate I (Competence) has developed the present online application to allow any modellers within the Commission to compute variance-based sensitivity indices also called Sobol' indices (Sobol', 1993) from given Monte Carlo samples. It is assumed then that the modeller has drawn *N* independent set of values of the model input **X** and for each draw has executed/run the model and calculated the response of interest *y*. For example, the modeller has the following samples at hand:

$\mathbf{X}=\begin{bmatrix} X_{11} & \cdots & X_{1d} \\ \vdots & \ddots & \vdots \\ X_{N1} & \cdots & X_{Nd} \end{bmatrix}$ and $\mathrm{Y} = \begin{bmatrix} Y_1 \\ \vdots \\ Y_N \end{bmatrix}$, where each corresponds to a model run.

The purpose is then to assess the relative importance of each input variable x_i against the output y. This can be achieved (under the independence assumption of the x-variables) by decomposing the variance of y in terms of partial contributions stemming from each input variable (so individually or in cooperation with others) as follows:

$$V(Y) = \sum_{i=1}^{d} V_i + \sum_{i=1}^{d}\sum_{j=1}^{d} V_{ij} + \sum_{i=1}^{d}\sum_{j=1}^{d}\sum_{k=1}^{d} V_{ijk} \ldots + V_{1,2,\ldots,d} \qquad (2.1)$$

where V_i is the individual contribution of x_i while V_{ij} is a mutual contribution of (x_i,x_j) called interaction, etc.

It is usually more convenient to normalise the variables., i.e. to have ranges [0.0, 1.0] which leads to the concept of variance-based sensitivity indices (or Sobol' indices),

$$1 = \sum_{i=1}^{d} S_i + \sum_{i=1}^{d}\sum_{j=1}^{d} S_{ij} + \sum_{i=1}^{d}\sum_{j=1}^{d}\sum_{k=1}^{d} S_{ijk} \ldots + S_{1,2,\ldots,d} \qquad (2.2)$$

with the nice property that they sum-up to one. They measure the amount of the variance of y due to x_i alone (i.e. S_i) or by its interactions with the other variables (e.g. S_{ij}, S_{ijk}). The higher its contribution the more y is sensitive to x_i. It is also convenient to introduce the total sensitivity index that capture the overall contributions of x_i (Homma & Saltelli, 1996),

$$ST_i = S_i + \sum_{j\neq i}^{d} S_{ij} + \sum_{k\neq j\neq i}^{d} S_{ijk} + \cdots \qquad (2.3)$$

If $ST_i = 0$, then x_i is deemed non-important for the model response.

Details about the Web-App

Step 1: uploading the data

By clicking on the link http://siprapp01-riod.jrc.org:3838/SA_app/ the user is connected to the remote application. The welcome page is depicted in fig. A1. On the left-hand side, the user has to specify the format of the data to be uploaded. The latter can be a csv file or any ASCII format like *'txt'*, data with a specific separator (comma, semicolon, tabulation). It is not mandatory but the first row should contain the name of the variables (e.g. x_1;x_2;….;x_d;y).

On this page, one must:

- Click on **Browse** to upload the data from your computer,
- Select or unselect **Header**,
- Specify the **Separator**,
- And possibly indicate whether the header (when any) is **quoted** or not (e.g. "x_1" instead of x_1, …),
- If the data upload is successful, then one can **Execute/Run** the program.

If the data upload is successful one should obtain a result similar to what is depicted in fig. A2, otherwise the results will look like fig. A3.

