

## JRC TECHNICAL REPORTS

# Dealing with uncertainty in sustainability assessment

Report on the application of different sensitivity analysis techniques to fieldspecific simulation models



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JRC68035

EUR 25166 EN

ISBN 978-92-79-22726-4 (PDF) ISBN 978-92-79-22725-7 (print) ISSN 1831-9424 (online)

ISSN 1018-5593 (print) doi:10.2788/57452

Luxembourg: Publications Office of the European Union, 2012

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Printed in Italy

#### **Executive Summary**

Assessing sustainability is more and more becoming a common practice in products, policies and institution appraisals. However, increasing concern has been recognized in the scientific community regarding whether the various available examples of sustainability assessment are really comprehensive and able to judge in a robust and reliable way if new developments "meet the needs of the present without compromising the ability of future generations to meet their own needs". Concerns are mainly related to intrinsic vagueness of the sustainability concept itself (sustainable development is, like social justice, a value-laden concept that has many different perceptions) and to the capability of addressing environmental, economic and social issues and their interactions with robust and meaningful measures.

In a sustainability assessment framework, the main sources of uncertainty can be: i) the "sustainable development" concept and the definition of boundaries (physical, economic and social) to assess it, ii) the intrinsic subjectivity of many assessment tools, and iii) the incapability of many available modelling activities to mimic our world. In order to deal with them, it is necessary to identify a suitable conceptual framework able to guide the analysts through a path aimed at increasing their capability to understand the main drivers of their analysis. Only in this way they will be able to quantify the robustness of the results of any assessment.

The problem is that uncertainties behind the comprehension of our world are probably too high to allow us presuming always to provide clear and certain answers on what is sustainable and what is not. All we can do now is trying to find the main sources of uncertainty and to deal with them, so that our answers can include also how confident we might think to be on them.

This report defines a conceptual framework centred upon the phases of sensitivity and uncertainty analysis. The former tries to individuate how the uncertainties in the outputs of the assessment can be apportioned into its inputs. The latter tries to understand how the uncertainty in the inputs affects the outputs of the assessment. In this way the analysts have all the instruments to comprehend to which extent the conclusions of their study are jeopardised by possible errors in the hypotheses made during the assessment itself.

For both sensitivity and uncertainty analysis, different techniques can be adopted. Some of these techniques have been here discussed and applied to field specific models to test their powerfulness in dealing with uncertainty. The report shed light also on some properties of the two modelling framework tested: i) two microscopic traffic simulation models and ii) a site specific spatially resolved model for calculating the fate of contaminant in the environment at a global scale. In this way it also represents a useful guide for the application of sensitivity and uncertainty analysis techniques.

The report is organized as follows: in the first section the main sources of uncertainty and a suitable conceptual framework to deal with them while assessing sustainability are presented. In section 2 and 3 some of the most widely adopted techniques sensitivity and uncertainty analysis are described. Sections 4 and 5 present the results of the application of variance-based sensitivity analysis techniques to i) microscopic traffic simulation models and ii) site specific spatially resolved model for calculating the fate of contaminant in the environment at a global scale. Section 6 reports on the application of uncertainty analysis techniques to a sustainability assessment case-study. In section 7, the intrinsic difference between uncertainty and fuzziness and possible implications for sustainability assessment are introduced, whereas in section 8 the concluding remarks of the work carried out are reported.

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#### 1. Introduction

Assessing sustainability is more and more becoming a common practice in products, policies and institution appraisals. However, increasing concern has been recognized in the scientific community regarding whether the various available examples of sustainability assessment are really comprehensive and able to judge in a robust and reliable way if new developments "meet the needs of the present without compromising the ability of future generations to meet their own needs" (WCDE 1987). Concerns are mainly related to intrinsic vagueness of the sustainability concept itself (sustainable development is, like social justice, a value-laden concept that has many different perceptions) and to the capability of addressing environmental, economic and social issues and their interactions with robust and meaningful measures (Bohringer and Jochem 2007).

Furthermore, there is a lack of both science-based and policy-based boundaries able to define thresholds between what does contribute to a sustainable development and what does not. As a matter of fact, in the common practice, the option selected after a sustainability assessment has no guarantee to contribute to a sustainable development in the sense previously defined.

This issue can be seen under the following light: sustainability assessment should aim at providing a clear answer about the impact on the development of "our" world caused by a certain element of the world itself. This is therefore connected with our capability to foresee this impact. So the real question appears to be: are we able to give such an answer? Is our knowledge sufficient to judge what will help "our" world (here "world" it is not necessarily referred to as ecosystem but more as the way in which we live) to survive like it is now (or even to improve its conditions) and what will instead cause devastating changes?

The answer is, probably, not. Uncertainties behind the comprehension of our world are probably too high to allow us presuming always to provide clear and certain answers on what is sustainable and what is not. All we can do now is trying to individuate the main sources of uncertainty and to deal with them, so that our answers can include also how confident we might think to be on them.

In the present work we have tried to identify and describe the main sources of uncertainties connected with a sustainability assessment. Then, we have proposed a conceptual framework to deal with these uncertainties considering the experience carried out in different scientific fields. Sensitivity and uncertainty analysis are the key components of this framework. The former tries to individuate how the uncertainties in the outputs of the assessment can be apportioned into its inputs. The latter tries to understand how the uncertainty in the inputs to the assessment affects its outputs. In this way the analysts have all the instruments to comprehend to which extent the conclusions of their studies are jeopardised by possible errors in the hypotheses made during the assessment itself.

For both sensitivity and uncertainty analysis, different techniques can be adopted. Some of these techniques have been here discussed and applied to field specific models to test their powerfulness in dealing with uncertainty.

Dealing with uncertainty is a big issue especially for policy makers. It can confuse them, but it can be made policy relevant if results are translated into the likelihood that policy targets will be met. Policy makers,

then, have the choice to either accept the risks, or to take actions that increase the certainty that targets will be met. Basically there are two types of policy risks, i) doing too much (and spoil public money) or, ii) doing too little (and be confronted with irreversible environmental problems later). The acceptance of the different types of policy risks will depend on the preference of the chosen politicians and the priorities they will give to environmental, social and economic stakes. The careful politician will easily realize that policies can be made more robust when risks are acknowledged and adaptations are made to minimize the risks (or to define a strategy on how to respond when risks would really occur).

#### 1.1. Uncertainty sources in sustainability assessment and strategies to deal with them

Given the previous definition of sustainability assessment, it is possible to identify three main sources of uncertainty:

- 1. the "sustainable development" concept and the definition of boundaries (physical, economic and social) to assess it;
  - 2. the intrinsic subjectivity of many assessment tools;
  - 3. the incapability of many available modelling activities to mimic our world.

The first source of uncertainty is so painful that almost all sustainability assessment studies end up comparing different alternative scenarios, with the assessment trying to individuate which alterative may lead to a more sustainable development. The problem is that, even if some global boundaries may exist (scientists are proposing some environmental boundaries for our planet, see, e.g. Rockstrom et al. 2009, Sverdrup and Ragnarsdottir, 2011), it is very difficult to assess how much a certain product, policy or institution can contribute to its fulfilment. The only possibility would be if thresholds are defined at a political level, with policy makers taking the responsibility of deciding each sector how much has to contribute to the achievements of global goals. It is basically what initiated by European Commission with the Europe 2020 strategy (http://ec.europa.eu/europe2020/index\_en.htm), but that should have been further specified by the governments of the members states in order to direct the national development strategies in a more effective way. Thresholds approach in decision theory (sometimes also known as "what to" approach) is very important when there are boundaries that can lead to major consequences if crossed (Polasky et al., 2011). This is the case of climate change: if we will maintain the CO2 concentration in atmosphere above the safety threshold of 350ppm (Rockstrom et al. 2009) for long time, we are not able to foreseen towards which new equilibrium configuration our ecosystem is moving. Our ecosystem is, indeed, a complex system, and a new equilibrium configuration can result to be very different from the present one, with many, unexpected, mechanisms activated without any possibility of control. At the same time focussing only on thresholds can give the misleading impression that "degradation below the threshold level is safe and improvements beyond it are of no value" (Polasky et al., 2011). In addition, most of the thresholds hide considerable and difficult to quantify level of uncertainty and, thus, only relying on some fixed values may turn not to be worthwhile. For this reason any threshold should always be coupled to the level of confidence that has been assumed in its definition (and preferably also to its probability distribution). It is worth noting that some threshold can also assume "fuzzy" values at the beginning of the decision process (e.g. considerations like "concentration of pollutant in urban cities has to be reduced" is a typical example). This has not to be confused the concept of uncertainty. The decision process acts as de-fuzzyfying filter in the sense that takes the fuzzy information as input and produces the clear threshold as output (Boschetti, 2011). The uncertainty has to be searched in this latter. Further details on this will be provided in section 7.

Alternative to the thresholds approach is the scenario planning (also known as "what if" approach). Scenarios are set of possible futures that are evaluated on the basis of different criteria. In sustainability assessment, scenarios need to be evaluated using criteria pertaining to the three different pillars of the sustainability. In this way it is unlikely to find a scenario that outperforms all the others over all the criteria adopted. For this reason, even with different approaches, in most cases, a single indicator is evaluated as a weighted combination of the criteria (e.g. multi-criteria assessment). In this way it is possible to rank the different options, but, depending on how the criteria are aggregated the order may be very different. This represents the second source of uncertainty that has be considered for sustainability assessment.

Both for the thresholds definition and the appraisal of the different scenarios, sophisticated analyses are required. Independently if they adopt modelling/simulation based approaches or experience based approach (e.g. by means of time series analysis) such analyses require an in-depth understanding of how our world behaves, especially in reaction to the pressure imposed by our society. This is more significant as we consider the world in which we live as a complex system, involving many sub-systems closely interrelated among each other. This is the third source of uncertainty, which rises as soon as we try to understand the system ("What makes modelling and scientific inquiry in general so painful is uncertainty. Uncertainty is not an accident of the scientific method, but its substance", Saltelli et al., 2008). In this case it is not occasional to have the uncertainty used to hide or neglect a problem. A typical example is the Climate Change. Even if the problem is now widely accepted and has rapidly reached the attention of the broader audience, this was not exactly the case up to few years ago. Many sources of uncertainties indeed exists, such as the uncertainty of the likelihood of adverse effects, the uncertainty over the consequences of change, the uncertainty over the speed of changes, the uncertainty about discontinuities, the uncertainty over the effectiveness of policy instruments and so on (Mabey et al. 2011). As it usually happens, focussing the attention on the possible sources of uncertainty has been the way to delay policies able to reduce greenhouse gas emissions (Hansen 2009). It is straightforward that, in this case, all the sources of uncertainty arise from the attempt of modelling several complex processes, like the climate response to the natural and anthropogenic forces and its impact of our society, often mixed in a complex way. To this aim, different kind approaches can be used in order facilitate the public debate (considering again the Climate Change problem, please refer to Boschetti 2011).

In any case, in this third source of uncertainty, part can be directly imputed to the (in)adequacy of the models to reproduce the reality, while another part depends on the (uncertain) model inputs<sup>1</sup>.

Uncertainty due to the inadequacy of models arises from a number of sources. First of all, any kind of model is developed based on the human comprehension of the modelled phenomena. This comprehension is always limited. Though evident and clear since Socrates ("I only know that I know nothing") this seems not always to be clear nowadays in modelling practice (Kay 2011). In any case we should never expect to have model being able to predict the world's evolution under all the possible conditions. Further to this, other sources of uncertainty can be the modelling basic assumptions, the structural equations, the level of discretization, the numerical resolution method, etc. Such sources of uncertainty can be reduced by 'improving' the model concerning one or more of these aspects. As the cost of reducing such uncertainties often results in the increasing of computing time, the choice of the most appropriate modelling framework depends on the specific application and stems from a trade-off between model adequacy and computing time.