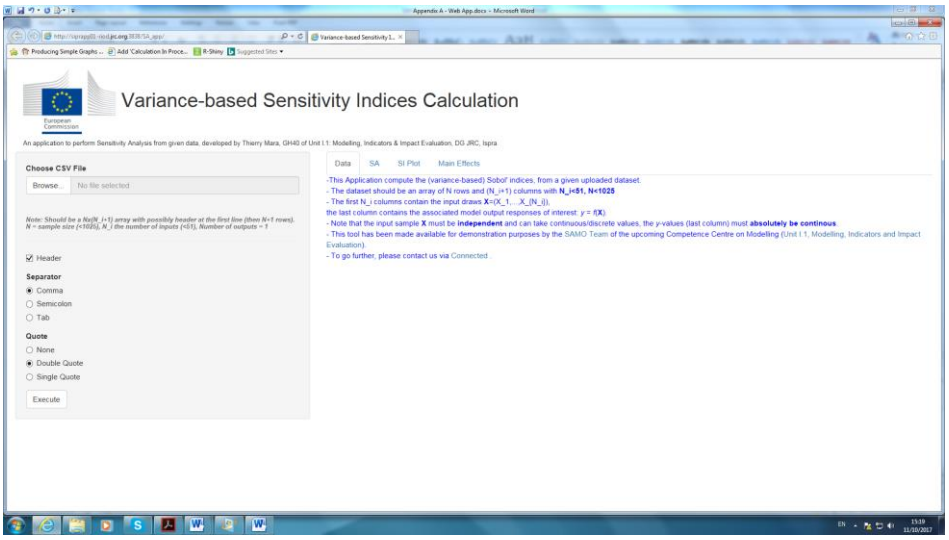


Fig. A1: Welcome page of the Web-App dedicated to sensitivity analysis of model response

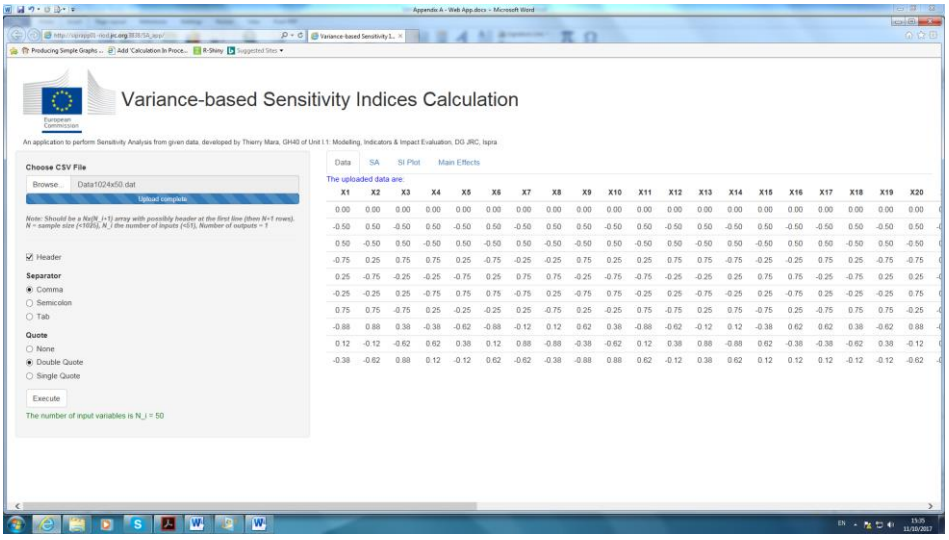


Fig. A2: Successful data upload. The program recognizes the number of input variables.

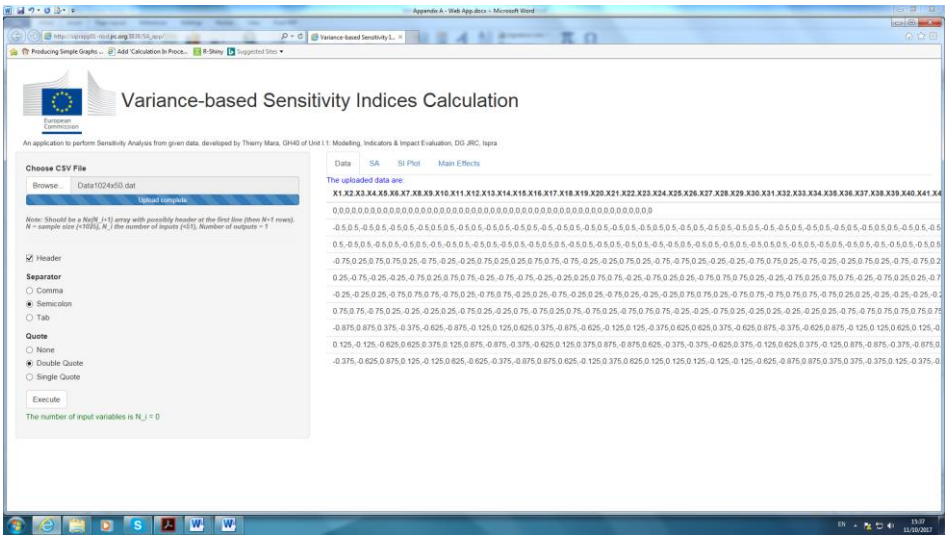


Fig. A3: Failure of the data upload. The program is not able to recognize the number of input variables and the array is not displayed properly.