As regards the uncertainty in the model inputs, we must distinguish between those inputs which are observable and those which are not. Such distinction is crucial as it affects the possibility, or the cost, of reducing the uncertainty they are responsible for:

- As **observable** we intend those model inputs which have a measurable equivalent in the reality. Thus
  they can be *directly estimated* and used to feed the models.
- Unobservable inputs are those which either are hardly measurable<sup>2</sup>, or have not an actual equivalent in the reality. Many model parameters, for example, either do just not have a physical interpretation (i.e. they are simply model constants), or they are deliberately considered uncertain by the modeller. In facts, as models are necessarily only coarse representations of the real system, considering modelling parameters as uncertain inputs is commonly taken to cover both the epistemic uncertainty regarding the un-modelled details of the phenomena and the ontological (or aleatory) uncertainty not predicted by the average models<sup>3</sup> (e.g. the variability in time of driver's behaviour). Such parameters can be therefore only *indirectly estimated* by means of inverse analysis, calibration, etc. (see also section 5.2)

Since the uncertainty in both the model and the inputs is propagated into the outputs, such uncertainty has to be assessed and, whenever possible, reduced. In facts, a model encompassing a disproportionate amount of uncertainty and thus returning unreliable results, turns out to have no practical utility for the analyst.

<sup>&</sup>lt;sup>1</sup> Also in this case several authors have proposed different classifications of the possible typology of uncertainty. The reader can for example refer to van Asselt et al. (1999)

<sup>&</sup>lt;sup>2</sup>In this context the immeasurability is intended practical rather than theoretical. Some quantities may be not measurable because of operational or economic constraints.

<sup>&</sup>lt;sup>3</sup> Epistemic, or reducible uncertainty, refers to types of uncertainty which can be directly reduced by an increase in available data. Ontological, or irreducible uncertainty, refers to events which remain unpredictable whatever the amount of data available. The difference is clear when looking at the failure rate of an industrial component (epistemic) against its instant of failure (ontological).

In the field of environmental assessment, considerable efforts for quantifying and managing uncertainty have been carried out by many research Institutes.

In the present work we adopt the conceptual framework presented by de Rocquigny et al. (2008) and reported in Figure 1.

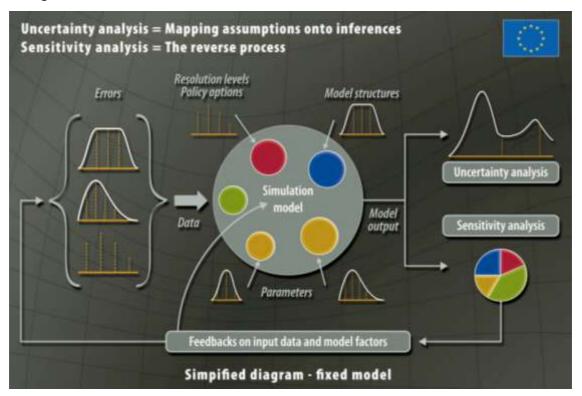


FIGURE 1. Conceptual framework for sensitivity and uncertainty analysis (copyright JRC)

The first step consists in the problem's specification, which involves the definition of the input and the output variables, the model specification and the identification of the quantity of interest for measuring the uncertainty in the outputs. Input variables may be uncertain or fixed mainly being a choice of the analyst. Depending on the problem setting the uncertain model inputs may include all the sources of uncertainty like the parametric or the model uncertainty. Other variables may be fixed, for example, in risk scenarios for comparative studies or, more in general, when the uncertainty of such variable is deemed negligible with respect to the output variables of interest.

The second step is the quantification of the uncertainty sources (uncertainty modelling). In a probabilistic setting this phase implies defining the joint probability density function (pdf) of the uncertain inputs or their marginal pdf with simplified correlation structures or even independence assumptions. It involves gathering information via direct observations, expert judgements, physical arguments or indirect estimation (as for the unobservable inputs in table 5.1) and it is often the most expensive phase of the analysis.

The propagation of the uncertainty is necessary to map the uncertainty in the inputs into the uncertainty measures in the outputs (this is usually referred to as uncertainty analysis, UA). A Monte Carlo simulation framework is often adopted to this aim. In a probabilistic framework the propagation entails the

estimation of the pdf of the output variables of interest, given the pdf of the uncertain inputs, the values of the fixed inputs and the model.

The sensitivity analysis (SA) or *importance ranking* represents the feedback process in the complex of the uncertainty management, and aims at understanding "how uncertainties in the model outputs can be apportioned to different sources of uncertainties in the model inputs" (Saltelli et al., 2004). In other words *the objective of the sensitivity analysis is to instruct the modeller with regards to the relative importance of the uncertain inputs in determining the variable of interest.* In this way the modeller is aware of which model's components deserve more attention in the estimation phase and which can be fixed without affecting too much the results of the assessment. As already pointed out, however, the modeller has few chances to nullify the uncertainty in the model inputs. Therefore, at the end of the analysis, he may fruitfully use an uncertainty analysis to determine the effect of this residual uncertainty on the results of the assessment study.

In conclusion, sensitivity and uncertainty analysis play a fundamental role for increasing the quality and the robustness of the answer provided by a sustainability assessment. In the following the report is providing some details on how to perform them.

#### 2. Model sensitivity analysis. Background

In the present section, we deal with the issue of model sensitivity analysis. Our principal source on this topic is Saltelli et al. (2008) to which the reader who would like to go deep to heart of the subject is suggested to refer. Also the notations used hereafter are the same than those reported in Saltelli et al. (2008) for the sake of simplicity. The sensitivity analysis is an important step to deal with the uncertainties hidden behind the modelling activities. This task is of fundamental importance in order to fight the scepticism that in the recent years the application of models to forecast the effect of policies and measures is attracting (being brought to the attention of a wider audience even by novelists like M. Crichton, Crichton 2004).

Econometricians have been among the first adopting techniques for sensitivity analysis to deal with the uncertainty in their models. Leamer (1983) proposed to use "Global sensitivity analysis" to investigate what happens in the neighbourhood of alternative assumptions and concluded that only if the neighbourhood is wide enough the results of the analysis can be really credible and useful.

Today, sensitivity analysis practices are highly recommended in many guidelines for assessments (e.g. in the 2002 Guidelines for Ensuring and maximizing the Quality, Objectivity, Utility and Integrity of Information Disseminated by Federal Agencies of the U.S. Office of Management and Budget<sup>4</sup>, in the 2009 Impact Assessment Guidelines by the European Commission<sup>5</sup> or in the 2009 Guidance on the Development, Evaluation and Application of Environmental models by U.S. Environmental Protection Agency<sup>6</sup>).

Despite their popularity, it is worth mentioning from the beginning that their use requires a thorough knowledge of the model and of the different techniques that one can think to apply. A non careful application of such techniques to the specific case study may indeed lead to three types of errors: i) assessing as important a non important factor (type I error), ii) assessing as non important an important factor (type II error) and iii) analysing the wrong problem (type III error). For this reason, in the following, different techniques for sensitivity analysis are first described and then, some of them are applied to field specific models, also showing the possible errors one can incur into when performing sensitivity analysis.

Several techniques can be fruitfully exploited to analyze the sensitivity of a model. Among the other we have, i) input/output scatter-plots, ii) Sigma-normalized derivatives, iii) standardized regression coefficient, iv) elementary effects, v) variance-based techniques, vi) Monte Carlo filtering and vii) meta-modelling. In the following some elements of each technique are presented.

#### 2.1. Input/output scatter-plots

Let the model considered be in the form

$$Y = f Z_1, Z_2, \dots, Z_r \tag{1}$$

πιιμ .

<sup>4</sup> http://www.whitehouse.gov/omb/inforeg/

<sup>&</sup>lt;sup>5</sup> http://ec.europa.eu/governance/impact/index\_en.htm

<sup>&</sup>lt;sup>6</sup> http://www.epa.gov/nscep/index.html

being  $Z_i$  (i:1,...,r) the model's input and Y its output. Let's perform a Monte Carlo experiment with our model. This means that, given the statistical distribution of the model inputs, we sample N possible combination of them in order to achieve the following matrix:

Computing Y per each row of the matrix in equation 2 we obtain the vector of model outputs Y.

$$\mathbf{Y} = \begin{array}{c} Y^{(1)} \\ Y^{(2)} \\ \dots \\ Y^{(N)} \end{array}$$

$$(3)$$

If we now plot the elements of  $\mathbf{Y}$  against the correspondent elements of each column of  $\mathbf{M}$ , we obtain r scatter-plots. From the visual analysis of the different scatter-plots it is possible to identify those parameters which have an influence on the model outputs and those parameters which do not. For the parameters able to influence the model outputs, the cloud of points of the scatter plot will have a more or less defined shape. For the others it will approximately resemble a circle. In this way it represents the simplest way to perform sensitivity analysis. The problem is that increasing the variables number, this method becomes unpractical. In addition it does not allow for the sensitivity of group of variables to be investigated.

As an example, let consider the well-known Ishigami test function (Ishigami and Homma 1996):

$$Y = \sin Z_1 + 7 \cdot \sin^2 Z_2 + 0.1 \cdot Z_3^4 \cdot \sin Z_1 + 0 \cdot Z_4 \tag{4}$$

with  $Z_i \sim U - \pi$ ,  $\pi$ . The scatter-plots of the Ishigami model resulting from  $10^4$  samplings from the parameters distributions are reported in Figure 2. From them it is possible to argue that the most important parameter is  $Z_2$ , being that parameters impacting the most on the shape of the scatter-plot.  $Z_4$  does not account for any share of the output variance (it was purposefully added to the model).  $Z_1$  and  $Z_3$  have some impacts on the model outputs ( $Z_1$  more than  $Z_3$ ). These considerations are confirmed by the analysis of the model formulation as in equation 4. However the scatter-plots do not allow understanding that  $Z_3$  has an impact on the model outputs only for its interaction with  $Z_1$ . At the same time  $Z_1$  has a per se impact on the outputs and also with its interaction with  $Z_3$  and this is not taken into account by the scatter-plots.

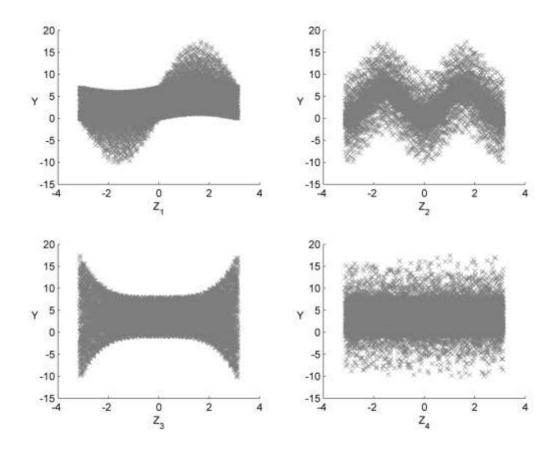


FIGURE 2. Scatter-plots of the Ishigami function

#### 2.2. Sigma-normalized derivatives

Function's derivatives seem to be the most natural way to perform sensitivity analysis, especially for analytical models. In truth derivatives are not always suitable (Saltelli et al. 2008) for this aim. In their place, sigma normalized derivatives are used instead. Considering the previous example, the formulation for sigma-normalized derivatives is the following:

$$S_{Z_i}^{\sigma} = \frac{\sigma_{Z_i} \partial Y}{\sigma_Y \partial Z_i} \tag{5}$$

in which  $S_{Z_i}^{\sigma}$  represents the sensitivity index for the variable  $Z_i$  and  $\sigma$  the standard deviation. It is worth noting that, sensitivity index as in equation (5) is recommended for sensitivity analysis by the Intergovernmental Panel for Climate Change (IPCC, 1999).

The main shortcoming of this approach is for the application with black-box models (like simulation). In this case the derivatives' computation can be very expensive in terms of time. For this reason, in this case, they are usually evaluated only in the middle of the distribution of the single variables and then some hypothesis on the function is made to extrapolate the results obtained to the entire function. When the hypotheses result false, the results achieved may be misleading.

#### 2.3. Standardized regression coefficient

Another possibility for black-box models is to create a regression model on the basis of the evaluations of the function. If we consider again elements of equation 2 and 3, a linear regression model can be written in the form:

$$y^{i} = b_{0} + \sum_{j=1}^{r} b_{Z_{j}} Z_{j}^{i}$$
 (6)

in which  $b_{Z_j}$  are the coefficient of the regression model. Normalizing these coefficients with the standard deviations of input and output, we obtain the sensitivity index

$$\beta_{Z_i} = b_{Z_j} \frac{\sigma_{Z_i}}{\sigma_V} \tag{7}$$

For linear models the sensitivity index in equation (7) coincides with that of equation (5). This holds only in this case. In general standardized regression coefficients are more robust and reliable than sigmanormalized derivatives, resulting from the exploration of the entire space of the input variables. Their precision is however connected with the size of the Monte Carlo experiment, N.

#### 2.4. Elementary Effect Test

It basically consists of an average of derivatives over the space of factors. If the r input variables vary across p levels, the elementary effect of the i-th input variable at the level j is given by:

$$EE_{i,j} = \frac{Y Z_1, \dots, Z_i + \Delta_j, \dots, Z_r - Y Z_1, \dots, Z_r}{\Delta_j}$$
(8)

In which  $\Delta_i$  is the width of the level j.

The sensitivity index for the i-th variable is then evaluated by the following:

$$\mu_i = \frac{1}{p} \sum_{i=1}^p EE_{i,j} \tag{9}$$

which allows for the variables to be ranked. In this way, it can be considered as a screening method, to be preferably used before the application of a more sophisticated method in order to reduce the number of input variables to consider.

#### 2.5. Monte Carlo filtering

When one is not interested at studying the specific value of Y, but if Y is above or below a certain threshold (that is to say if Y creates or not a certain effect), a Monte Carlo filtering can be used. Indeed using a Monte Carlo setting to produce matrix and vector of equations 2 and 3, and then applying the filter of interest to the values of Y, it is possible to divide the matrix M in two groups, one for the variables' values producing one effect and the other for those which not produce it. At this point a statistical test can be carried out to check whether each of the inputs is statistically responsible for the effect to be produced.

#### 2.6. Meta-modelling

A possible way to perform sensitivity analysis of complex black-box models is to use a meta-model able to approximate the output of the model itself. In this way the time required is used to create the meta-model, while the analysis can be then easily performed using its analytical formulation. This topic is attracting the interest of researchers, in particular for some interesting properties of some meta-models. An interested reader can refer to the Chapter 5 of Saltelli et al. (2008).

#### 2.7. Variance-based methods

Variance-based methods have been left to the end of the list since this is the method chosen in our application. For this reason they deserve some more details. Variance-based methods for sensitivity analysis were first employed by (Cukier et al., 1973) and generalize by Sobol to provide a Monte Carlo-based implementation of the concept.

Let us consider again the general model of equation (1). We want to see what happens to the uncertainty of Y if we fix one of the input variables  $Z_i$  to a specific value  $z_i^*$ . The resulting variance of Y, that we call conditional variance, will be  $V_{\mathbf{Z}_{\sim i}}$  Y  $Z_i = z_i^*$ . In which the symbolism in  $\mathbf{Z}_{\sim i}$  means that we are considering the variance across all the variables but the i-th. It is expected that the conditional variance will be as lower than the total variance of Y as bigger is the influence of the variable  $Z_i$ . For this reason the conditional variance can be considered as an index of the sensitivity for  $Z_i$ . The problem with this formulation is that the sensitivity index would depend on the specific value  $z_i^*$  considered. For this reason, we consider the average of this measure over all possible points  $z_i^*$ ,  $E_{Z_i}$ ,  $V_{\mathbf{Z}_{\sim i}}$  Y  $Z_i$ . Furthermore it is known that

$$V Y = E_{Z_i} V_{\mathbf{Z}_{\sim i}} Y Z_i + V_{Z_i} E_{\mathbf{Z}_{\sim i}} Y Z_i$$
 (10)

Equation (10) shows that for  $Z_i$  to be an important factor we need that  $E_{Z_i}$   $V_{\mathbf{Z}_{\sim i}}$  Y  $Z_i$  is small, that it is to say that the closer  $V_{Z_i}$   $E_{\mathbf{Z}_{\sim i}}$  Y  $Z_i$  is to the unconditional variance V Y the higher the influence of  $Z_i$ . Thus we may define our first order sensitivity index of  $Z_i$  with respect to Y as:

$$S_i = \frac{V_{Z_i} \quad E_{\mathbf{Z}_{\sim i}} \quad Y \quad Z_i}{V \quad Y} \tag{11}$$

For a comprehensive physical interpretation of such index refer again to Saltelli et al. (2008).

The first order sensitivity index is a very important measure to understand how much the correct definition of an input to the model may reduce the overall variance of the results. From equations (10) and (11) we have  $S_i \leq 1$ . It is possible to define a model as additive if

$$S_i = 1$$

$$i=1$$
(12)

In this case, indeed, the unconditional variance of the model can be decomposed in the sum of the first order effect of each single variable. Usually this is not the case, meaning that the joint combination of some variables can be responsible for a certain share of the unconditional variance, that is just the definition

of non-additive models. In this case, a low first order sensitivity index does not necessarily imply that the corresponding variable has scarce effect on the output variance, since it might considerably contribute to the total output variance, by means of its combination with the other variables. For this reason, using the so-called ANOVA-HDMR (Analysis of Variance-High Dimensional Model Representation) decomposition developed by Sobol (1993), it is possible to say that a full analysis of a model with r variables requires for all the elements of the following equation to be discovered (in number of  $2^r - 1$ ):

However, the characterization of all the sensitivity indices in equation (13) would require a very expensive experimental work. In order to reduce the efforts required, a synthetic indicator to be coupled with the first order sensitivity index is the total effects index, defined as follows (Homma and Saltelli 1996, Saltelli 2002):

$$S_{T_i} = 1 - \frac{V_{Z_{\sim i}} E_{\mathbf{Z}_i} Y Z_{\sim i}}{V Y} = \frac{E_{Z_{\sim i}} V_{\mathbf{Z}_i} Y Z_{\sim i}}{V Y}$$
(14)

Total effects index of the input factor i provides the sum of all the elements in equation (13) in which the i-th is included. When the total index is  $S_{T_i}=0$  the i-th factor can be fixed without affecting the outputs' variance. If  $S_{T_i}\cong 0$  the approximation made depends on the value of  $S_{T_i}$  (Sobol et al. 2007). It is worth noting that while  $r_{i=1}^r S_i \leq 1$ ,  $r_{i=1}^r S_{T_i} \geq 1$ , both being equal to one only for additive models.

Using the definitions just provided to calculate the Sobol Indices for the parameters of the Ishigami function (equation 4), we obtain the values reported in the second column of the following table.

Index	Theoretical value	Approximated value			
	0.3139	0.3189			
$S_2$	0.4424	0.4459			
$S_3$	0	0.0103			
S <sub>12</sub>	0				
S <sub>13</sub>	0.2437				
S <sub>23</sub>	0				
S <sub>123</sub>	0				
$S_{T1}$	0.5576	0.5559			
$S_{T2}$	0.4424	0.4429			
$S_{T3}$	0.2437	0.2439			

Table 1. Sobol sensitivity indices for the Ishigami function (evaluated using both the definition and the approximated procedure)

The values of the Sobol indices for the input  $Z_4$  have not been reported since they are always 0. The results clearly show what anticipated previously. In addition the allow to prioritize the models inputs:  $Z_2$  is the variable accounting for the highest variance of the outputs without considering second or third order interactions.  $Z_1$  is the variable accounting for the highest share of the output variance considering all the interactions.  $Z_3$  accounts for a good variance share, but only with its interaction with  $Z_1$ .

#### 2.7.1. Variance-based methods. Implementation

In the previous section we have presented the first order and total effects sensitivity indices which will be used in our application. Their simultaneous evaluation, however, is not straightforward. In the present work we use the methodology described in (Saltelli et al. 2008, 2010) and presented hereafter.

The more immediate way for the evaluation of the sensitivity indices, would be the computation of the multidimensional integrals (in a Monte Carlo setting) in the space of the input variables. This would require  $N^2$  model evaluations, for each sensitivity index, being N, again, the size of the Monte Carlo experiment.

This has been revealed to be not necessary (Saltelli 2002). The following procedure has been then adopted:

- two (*N*, *r*) matrix of quasi-random numbers (Saltelli et al. 2010) are generated. Using the random numbers two matrices of values for the input variables of the model as in equation (1) are generated (called **A** and **B** in the following). The tool for quasi-random number generation is freely available on the internet (SIMLAB 2010).

$$\mathbf{A} = \begin{array}{ccccc} z_1^{(1)} & z_2^{(1)} & \cdots & z_r^{(1)} \\ z_1^{(2)} & z_2^{(2)} & \cdots & z_r^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ z_1^{(N)} & z_2^{(N)} & \cdots & z_r^{(N)} \end{array}$$
(15)

$$z_{r+1}^{(1)} \quad z_{r+2}^{(1)} \quad \cdots \quad z_{2r}^{(1)} 
\mathbf{B} = z_{r+1}^{(2)} \quad z_{r+2}^{(2)} \quad \cdots \quad z_{2r}^{(2)} 
\vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \quad \vdots \\
z_{r+1}^{(N)} \quad z_{r+2}^{(N)} \quad \cdots \quad z_{2r}^{(N)}$$
(16)

- a set of *r* matrices, **C**, is obtained assembling *r* matrices equal to **A** except for the *i*-th column (with *i* varying from 1 to *r* among the *r* matrices) that is taken from **B**.

1. the model is evaluated for all the  $[N \cdot (r+2)]$  combinations of input variables as given by matrices **A**, **B** and **C** so as to produce the vectors of outputs  $y_A = f$  **A**,  $y_B = f$  **B** and  $y_{C_i} = f$  **C**<sub>i</sub> for i=1...r. These vectors are sufficient for the evaluation of all the first order and total effects indices. This is the reason why, the application of this technique for variance-based methods requires  $[N \cdot (r+2)]$  which is still a not negligible number for complex and expensive models, but anyway definitely lower than  $N^2 \cdot r$ .

Sensitivity indices can be then evaluated using the following formulations (Saltelli et al. 2010):

$$S_{i} = \frac{\frac{1}{N} \sum_{j=1}^{N} y_{B}^{(j)} \oint_{C_{i}}^{(j)} - y_{A}^{(j)}}{\frac{1}{2N} \sum_{j=1}^{N} \oint_{A+B}^{(j)} \underbrace{}_{-}^{2} - \left(\frac{1}{2N} \sum_{j=1}^{N} y_{A+B}^{(j)}\right)^{2}}$$

$$(18)$$

$$S_{\pi} = \frac{\frac{1}{2N} \sum_{j=1}^{N} \oint_{A}^{(j)} - y_{C_{i}}^{(j)}}{\frac{1}{2N} \sum_{j=1}^{N} \oint_{A+B}^{(j)} - \left(\frac{1}{2N} \sum_{j=1}^{N} y_{A+B}^{(j)}\right)^{2}}$$

$$(19)$$

The choices of N and the input variables distribution are the last points to be discussed in this section. There are no universal recipes in both the cases. N can vary from few hundred to several thousands. A possible strategy to be adopted is to evaluate the indices per each N in the range [1,N], being N a "sufficiently" large number. Then, plotting the sensitivity indices against N, it is possible to recognize if they have reached a stable value (i.e. a value in which they do not depend anymore from N) or not. In case they are not it is possible to increase again N. For this reason, in the following, the results of the sensitivity analysis will be shown in this graphical form.

Instead for what concerns the distribution of the input variables, the only think one can do is to rely upon a priori information (physical meaning of the variables, previous studies, experts' suggestion, etc.). In case they are not available, some preliminary tests should be performed to find the best settings. It is worth considering that an inappropriate definition of the distributions of the input variables may lead to misleading results from the sensitivity analysis. This is the reason why this phase of the study (also referred to as data-assimilation) can be considered as the most crucial one, deserving a lot of attention and efforts.

In Table 1, results of the application of equations (18) and (19) to the Ishigami function are also reported. As one may see, they produce a good approximation of the correct values. The Monte Carlo experimental size *N* was set to 3.000 and the previously mentioned check on the indices stability gave positive results.