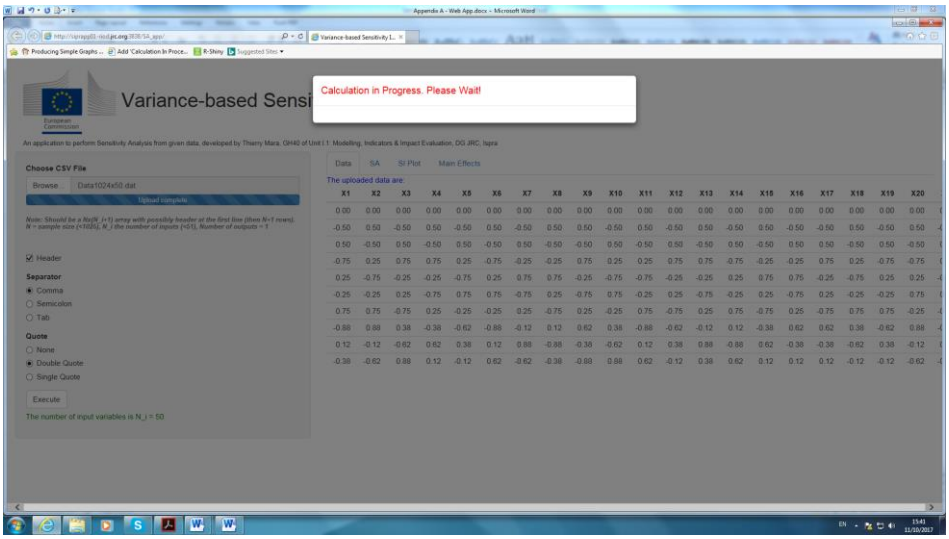


Fig. A4: Window displayed during the program execution.

Step 2: Execution and analysis of the results

When executing/running the program, a message is displayed indicating that the calculation is in progress (see fig. A4). Once the calculation has finished a message appears to warn the user. Then, one can check the results. To this end, three types of result presentation are proposed in different tabs:

- Tab SA (fig. A5): Gives some information about the results of the polynomial chaos expansion (PCE), the N_{pce} (Number of terms in the expansion), the $Q\varepsilon 2$ (amount of variance unexplained by the PCE approximation, a value < 0.10 is recommended), the first-order and total index of each variable, and the variance decomposition as shown in (2.1) and (2.2),

- Tab **SI Plot** (fig. A6): In this tab, the first-order (i.e. S_i) and total-order (i.e. ST_i) are displayed graphically for a faster inference,
- Tab **Main Effects** (fig. A7): Display the marginal effect of each variable (univariate effect) versus the scatterplots. The marginal effect normally shows the trend of the effect of each variable onto the model response *y*.