#### 3. Uncertainty analysis. Background

In our report we refer to the uncertainty analysis considering those techniques allowing identifying how the uncertainty in the inputs and the parameters of the model propagates into the outputs. With the sensitivity analysis it is possible to individuate those parameters/inputs accounting for the highest share of the uncertainty in the outputs. In this way the analyst knows where to focus his attention in order reduce the uncertainty in the outputs. With the uncertainty analysis we are willing to know how uncertain is the answer that we will give based on the outputs of the model. In this phase, thus, the focus is not on the uncertainty reduction, but, rather, on its quantification (see, e.g. Muleta and Nicklow 2005).

Uncertainty analysis of model outputs is becoming a common practice in many fields (see e.g. the indications reported by the Journal of Fluid Engineering Policy Editors to their authors, Rood and Telionis 1991 and the critics to the authors who do not consider uncertainty analysis as an important phase reported in Pappenberger and Beven 2006). Many techniques have been developed over the last decades. However, all the techniques require an a priori knowledge of the uncertainty in the model inputs. This phase is crucial as this a priori knowledge is usually almost unknown or hardly quantifiable. In the last years, a technique which has become widely adopted is based on structured expert judgement. According to Kurovicka and Cook (2006), main features of the structured (in the sense that the experts are identifiable, the assessments are traceable and the computations are transparent) expert judgements are the following:

- 2. expert are selected;
- 3. experts are asked individually about the uncertainty in measurements and observations in their field of expertise;
- 4. experts are tested to give values to measures within their field;
- 5. experts are treated as statistical hypotheses and are scored "with regard to statistical likelihood and informativeness";
- 6. scores are used to create weights.;
- 7. likelihood and informativeness scores are used to derive performance-based weighted combinations of the experts' uncertainty distributions.

According to Kurovicka and Cook (2006) this objective approach has proven its usefulness, in particular if compared with equal weight combinations of expert distributions.

At the end of the survey with the experts, the analyst should have gathered an estimation of two important elements: the marginal distribution of each uncertain variable and the correlation structure among the different variables. Given such information, a Monte Carlo based approach can be fruitfully used to perform uncertainty analysis (see e.g. Thompson et al. 1992).

As described in section 2.7.1, in a Monte Carlo setting N different model inputs combination are extracted from their estimated multivariate distributions, being N, again, the size of the Monte Carlo experiment (also in this case Sobol sequences can be adopted, Sobol, 1976). Per each inputs combination, the model is evaluated. At the end of the process, the analyst will have the results from N model evaluations.

From these evaluations he can draw inference about the (empirical) distribution of the uncertainty in the outputs. At this point, providing information about the confidence of the results achieved by the model is straightforward.

Main issue of this approach is the specification of reliable multivariate distributions of the model inputs. Providing more details on this issue is, however, beyond the aim of the present study. In Section 6 we will present an application of Monte Carlo base Uncertainty analysis to the sustainability assessment case study reported in Dorini et al. (2011).

Finally, as highlighted for sensitivity analysis in section 2.8, the correlation of the parameters may have a relevant and misleading role also for the uncertainty analysis. Let, for example, consider a model with two parameters with a strict correlation (e.g. a linear dependence between the two). Adopting a Monte Carlo approach to perform uncertainty analysis without considering this correlation means that we are extracting several combinations of the two parameters that do not satisfy their correlation structure (being therefore not admissible). In this way the model uncertainty would necessarily be overestimated (having been considered several meaningless parameters combinations) with the results of providing a misleading figure of the model performances.

Dealing with correlations is, however, not a trivial task. For further details, please refer to Kurovicka and Cooke (2006).

#### 4. Sensitivity analysis in traffic modelling

The choice of considering traffic models as a case study for the application of sensitivity analysis techniques has basically two motivations. First of all, road traffic, and the transportation system in general, is a significant driver of impacts on our society. These impacts, such as, air pollution, global warming, people frustration, economic losses connected to delays, accidents, and so on, play an important role in the sustainability of the development of our society. For this reason traffic/transportation models are likely to be intensively used in sustainability assessment exercises. Secondly, the intrinsic nature of how traffic generates and evolves makes the assessment of uncertainty in the results of traffic/transport model outputs a very important issue. Nevertheless uncertainty and sensitivity analysis in traffic modelling is an almost novel topic.

To understand how uncertainty enters traffic modelling is useful to make some reasoning on the sources and the nature of uncertainty in traffic systems/models.

Following the distinction made in the introduction between observable and unobservable inputs, in a traffic microscopic model, observable inputs are the network characteristics, the traffic lights timing, the traffic composition, the distribution of vehicles size, etc. Unobservable inputs are instead, for example, the origin-destination (OD) traffic demand, but also most of traffic model parameters that either do just not have a physical interpretation (i.e. they are simply model constants), or they are deliberately considered uncertain by the modeller.

In this way, it is common practice to consider the model uncertainty alongside the parametric inputs. Calibrating the uncertain model parameters against real world outputs allows covering both the ontological (aleatory) uncertainty of the phenomenon and the inaccuracies of the model.

The problem with reducing the parametric inputs uncertainty via inverse analysis – such as indirect estimation or calibration - mainly deals with three factors:

- the scarceness, incompleteness or inconsistency of data as to the model complexity;
- the data measurement errors;
- the computational complexity of the analysis;
- the asymmetry in the importance of uncertain inputs.

The scarceness, incompleteness or inconsistency of data with respect to the complexity of a model may lead either to ill-posed inverse problems - such as the case of the OD matrix estimation - or to biased or not robust estimates of the parameters' pdf, as also in presence of measurement errors. In addition, a high number of parameters can make computationally unfeasible the analysis.

Moreover, most of the models present a pronounced asymmetry in the influence of the parametric inputs on the model outputs, with a small subset of the input parameters accounting for most of the output uncertainty and the others playing little or no role. The calibration of parameters with scarce influence on the outputs and then flat objective functions, for instance, is a hard challenge for any optimisation algorithm.

In this picture, a key role is played by the sensitivity analysis which may serves to a number of useful purposes, depending on which different settings may be defined. The importance ranking of the inputs with

regards to their influence on the outputs uncertainty is the most common function of SA (factor prioritization setting). The analysis can be applied to identify which input parameters really need to be calibrated (factor fixing setting) and which are the observations that are really sensitive to the inputs and therefore useful for the estimation. Reducing the number of parameters to calibrate may make feasible an otherwise unfeasible problem while the definition of the most appropriate observations is crucial to guide in the allocation of resources for the collection of new data. Both are obviously crucial to succeed in the analysis and reducing the analyst' costs.

A part from the importance ranking of the uncertainty sources the sensitivity analysis may be useful to identify the elements of the modelling process (inputs, assumptions, etc.) or the regions of the inputs which are most responsible for the model realizations in the acceptable region or, at the contrary, which cause the exceeding of specific thresholds (i/o mapping setting).

For all these reasons sensitivity analysis may be viewed as a formalized and efficient space-exploring mathematical tool to understand upstream models. It is not surprising that the sensitivity analysis may allow technical errors in the model to be uncovered or may lead to the simplification of model. Often it guides in modifying the uncertainty model or in taking action on the system or design to reduce uncertainty.

Despite of the importance of sensitivity analysis as a preliminary step for model use and analysis, very few examples exist in the literature on traffic modelling. In addition (commonly also to other fields), only a minority of sensitivity analysis practitioners make use of the most sophisticated techniques made available in the recent years.

These few examples basically adopt two main categories of sensitivity analysis approaches:

- One at time (OAT) sensitivity analysis;
- Analysis of Variance (ANOVA) based on experimental design (DoE);

In the first group, the effect of model inputs (parameters) on model outputs are evaluated one at time. This means that one studies the variation in the models outputs connected with the variation of one model input (parameter) at time, while the others are taken fixed to a certain value. This approach, however, completely hides the effect of parameters interaction on model outputs and thus can be used only for purely additive models. This approach has been used by Lownes and Mechemel (2006) and in Mathew and Radhakrishnan (2010) on the VISSIM model in order to prioritize model parameters in terms of effects on the model outputs (the former) and to select the parameters to calibrate (the latter). In Kesting and Treiber (2008) the authors follow the same approach in order to get additional insight on the meaning of the parameters values resulting from the calibration of two car-following models.

In the second group ANOVA technique is used to derive the share of variance in the model output explained by each parameter (and their combinations). Models are evaluated on a certain number of parameters combinations resulting from a Design of Experiment (DoE).

The adoption of this approach allowed Bartin et al. (2006) and Li et al. (2009) to draw inference about the first order effect of the parameters of the Paramics traffic model. The parameters' interaction effects were

not captured since the adopted a two levels (the number of levels represents the number of values considered per each parameter) factorial design. A three levels factorial design has been used in Beegala et al. (2005), in Ciuffo et al. (2007) and in Punzo and Ciuffo (2009) for the AIMSUN traffic model. In the former, however, a fractional factorial design has been considered (in a full factorial design all the parameters combinations at the defined levels are evaluated, while in a fractional factorial design, some of them are avoided, resulting in a weaker coverage of the input space and then in the impossibility to get information on some interactions), and therefore also in this case it was not possible evaluating the effect of parameters combinations. On the contrary, in the other two studies, a three levels full factorial design was used, allowing for the evaluation of the variance explained by the second order interactions between parameters (it is worth knowing that a full factorial design with k levels allows for the identification of all the interactions of order lower than k).

The limitation of the variance based method previously described, mainly lies in the scarce capacity of commonly used DoE techniques in providing a satisfactory exploration of the inputs domain (the model is indeed evaluated for the inputs moving on the edges of the hypercube identified by their levels). A Montecarlo framework, like that presented in Section 2, might overcome this problem, allowing for a deeper exploration of the input space, not necessarily with an increase of models evaluations. For this reason, variance based sensitivity analysis techniques based on quasi-Montecarlo sampling in the parameters space have been used in the present study in order to prioritize the parameters of two car-following models with the purpose of reducing the complexity of the optimization problem connected to their calibration. The authors aim, on one hand, at presenting sufficient elements to demonstrate the usefulness of (variance-based) sensitivity analysis techniques for improving our capabilities of understating and using traffic simulation models, and, on the other hand, at providing some innovative insights into the two car-following models that have been chose as case studies.

The next section describes the two car-following models considered in this preliminary investigation. The description of the case study and of the result achieved will follow. In section 4.4 the calibrations of different sets of parameters for the two models is presented, followed by the section 4.5 summarising the main findings of the study and offering concluding remarks.

#### 4.1. Car-following models

The car-following models selected in this study are the Gipps' car-following model (Gipps 1981) and the Intelligent Driver Model (Treiber et al. 2000). In the following sections, a brief description is presented.

#### 4.1.1. Gipps's car-following model

The Gipps' car-following model is the most famous model pertaining to the class of the "safety distance" or "collision avoidance" models. Models of this class aim to specify a safe following distance and to adapt the driver's behavior in order to always keep it. In practice, the Gipps' model assumes that the following driver chooses his speed such that he is able to keep the minimum distance at a standstill whenever the leader

brakes at its maximum deceleration rate. In case the driver has no vehicles in front, the model defines an acceleration profile able to make the vehicle reaching and maintaining his desired speed.

According to Gipps' model, then, the speed attained by a vehicle at a given time instant  $t + \tau$  (in which the delay  $\tau$  is the "apparent" driver's reaction time (Gipps 1981)), is given by:

$$s_{f} t + \tau$$

$$= min$$

$$b_{f} \cdot \frac{\tau}{2} + \theta + b_{f}^{2} \cdot \frac{\tau}{2} + \theta^{2} - b_{f} \cdot 2 \cdot s_{l} t - s_{f} t - L_{l} + \Delta S^{0} - s_{f} t \cdot \tau - \frac{s_{l}^{2} t}{b}$$

$$(20)$$

in which f and I indicate the follower and the leader, respectively, s is the space travelled by a vehicle and s its speed.  $S_f$  and  $S_f$  are, respectively, the follower's maximum desired speed and maximum acceleration.  $b_f$  and b are, respectively, the "most severe braking that the driver of the following vehicle wishes to undertake" and his estimate of the leader's most severe braking capabilities (in the formulation are considered with their sign). L is the leader's vehicle length and  $\theta$  is a safety margin introduced by Gipps to avoid that the follower decelerates always at his maximum rate.  $\Delta S^0$  is the inter-vehicle spacing at a stop.  $\alpha$ ,  $\beta$  and  $\gamma$  are model parameters that, in the original formulation by Gipps (1981), as well as in the following literature (e.g. Ossen and Hoogendoorn 2008, Wilson 2001, Punzo and Tripodi 2007), are assumed equal to 2.5, 0.025 and 0.5, respectively. As from a modelling point of view they are parameters like the others, in this context we do want understand the part of the total output variance that they explain and if their calibration is necessary in order to improve model performances. However, in order to consider only values which may be really used in the formula, we adopted the modified version presented in Ciuffo et al. (2012), in which  $\alpha$ =1 and  $\beta$ = $\beta$ ( $\gamma$ ).

Finally, in order for equation (20) not to loose global existence, according to Wilson (2001), the following condition must hold:

$$S_f \cdot \frac{1}{b} - \frac{1}{b_f} - \tau - \theta \le 0 \tag{21}$$

For this reason, in the Monte Carlo framework, we discarded all the parameters combinations, which did not respect equation (21). It has to be said that this potentially introduces correlation among parameters, which are the inputs of our sensitivity analysis. As anticipated, this condition imposes careful consideration in setting the analysis, as also mentioned in the presentation of results on Gipps' model.

#### 4.1.2.Intelligent Driver Model (IDM)

The Intelligence Driver Model developed by Treiber et al. (2000) is part of the class of social force models. It is developed by an analogy of the molecular-dynamics method (Helbing and Tilch 1998). The social force concept states that the driving behavior is driven by a sum of social forces, including both the force that pushes the

vehicle to reach the driver's desired speed, and the interaction force that compels the vehicle to keep a suitable distance from the previous vehicle (Wang et al. 2010), definition which, however, does not highlight the theoretical difference with the Gipps's model, for instance.

It is a simple car-following model with descriptive parameters (Treiber et al. 2006), describing the acceleration of a driver as a continuous function of its speed, distance and relative speed with respect the vehicle it has in front (i.e. its leader). The model formulation is the following:

$$s_f t = S_f \cdot 1 - \frac{s_f t}{S_f} - \frac{\Delta S^* t}{\Delta s t - L_l}$$
(22)

where

$$\Delta S^* \ t = \Delta S^0 + max \quad T \cdot s_f \ t + \frac{s_f \ t \cdot s_f \ t - s_l \ t}{2 \cdot S_f \cdot b_f}, 0 \tag{23}$$

According to the original interpretation (Treiber et al. 2000), in equations (22) and (23), f and l, respectively, indicate the follower's and leader's vehicles, s is the space travelled by a vehicle and s and s its speed and acceleration.  $\Delta S^*$  t is the desired distance between leader and follower.  $S_f$  and  $S_f$  and are, respectively, the follower's free flow speed and maximum acceleration.  $b_f$  is the follower comfortable deceleration.  $L_l$  is the leader's vehicle length. T is the minimum time headway and  $\Delta S^0$  the stopping distance.  $\alpha$  and  $\beta$  are other model parameters. As for the Gipps' model, also for the IDM, parameters  $\alpha$  and  $\beta$  have been usually considered fixed at specific values. In particular in the original paper (Treiber et al. 2000),  $\alpha$  was not fixed at a specific value, while  $\beta$  was set to the value of 2. According to the author this value (which is not derived from any physical analogy) allows for the "intelligent" braking strategy to be effective, that is critical situations are resolved by dynamically reverting to a "safe" driving defined by a required minimum deceleration that is at or below the comfortable deceleration (model parameter  $b_f$ ). However, in Treiber et al. (2000) it is only demonstrated that the  $\beta$  needs to be greater than 1 in order for the model to remain a collision free model. For this reason, in the remainder, we will consider it as a parameter, just imposing the condition  $\beta > 1$ . In Treiber et al. (2000) it is also showed that  $b_f$  represents a sort of threshold between normal and emergency braking conditions. This implies that its value can hardly be measured from real driving, but it has to be calibrated.

Differently from the Gipps's model, no constraints have to be imposed on the parameters' values.

All the considerations made concerning the meaning of the parameters for the two car-following models have the role of driving the successive phases in which the variance based sensitivity analysis techniques have been applied.

#### 4.2. Application

#### 4.2.1. Fixed input data

The two car-following models described in the previous section have been fed with the vehicles' trajectories

shown in Figure 3.

Such trajectories were obtained from a series of experiments carried out along roads in areas surrounding Naples, Italy, under real traffic conditions between October 2002 and July 2003. Experiments were performed by driving four vehicles in a platoon along urban and extra-urban roads under different traffic conditions. All vehicles were equipped with kinematic differential GPS receivers that recorded the position of each vehicle at 0.1second intervals. More details on data, including the description of the experiments for their collection and the filter designed to process raw them, can be found in (Punzo et al. 2005 and Punzo and Simonelli 2005).

The trajectory data used here are named in Figure 3 as 30C (on the left) and 30B (on the right). Set 30C is for one-lane urban road and is 6 minutes long, while Set 30B is for a two-lane rural high-way and is 4.2 minutes long. In this study we considered only the trajectories of the first and the second vehicle of each platoon (as shown in the figure). In particular inputs to the models are the trajectory of the first vehicle and the initial position and speed for the second vehicle. The model has to reproduce the whole trajectory of the second vehicle.

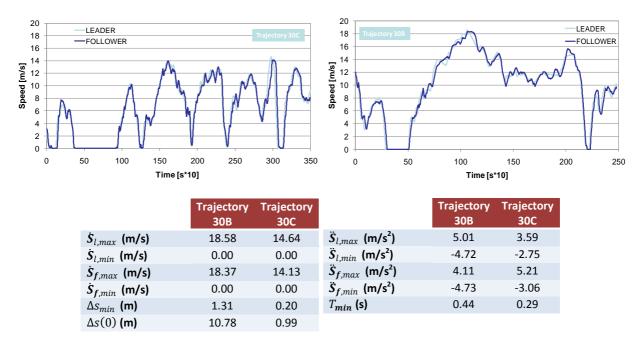


FIGURE 3. Trajectories used in the analysis and main kinematic characteristics. Diagram on the left refer to congested urban conditions (30C), while that on the right to extra-urban conditions (30B). For the two trajectory pairs maximum and minimum speed and acceleration, minimum time headway, minimum spacing and spacing at the beginning of the simulation are reported.

#### 4.2.2. Setting up the method for car-following models

For all the model evaluations required to perform the sensitivity analysis, data described in section 4.1 are used always in the same way (they are fixed inputs). The inputs that will vary are instead the model parameters (that we have described in section 4.1). In this way, the analysis will inform the modeller only on the importance in influencing the outputs of those inputs that are left to vary, but neither of other parameters

kept fixed, nor of any other information fed into the model. Therefore results are conditional on the rest of information fed into the model, namely on the leaders' trajectories. We will see if and how such fixed inputs influence results. Conversely, the analysis will inform us about the richness of trajectory data needed in order to perform a correct analysis and successive calibration.

In general methodology to perform a sensitivity analysis consists of three steps:

- Data assimilation
- Uncertainty propagation
- Computation of sensitivity indices

Characterizing uncertainties in the inputs is the objective of the first phase. In our analysis we seek for the appropriate space of car-following parameters. "Appropriate" meaning that a too tight range for a parameter might fictitiously limit its influence on model outputs, whereas a too large space implies incorporating so much uncertainty to make model predictions of no practical use. To accomplish this task it is possible to rely on experimental observations, theoretical arguments, inverse analysis results (e.g. model parameter estimation) or expert opinions.

The second step consists in propagating the uncertainty in the inputs into the outputs by means of the model, in order to be able to evaluate which portion of the output uncertainty each input factor accounts for. Such propagation may be done in a Monte Carlo framework which allows us to select quasi random combinations of the inputs assuring undistorted and wider coverage of the input space with respect to fixed grid approaches. This phase has been carried out following the method described in section 2.7.1, in particular, equations (15), (16) and (17).

Finally the sensitivity analysis is here performed applying first order sensitivity indices and total effects as described by the formulas (18) and (19).

It is worth noting that, in our setting, the output uncertainty resulting from each simulation is quantified through the distance between the follower's trajectory simulated by the model and the one measured in the reality (the blue ones in Figure 2). Such distance has been evaluated by the Root Mean Square Error (RMSE):

$$RMSE \ x, y = \frac{1}{H} \int_{i=1}^{H} x_i - y_i^2$$
 (24)

where x and y are, respectively, the simulated and observed measurements and H is the length of the time series (in this case the number of observations in the trajectory). In order to check also the influence of the measure adopted on the sensitivity analysis results, two different measures were considered: the vehicle's speed and the spacing with respect to his leader.

Table 1 presents the results of the data assimilation phase, commented below together with the results of the sensitivity analysis for each model.

	IDM				Gipps					
Parameter	LB1	UB1	LB(B)	UB(B)	LB(C)	UB(C)	LB(B)	UB(B)	LB(C)	LB(C)
$\alpha$	0.1	10.0	1.0	8.0	1.0	8.0				
β	0.1	10.0	1.0	5.0	1.0	5.0				
$S_f$	0.5	2.5	1.0	8.0	1.0	8.0	4.7	8.0	3.4	8.0
$b_f$	0.0	2.5	0.5	7.5	0.5	7.5	2.0	8.0	2.0	8.0
$\Delta S^0$	5.0	25.0	0.1	2.0	0.1	1.0	0.1	2.0	0.1	1.0
<i>T</i>	0.0	2.0	0.1	1.0	0.1	1.0				
$S_f$	20.0	60.0	18.4	2.05	14.1	25.0	18.4	25.0	14.1	25.0
γ							-4.0	4.0	-4.0	4.0
b							2.0	8.0	2.0	8.0
$\boldsymbol{\theta}$							0.05	0.5	0.05	0.5
τ							0.1	1.0	0.1	1.0

Table 2. Input factors space adopted. Additional columns for IDM model derive from information reported in Hoogendoorn and Hoogendoorn (2010). Letters C and B among parentheses respectively refer to trajectories 30C and 30B mentioned in section 4.1.

#### 4.2.3.Results – Intelligent Driver Model

Data assimilation phase for the IDM was based on the results of the parameter estimation carried out in (Hoogendoorn and Hogendoorn 2010). In that work, the distributions of five model parameters (i.e. excluded  $\alpha$  and  $\beta$ ) were estimated on four datasets of different size (1, 10, 25 and 100 trajectories). With the increase of size it was observed an improvement of estimation results as well as a decrease of the input space amplitude. Not to have too tight ranges it was decided to take values from the estimation results on the sample of 25 trajectories. Corresponding upper and lower bounds are reported in Table 1 as LB1 and UB1. For the sake of simplicity and to be fair with the other model, the parameters were assumed to be uniformly distributed over their domain.

As the IDM model counts for seven input factors (parameters) the evaluation of the sensitivity indices required  $N\cdot(7+2)$  model simulations. As previously stated, we considered increasing values of N, and then checked a posteriori if those values were sufficiently high to obtain stable indices (we stopped our analysis at N=10.000, that is after 90.000 model runs).

Figure 4 shows the results are for the model fed with the urban congested trajectory (30C). Results are presented in terms of total sensitivity indices of each parameter, for the speed and the spacing measures (left and right plots, respectively).

Regarding to the number of model evaluations, N=3000 proved to be sufficient for the indices to be stable. Results for both the measures were similar, that is, the maximum speed explaining (with all its interactions) around the 80% of the outputs' variance, followed by the two exponents  $\alpha$  and  $\beta$ . All the other parameters resulted not significant.