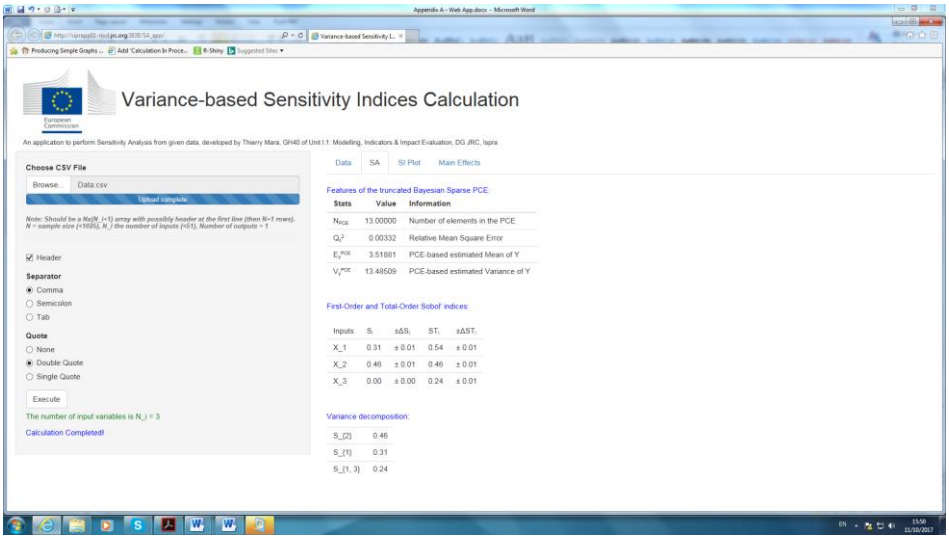


Fig. A5: Results displayed in the tab SA. The results indicate that the PCE contains 13 terms. The unexplained variance is about 3/1000. The estimated first-order sensitivity indices are respectively: S_1=0.31, S_2=0.46 and S_3=0. The total-order sensitivity indices are respectively: ST_1=0.54, ST_2=0.46 and ST_3=0.24. One can infer that x_3 is not important alone but is important because of its interaction with x_1 (S_{13}=0.24). The variance decomposition is: 1 = S_1 + S_2 + S_{13}.

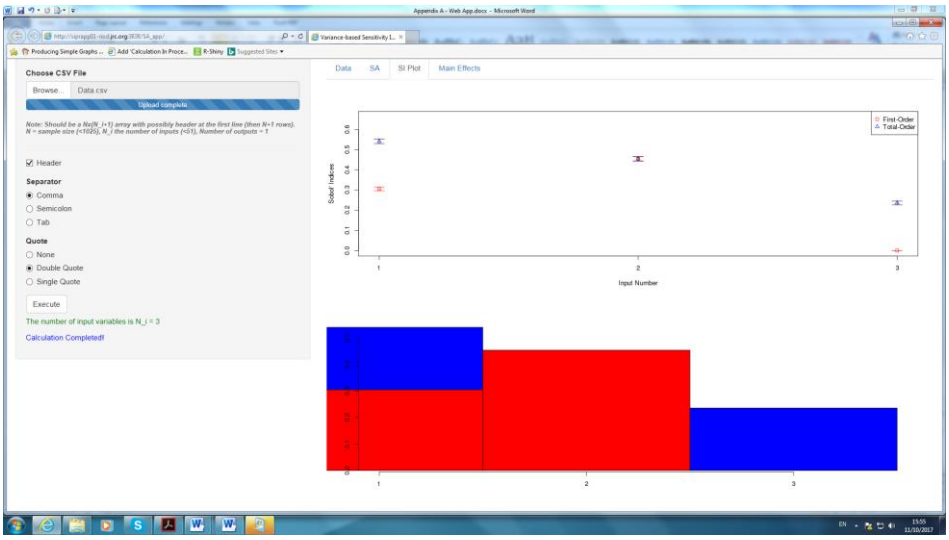


Fig. A6: Results displayed in the tab SI Plot.

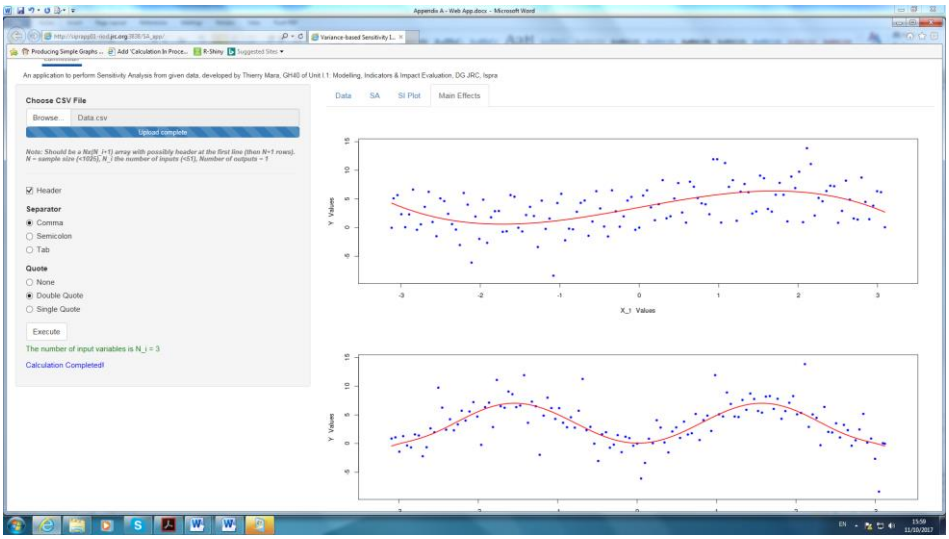


Fig. A7: Results displayed in the tab Main Effects.

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