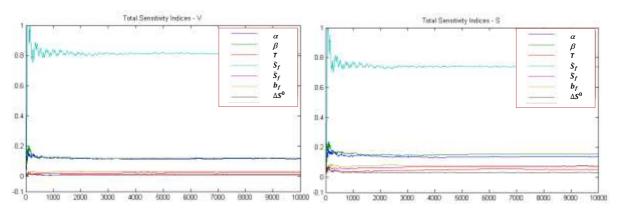


FIGURE 4. Total sensitivity indices for IDM parameters based on speed (left) and spacing (right) measures. Model is fed with the 30C leader's trajectory, and with parameter values sampled from the ranges defined by LB1 and UB1 in Table 1.

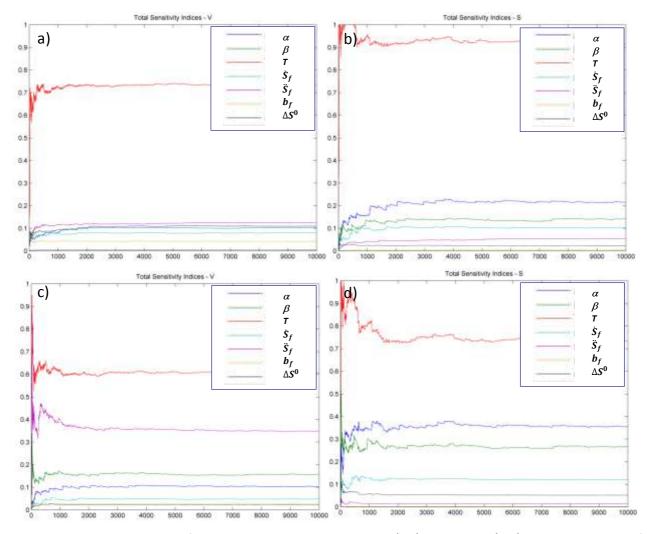


FIGURE 5. Total sensitivity indices for IDM parameters based on speed (a-c) and spacing (b-d) measures. Model is fed with the 30C (a-b) and 30B (c-d) leader's trajectories, and with parameter values sampled from the ranges defined by LB(C), UB(C), LB(B) and UB(B) in Table 1

Given such results it was decided to repeat the analysis enlarging the parameters space. This was done considering the parameters physical meaning outlined in the previous section and the kinematic characteristics of the trajectories as reported in Figure 3. As a result we considered the ranges LB(C)-UB(C) and LB(B)-UB(B) reported in Table 1. In particular we considered a wider interval for  $S_f$  and  $b_f$ , being their meaning

not as clear as one can imagine (as detailed in the previous section), and a narrower interval for  $\Delta S^0$  and  $S_f$  in order to be more in line with the trajectories peculiarities.

Figure 5 shows the results, which are completely different both for what concerns the speed and the spacing. Actually the new pattern of results in Figure 5 confirmed the guess that results of the first data assimilation phase were not satisfactory. The excessive importance of the maximum speed, accounting for the most of the output variance (see Figure 4), suggests indeed that the problem was in the range adopted for the maximum speed (taken from Hoogendorn and Hoogendoorn 2010) which is clearly not consistent with trajectory 30C used to fed the model here (in Hoogendoorn and Hoogendoorn 2010 freeway trajectories were collected). This is a typical example of the type I and type II errors one can make when performing sensitivity analysis without a proper knowledge on the range in which the model inputs may really vary.

With the second setting all the parameters turned out to be significant, apart from the stopping distance. This suggests that it is the only parameter for which the calibration might be avoided (but kept fixed at a reasonable value), as it does not account for a significant portion of the output uncertainty.

The most influencing parameters turned out to be the minimum time headway for both trajectories and measure considered. Also the two exponents  $\alpha$  and  $\beta$ , accounted for a significant share of the output variance confirming the necessity to include them in any model calibration. Considering Figure 5(a-c), it resulted that also the maximum acceleration explained a significant share of the speed variance, while in Figure 5(b-d) it is shown that the maximum speed accounts for a certain share of the spacing variance. This also highlights the differences arising using different measures for the sensitivity analysis.

The impact of choosing different fixed inputs to the model can be also investigated. Indeed comparing Figure 5(a-b) with Figure 5(c-d), it is possible to notice that the parameters' prioritization, in terms of share of variance explained, does not change. However the share specific portion of the output variance explained by each single parameter may vary significantly (see for example the  $S_f$  that in Figure 5(a) results accounting for the 10% of the outputs' variance while in Figure 5(c) for approximately the 40%).

The impact of these considerations on model calibration will be analyzed in section 5.

## 4.2.4.Results – Gipps' car-following model

As shown in Table 1, the Gipps' model counts for 8 input factors (parameters). This means that the computation of the sensitivity indices requires N·(8+2) model evaluations. Also in this case N=10.000 was considered, thus requiring 100.000 evaluations. Parameters distribution was assumed to be uniform as in the IDM case. Upper and lower bounds of parameters were initially chosen basing on the authors experience and successively refined through some preliminary tests (in particular the values of  $\gamma$  which is usually kept fixed). Final values are reported in Table 1 and purposefully consider the trajectories kinematic characteristics reported in Figure 3.

In Figure 6 the first results are presented for the trajectory 30C. Besides the total sensitivity indices (Figure 6b-d), here also the first order sensitivity indices (a-c) for spacing (a-b) and speed (c-d) are shown. Also

in this case all the results are almost stable for N higher than 6000.

From the picture it is possible to observe a slight difference between the results achieved using the spacing and those using the speed. In both the cases the most important parameter is  $b_f$ . This was expected, being the trajectory characterized by frequent and intense acceleration and deceleration phases. Other parameters explaining a considerable share of the outputs' variance are the apparent reaction time  $\tau$  and the follower's estimation of the leader maximum deceleration b. It is interesting to notice the difference between the first order and the total sensitivity indices. The outputs' variance explained by b is indeed approximately constant, meaning that this parameter has few interactions with the others. On the contrary both  $b_f$  and  $\tau$  increase the share of variance explained in combination with other parameters approximately of the same magnitude. It is therefore presumable that their interaction has an important role on the model outputs. This is of course confirmed by the model formulation and in particular by equation (20). Even more interesting, in this light, are the results for  $\gamma$ ,  $S_f$  and  $S_f$ : looking at Figure 6(c), they appear to have negligible influence on the outputs, but looking at Figure 6(d) they reveal a high impact (with  $\gamma$  scoring as second most influent parameter). This means that their combinations have an important role in the model. This can be clearly seen from equation (22) where they are all part of the second term of the equation.

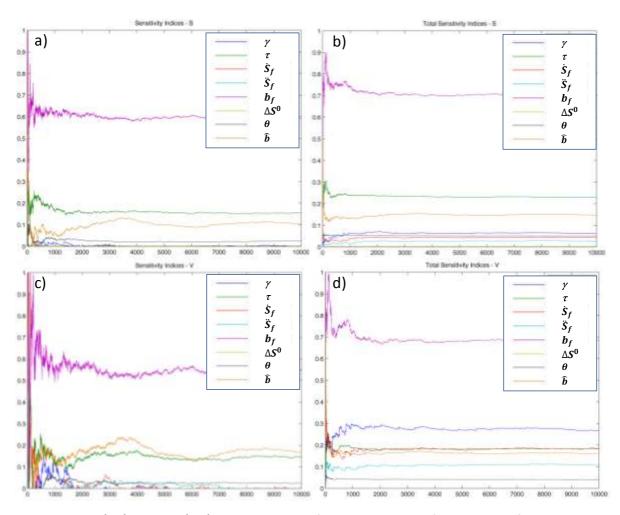


FIGURE 6. First order (a-c) and total (b-d) sensitivity indices for the parameters of the Gipps car-following model on the 30C trajectory, considering the vehicle's speed (c-d) and the vehicles' spacing (a-b)

This is an important outcome of the present study, since it clearly demonstrates that all the studies where only the first order sensitivity indices are provided might lead to erroneous and misleading results. In Addition it further confirm the necessity of calibrating the  $\alpha$ ,  $\beta$  and  $\gamma$  parameters of the acceleration portion of the Gipps' model.

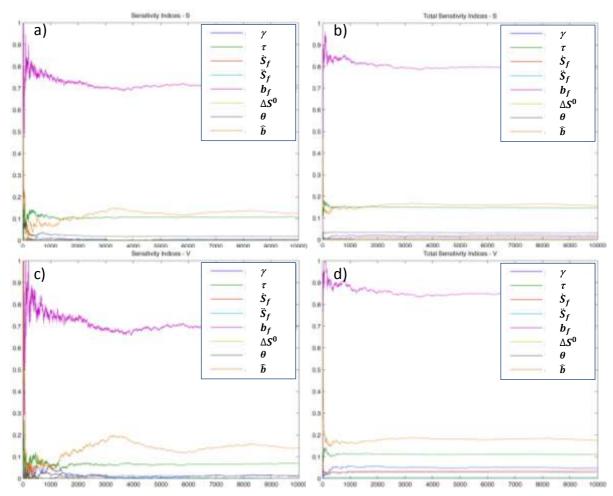


FIGURE 7. First order (a-c) and total (b-d) sensitivity indices for the parameters of the Gipps car-following model on the 30B trajectory, considering the vehicle's speed (c-d) and the vehicles' spacing (a-b)

The previously outlined behaviour is less evident if we consider the results of the sensitivity analysis on the trajectory 30B. In this case, the parameters' prioritization is the same as for trajectory 30C, apart from the total sensitivity indices using the speed as measure. Here the role played by the acceleration part of the model is less significant, being much less frequent and important the acceleration/deceleration phases.

Before concluding the discussion, it is worth noting that the results for the Gipps model might require further investigations mainly because of the correlation introduced by equation (21) among parameters and of the approach adopted here for their generation. Indeed, not to incur in model solution existence problems and to assure a random coverage of the input space, a rejection approach was here adopted in the generation of the  $N \cdot (r+2)$  combinations of inputs (that is discarding the quasi-random numbers that led to the violation of condition in equation 21). To the authors' opinion this should not introduce real correlations, since equation (21) just introduce a discontinuity in the parameters' domain. Outside this discontinuity, however, the parameters domains are equally covered by the experimental procedure.

## 4.3. Impact of sensitivity analysis on model calibration

In this section we test the results of the sensitivity analysis for the two car-following model on their calibration against the two trajectories considered. In particular, we want to investigate what happens if those parameters showing a negligible impact on the outputs' variance are considered fixed (to randomly extracted values) during the model calibration. It is worth underlying here, that with the present analysis, we do not yet intend to propose a methodological framework for calibrating car-following models, since many aspects are still under investigation and will be presented in future works. Here we want to use the calibrations just as a case study to show how useful can be the results of a model sensitivity analysis.

To this aim, looking at the total sensitivity indices of both the models' parameters on the different trajectories/measures combinations, we performed 40 calibration experiments as detailed in the following table. In the table, calibrations defined as "complete" consider all the parameters revealed by the models' formulations, while those defined as "classic" consider only the parameters that in the classical version of the model are not considered as fixed (i.e.  $\beta$ =2 in IDM classic and  $\alpha$ =2.5,  $\beta$ =0.025 and  $\gamma$ =0.5 in Gipps classic).

	IDM Mod	el	Gipps' model				
Calibration	Calibration	Parameters involved	Calibration	Calibration	Parameters		
ID	Reference		ID	Reference	involved		
1	B_complete_S	All	19	B_complete_S	All		
2	B_classic_S	All classic	20	B_classic_S	All classic		
3	B_6_S	$\boldsymbol{b}_f$ , $\Delta S^0$ , $S_f$ , $T$ , $\alpha$ , $\beta$	21	B_3_S	$\boldsymbol{b_f}$ , $\boldsymbol{b}$ , $\tau$		
4	B_4_S	$S_f$ , $T$ , $\alpha$ , $\beta$	22	B_1_S	$b_f$		
5	B_3_S	Τ, α, β	23	B_1_S	b		
6	B_1_S	T	24	B_1_S	τ		
7	C_complete_S	All	25	B_1_S	$S_f$		
8	C_classic_S	All classic	26	C_complete_S	All		
9	C_4_S	$S_f$ , $T$ , $\alpha$ , $\beta$	27	C_classic_S	All classic		
10	C_1_S	T	28	C_3_S	$\boldsymbol{b}_f$ , $\boldsymbol{b}$ , $\tau$		
11	B_complete_V	All	29	C_1_S	$b_f$		
12	B_classic_V	All classic	30	C_1_S	b		
13	B_4_V	$S_f$ , $T$ , $\alpha$ , $\beta$	31	C_1_S	τ		
14	B_2_V	$S_f$ , $T$	32	C_1_S	$S_f$		
15	C_complete_V	All	33	B_complete_V	All		
16	C_classic_V	All classic	34	B_classic_V	All classic		
17	C_5_V	$S_f, S_f, T, \alpha, \beta$	35	B_3_V	$\boldsymbol{b_f}$ , $\boldsymbol{b}$ , $\tau$		
18	C_1_V	T	36	B_1_V	$b_f$		
			37	C_complete_V	All		
			38	C_classic_V	All classic		
			39	C_5_V	$\gamma$ , $\boldsymbol{b}_f$ , $\boldsymbol{b}$ , $\tau$ , $S_f$		
			40	C_1_V	$b_f$		

Table 3. Calibration experiment table. We refer to as "complete" those calibration involving all the parameters reported in the models formulation, while as classic those calibrations involving all the parameter considered in the original models' formulations. "S" indicates those calibration performed using the spacing as model measure, while "V" those calibrations adopting speed. As before "B" indicates the trajectory 30B and "C" the trajectory 30C.

## 4.3.1. Formulation and solution of the calibration problem

Calibrating a simulation model consists of finding the values of its parameters allowing the model itself to reproduce in the best possible way the behaviour of the real system simulated. It is equivalent to the solution of a constrained minimization problem in which the objective function expresses the deviation of the simulated measurements from those observed:

$$\min_{\beta,\gamma} f M^{obs}, M^{sim}$$
 (25)

possibly subject to the following constraints:

$$l_{\beta,i} \leq \beta_i \leq u_{\beta,i}$$
  $i = 1 \dots m$ 

$$l_{\gamma,j} \le \gamma_j \le u_{\gamma,j}$$
  $j = 1 \dots n$ 

and potentially also to other constraints:

$$g_k \beta_i, \gamma_j ? b_k \quad i = 1 ... m, j = 1 ... n, k = 1 ... l$$

where  $\beta_i$  and  $\gamma_i$  are, respectively, the vectors of continuous and discrete model parameters, potentially belonging to m different classes of simulation subjects; f · is the objective function (or fitness or loss function) to be minimized, which measures the distance between the simulated and the observed traffic measurements,  $\mathbf{M}^{sim}$  and  $\mathbf{M}^{obs}$ ;  $\mathbf{l}_{\beta,i}$ ,  $\mathbf{l}_{\gamma,i}$ ,  $\mathbf{u}_{\beta,i}$ ,  $\mathbf{u}_{\gamma,i}$ , are model parameters lower and upper bounds.  $g_k$   $\boldsymbol{\beta}_i$ ,  $\boldsymbol{\gamma}_j$  is a scalar valued linear or non-linear function of the model parameters  $\boldsymbol{\beta}_i$ ,  $\boldsymbol{\gamma}_j$ , that calculates the left hand side of the k-th constraint;  $b_k$  is a constant value equal to the right hand side of the k-th constraint and ? is one the following relational operators: " $\leq$ ", " $\geq$ " or "=".

The problem in equation (25) cannot be solved analytically, since we are dealing with a simulation model. For this reason an optimization algorithm is used instead. In the present case we have used the Opt/Quest Multistart algorithm as implemented in the optimization package Lindo API (Lindo 2003). The good performances of this algorithm in dealing with similar problems have been tested in several studies (see for example Ciuffo et al. 2008 and Ciuffo et al. 2011).

In the present study,  $M^{sim}$  and  $M^{obs}$  are respectively the simulated and observed trajectory data. A trajectory is defined as the time series of the positions or the speeds assumed by a vehicle during its path. In order to compare simulated and observed trajectories we need an appropriate measure of goodness of fit. (Punzo et al. 2011) has recently shown through an extensive experimental study that a car-following model should be calibrated using the Root Mean Squared Error (RMSE) of the time series of vehicle's speeds or spacing. For this reason we adopted here the same approach.

#### 4.3.2.Results

Calibration results are reported in Table 3 for the IDM model and Table 4 for the Gipps model.

As it is possible to see, the number of algorithms iterations considerably decreases with the number of parameters. This is an important feature, especially when the number of parameters si higher than 10-15. Contextually the value of the objective does not increase considerably as the less sensitive parameters are

removed from the calibration set. Indeed if we consider the calibration number 5, the IDM model has been calibrated (using the spacing for the trajectory 30B) with just 3 (out of 7) parameters ( $\mathbf{T}$ ,  $\alpha$ ,  $\beta$ ) and the result both in terms of spacing and speed is not considerably worse that the other calibration. This is particularly relevant with the Gipps' model. Indeed, if we compare calibrations 20 and 23 we have approximately the same result in terms of objective function value with more than three times less iterations (being just 1 parameter calibrated).

Calibration number 6, instead, considers calibrating the model with just the maximum headway parameter. In this case the results are worse. This was however expected as the maximum time headway (and its combinations with the other parameters) accounts only for 70% of the output variance (and for the 40% considering the first order index). The same holds also for calibration 10, in which the maximum headway accounts together with its combinations accounts for the 90% of the variance, but alone it accounts for only the 70%.

CalibrationID	numiter	ObjV	ObjS	$\ddot{S}_f$	$b_f$	$\Delta S^0$	$\dot{S}_f$	Т	α	β
1	5,030	0.509	1.416	2.06	7.50	1.94	18.90	0.55	8.00	5.00
2	3,464	0.501	1.421	2.83	2.92	2.00	20.58	0.54	8.00	2.00
3	2,338	0.506	1.431	4.73	1.00	2.00	22.40	0.54	8.00	1.00
4	2,214	0.503	1.478	4.73	1.00	1.31	23.33	0.61	8.00	1.00
5	1,864	0.562	1.610	4.73	1.00	1.31	18.37	0.59	8.00	5.00
6	1,556	0.583	2.343	4.73	1.00	1.31	18.37	0.42	4.00	2.00
7	4,228	0.542	1.469	1.41	0.84	0.61	18.26	0.49	1.00	5.00
8	5,287	0.524	1.539	1.41	0.50	0.25	18.44	0.40	1.00	2.00
9	1,991	0.643	2.207	3.06	1.00	0.19	14.13	0.52	1.00	5.00
10	1,598	0.710	2.878	3.06	1.00	0.19	14.13	0.61	4.00	2.00
11	3974	0.445	3.808	3.26	7.50	2.00	21.82	0.86	8.00	1.95
12	3732	0.445	3.799	3.17	7.50	2.00	21.73	0.86	8.00	2.00
13	2114	0.501	3.315	2.02	1.00	1.31	18.37	0.74	8.00	1.95
14	1504	0.518	3.509	2.03	1.00	1.31	18.37	0.62	4.00	2.00
15	3916	0.448	1.803	1.58	7.50	0.81	18.37	0.54	1.00	4.18
16	3652	0.458	1.909	1.57	3.79	0.24	18.97	0.40	1.00	2.00
17	3047	0.482	1.822	1.47	1.00	0.19	19.34	0.37	1.00	1.40
18	1344	0.683	3.653	3.06	1.00	0.19	14.13	0.86	4.00	2.00

Table 4. Results of the calibrations for the IDM model. Calibration Ids refer to Table 2. In red italic the calibrated parameters. The other parameters are kept fixed to random values. In bold the measure used for the calibration. Red lines refer to calibration using trajectory 30C, while the others are with trajectory 30B.

However, if we compare the results of calibrating only 1 non sensitive parameter, the results are not so bad. We made this attempt in calibration 25 and 32 where we only calibrated the maximum acceleration of the Gipps' model (accounting for a negligible portion of the outputs variance). The results are much worse than in the previous case. It has to be said, that this also depends on how distant are the sensitive parameters from their "best" values, but the results we achieved allow to highlight also this point.

CalibrationID	numiter	ObjV	ObjS	α	β	γ	$\ddot{S}_f$	ΔS <sup>0</sup>	$b_f$	$\widehat{b}$	θ	τ	$\dot{S}_f$
19	14,012	0.533	1.363	1.00	1.00	-2.90	4.93	1.99	-4.38	-3.88	0.50	0.20	21.71
20	21,767	0.524	1.515	2.50	0.03	0.50	5.59	1.67	-3.34	-3.38	0.11	0.52	21.98
21	16,439	0.531	1.549	1.00	0.97	-0.75	6.47	1.23	-3.50	-3.45	0.32	0.41	21.89
22	4,743	0.527	1.636	1.00	0.97	-0.75	6.47	1.23	-6.10	-5.56	0.29	0.48	21.48
23	5,594	0.529	1.590	1.00	0.97	-0.75	6.47	1.23	-5.56	-5.14	0.29	0.48	21.48
24	1,837	0.552	3.177	1.00	0.97	-0.75	6.47	1.23	-5.56	-5.19	0.23	0.55	21.48
25	3,931	0.657	7.128	1.00	0.97	-0.75	6.20	1.11	-5.56	-5.56	0.29	0.48	21.48
26	27,889	0.553	1.490	1.00	1.00	-3.75	3.36	0.84	-8.00	-7.16	0.22	0.45	25.00
27	16,157	0.678	2.779	2.50	0.03	0.50	3.36	0.43	-3.55	-4.25	0.11	0.70	14.13
28	15,207	0.696	2.546	1.00	0.97	-0.75	5.83	0.63	-3.87	-5.00	0.32	0.36	19.90
29	5,774	0.677	2.525	1.00	0.97	-0.75	5.83	0.63	-5.79	-5.56	0.29	0.48	19.23
30	7,465	0.682	2.502	1.00	0.97	-0.75	5.83	0.63	-5.56	-5.31	0.29	0.48	19.23
31	1,761	0.665	2.623	1.00	0.97	-0.75	5.83	0.63	-5.56	-5.19	0.23	0.55	19.23
32	5,664	0.810	4.721	1.00	0.97	-0.75	4.35	0.58	-5.56	-5.56	0.29	0.48	19.23
33	12,949	0.444	4.287	1.00	0.99	-2.25	4.78	2.00	-5.19	-4.37	0.18	0.95	21.86
34	7,832	0.472	4.292	2.50	0.03	0.50	6.91	2.00	-5.61	-5.27	0.07	0.96	20.58
35	8,221	0.478	3.860	1.00	0.97	-0.75	6.47	1.23	-7.13	-6.37	0.32	0.77	21.89
36	6,365	0.504	3.134	1.00	0.97	-0.75	6.47	1.23	-5.05	-5.56	0.29	0.48	21.48
37	12,879	0.493	2.107	1.00	1.00	-3.32	3.50	0.58	-5.71	-5.50	0.09	0.81	25.00
38	5,846	0.622	4.317	2.50	0.03	0.50	3.59	0.74	-5.75	-7.55	0.05	0.90	19.60
39	3,942	0.423	2.262	1.00	1.00	-0.58	1.34	0.81	-7.64	-7.77	0.29	0.13	20.60
40	5,162	0.639	3.323	1.00	0.97	-0.75	5.83	0.63	-4.54	-5.56	0.29	0.48	19.23

Table 5. Results of the calibrations for the Gipps' model. Calibration Ids refer to Table 2. In red italic the calibrated parameters (the other parameters are kept fixed to random values). In bold the measure used for the calibration. Red lines refer to calibration using trajectory 30C, while the others are with trajectory 30B.

For both the IDM and the Gipps' model the calibration of the parameters usually considered as fixed leads to an overall improvement of the objective function. This is more evident in the Gipps' model, where the results clearly confirm the outputs of the sensitivity analysis that, especially when the trajectory to reproduce has important acceleration phases (stop and go conditions).

In addition, if we compare the results of the calibrations using speed and spacing, we may see that spacing provide a better fit also of the speed profile, while this is not true if we calibrate using speeds. This would suggest to calibrate car-following model using the time series of spacing between leader and follower.

Finally, calibrations results also show that the introduction of the constraint of equation (21) has not affected the validity of the results of the sensitivity analysis, being the indications on the parameters importance widely confirmed.

## 4.4. Discussion

In this application variance-based techniques for model sensitivity analysis have been discussed and applied to two car-following models. Throughout the chapter it is argued that the application of such methods is crucial for a true comprehension and the correct use of these models. In particular, concerning the issue of model parameter estimation or calibration.

Such a guess has been supported by the outcomes of the technique here applied and by the calibrations of the two car-following models using only the parameters suggested by the sensitivity analysis. Indeed important issues arising when setting up a sensitivity analysis have been investigated and commented.

Firstly, the importance of the data assimilation phase has been highlighted through the presentation of the controversial results in Figure 4, yielded by an incorrect/inconsistent definition of the input space. They reveal the effect of cutting off a part of the input uncertainty by considering too tight boundaries for the parameters. This has notable implications also for model calibration, where the smallest possible searching space for the optimisation algorithms is generally sought. The recommendation is therefore that of getting prior information on the inputs distribution possibly from dataset covering a wide spectrum of traffic patterns (e.g. through preliminary parameters estimation). Alternatively, to perform a number of preliminary tests (sensitivity analyses) to find the right balance.

Figures 5 and 6 show an example of the influence on the results of the information used to feed the model. The use of trajectories containing different dynamics (urban vs. extraurban) allowed us to quantify the change in the relative importance of model parameters in affecting the output variance in presence of different traffic patterns. On the other hand, this showed that the application of such techniques may allow the richness of a particular dataset to be also investigated, once a priori information on the sensitivity indices of the model parameters is available e.g. calculated over wider datasets.

Comparison of first order sensitivity indices and total effects of a parameter tell us whether that parameter has higher order effect on model outputs. Such results and the ranking of parameters they allow for, provide crucial information for model calibration too, as shown both in the case of the IDM and the Gipps' model, where some parameters, generally considered fixed, were demonstrated to account for a not negligible share of the output uncertainty. This result requires that those parameters be calibrated in the future applications of such models.

The sensitivity analysis allowed us also to evaluate the parsimony of the two models that is the ability to describe reality with a minimum of adjusting parameters (Young et al. 1996). Both the model resulted not totally parsimonious, with one parameter showing higher relative importance with respect the others. In general, however, we can consider the IDM model more parsimonious, with all the parameters but one explaining a significant share of the output variance.

Results on the Gipps' model, on the other hand, might require further investigations, depending on the problem of inputs correlation introduced by the condition (21). Though such correlation is not expected to be strong, being not introduced by a structural equation of the model and being the rejection approach here adopted correct, in principle, further research is needed to ascertain results correctness. Calibrations results, however, seems confirming the reliability of the results achieved.

# 5. Sensitivity analysis of the Multimedia Assessment of Pollutant Pathways in the Environment (MAPPE) model

Nowadays multimedia models are increasingly used to perform chemical assessment in several scientific domains, such as Health and Environmental Risk Assessment (ERA) and Life Cycle Assessment (LCA). Historically, ERA, LCA and related impact assessment methods have mostly relied on site-generic models, not spatially resolved. In recent years, the relevance of accounting for spatial differentiation has been increasingly discussed to provide more realistic evaluations. There is continual debate whether the exclusion of spatial information in applications such as ERA and LCA may imply misleading results, influencing the decision on products environmental risk and performance.

Furthermore, toxicity related impacts are argued to present high variability among different models (Huijbregts et al 2003, Geisler et al 2005) and results are sometimes expected to be highly sensitive to spatial differentiation, depending on emissions' location patterns, chemical properties, and various landscape parameters. Contrary to the so-called global impact categories, such as Global Warming and Ozone depletion, the need to have spatially-differentiated models for so-called regional impact categories, has arisen under the evidence that differences in fate and exposure mechanisms and differences in sensitivity and background levels for effect can vary significantly depending on different geographical contexts (Udo de Haes et al. 2002). Environmental fate of chemicals presents an high variability depending on geographical location, due to a complex interaction between different chemical and landscape related inputs.

A complete assessment of spatial differentiation requires at least two levels of analysis (Sala et al 2011):

- Assessment of spatial distribution (the range of potential environmental geographical distribution of a chemical) in order to understand at which scale a chemical is typically distributed (local, regional, global etc) and
- Assessment of spatial variability (the variability of the distribution and fate of a chemical among various scenarios, countries, continents).

Hitherto, several spatially distributed fate and transport models of chemicals, i.e. models allowing spatially explicit assessment of contaminants from a given spatial distribution of emission, were developed at various resolutions (e.g. Wegener Sleeswijk and Heijungs 2010, Pennington et al 2005, Toose et al 2004 etc). These models allow assessing the distribution and fate of chemicals in the environment after their emissions, on the basis of chemical (viz. physical chemical) and landscape related properties.

Despite this underlying research work, practical recommendations how to reduce uncertainty and improve the relevance of environmental impact assessment results by addressing spatial differentiation have still not been implemented in the daily ERA or LCA practice. Moreover, asking a practitioner to address spatial differentiation has important drawbacks in term of workload (e.g. input data to be provided) and computational capacities. Sensitivity analysis techniques may be useful for addressing model uncertainty and reducing the computational complexity by highlighting those factors influencing the model outputs.

In literature, some attempts of applying sensitivity analysis techniques to spatial multimedia models exist and have been focussed on evaluating:

- the influence of integrating spatial resolved information within multimedia models comparing a spatially resolved model for Europe with a non spatial one (Pennington et al, 2005)
- the influence of a specific environmental input on the final result (e.g. analysis of role of forest Wania and McLachlan 2001, or the influence of precipitation Jolliet and Haushild 2005)
- the relative influence of environmental or chemical based inputs in affecting the final results (e.g. Hollander et al 2009, using stepwise multiple regression analysis; Wania and Dugani 2003 performing sensitivity analysis of four multimedia (box) models, processing various chemicals in order to support the assessment of the long range transport potential of the substances and the influence of both chemicals and environmental parameters in the final results; Schenker et al 2009 adopting rank correlation based approach to provide new insight into important processes that govern the global fate and persistence of DDT in the environment)

Hence, in the context of multimedia models, sensitivity analysis may play a relevant role in evaluating the robustness of models but also in supporting the assessment of spatial differentiation.

Approaches applied so far, however, do not perform an exhaustive exploration of the inputs' domains and therefore do not ensure the correct estimation of the relative influence of model inputs.

For this reason, in this report, we adopted a Monte Carlo framework to perform the sensitivity analysis of the multimedia model MAPPE Global.

Sala et al 2011 perform with MAPPE an analysis of relevant pattern associated to a set of 34 chemicals, representative of different physical chemical properties. The results for the atmospheric part of MAPPE showed that there are clear patterns of variability among different substances. This variability has to be further explored in order to be able to develop simplified archetypes and scenarios for reducing the computational complexity of the impact assessment. Therefore, the sensitivity analysis of MAPPE is conducted exploring both the influence of environmental and chemical related parameter and input.

## 5.1. The Multimedia Assessment of Pollutant Pathways in the Environment (MAPPE) model

MAPPE Global (Pistocchi et al 2011) is a GIS based model that builds on the concept of the European version (Pistocchi 2008; Pistocchi et al 2010) Currently, it computes only the removal rates of a substance with given physico-chemical properties, composed of atmospheric boundary layer, soil, inland and seawater, for the whole world, with a resolution of 1°x1° (except for land use parameters, which are defined at finer resolution). In MAPPE, the advection between cells is not yet accounted for. Hence, the influence of distributing an emission over a region, which would reduce the maximum potential variability for some types of chemical, is not modelled at the global scale. The detailed model description, background parameters and input data are reported in Pistocchi et al 2011.

MAPPE Global does not compute chemical transport in space at this time, but only the rate coefficients of a substance at each location. The MAPPE Global computes, for each grid cell, mass fluxes of

chemical that are available for transport outside of the cell, and their global variability. The model is developed specifically to answer questions concerning the environmental fate of contaminants taking into account the variability of environmental processes at the global scale. As such, the model can and should be used to answer questions related to the variability of fate in response to spatial variance of emissions and chemical fate processes, such as: distribution of a chemical cross different media in different climatic and landscape settings; relevance of the variability of environmental processes in determining the fate of chemicals across the globe; assessment of amount of a chemical emitted to air will result in a load to soil or waters.

With respect to spatial differentiation, MAPPE Global allows to adopt several scales of assessment by differentiating on the basis of grid cells (100x100 km), political boundaries (countries) or geographical borders (river basins, continents, global) and identification of specific pattern in the environmental behaviour of chemicals.

## 5.1.1. Calculation of Removal rates from air

The sensitivity analysis was performed on the model, assessing the variability of removal rate from air. MAPPE calculation of removal rates are as follows

Generally, let define the chemical mass,  $M_{i,j}$  [kg], in the medium j for a pollutant i emitted in the same medium j as:

$$M_{i,j} = \frac{E_{i,j}}{K_{i,j}} \tag{26}$$

where  $E_{i,j}$  [Kg day<sup>-1</sup>] is the mass of pollutant i emitted in the medium j and  $K_{i,j}$  [day<sup>-1</sup>] is the removal rate for pollutant i in the medium j.

Let also define the max fluxes  $L_{i,j}$  [kg day<sup>-1</sup>] of pollutant i originated from a cell and available for long range transport within the medium j, as

$$L_{i,j} = M_{i,j} \cdot K_{adv,i,j} \tag{27}$$

with  $K_{adv,i,j}$  representing the advection removal rate for pollutant i within medium j. If we consider as medium j the sole air, we can write:

$$K_{i,air} = 86400 \frac{K_{i,part} + 1 - \phi K_{i,gas} + K_{i,wet}}{ABL} + K_{i,deg} + \frac{u_{10}}{X}$$
 (28)

$$K_{i,air,no\_adv} = 86400 \frac{K_{i,part} + 1 - \phi K_{i,gas} + K_{i,wet}}{ABL} + K_{i,deg}$$
 (29)

For equations (28-29) it is evident that  $K_{i,air}$  is expressed in [day<sup>-1</sup>], while the other  $K_{i,\underline{\ }}$  are expressed in [s<sup>-1</sup>]. In equations (28-29):

$$K_{i,part} = \phi \frac{F_{OC}}{OC} \tag{30}$$

$$\phi = \frac{\vartheta_1 \cdot K_{OW} \cdot OC}{K_{AW} + \vartheta_1 \cdot K_{OW} \cdot OC} \tag{31}$$

$$K_{AW} = K_{AW_0} \cdot exp \ \gamma_1 T \tag{32}$$

$$K_{i,gas} = K_{GW} \frac{w}{100} + 1 - \frac{lmp}{100} \quad 1 - \frac{w}{100} \quad K_{GF} * \frac{Dec + Eve}{100} + K_{GS} \quad 1 - \frac{Dec + Eve}{100}$$
(33)

$$K_{GW} = \frac{v_a \cdot v_w}{v_a \cdot K_{AW} + v_w} \tag{34}$$

$$v_a = \vartheta_2 \cdot u_{10} + \vartheta_3 \quad \frac{\vartheta_4}{MW} \tag{35}$$

$$v_w = \vartheta_6 \cdot u_{10}^2 + \vartheta_7 \quad \frac{\vartheta_8}{MW} \tag{36}$$

$$K_{GF} = \vartheta_{10} \frac{Dec}{100} + \vartheta_{11} \frac{Eve}{100} + \vartheta_{12} \frac{Eve}{100} \frac{Bro}{100} + \vartheta_{12} \frac{Eve}{100} \frac{Bro}{100} - \frac{\vartheta_{13}}{MW}$$
(37)

$$K_{GS} = \vartheta_{14} \frac{\vartheta_{15}}{MW}^{0.5} \tag{38}$$

$$K_{i,wet} = S \cdot \phi + \frac{1}{K_{AW}} 1 - \phi \frac{P}{86400}$$
 (39)

$$K_{i,deg} = K_{deg0} \cdot exp \ \gamma_2 T \tag{40}$$

	t of inputs eir descript	and outputs used in MAPPE and ion	Unit in MAPPE	Model parameters	Value
1	$L_{i,j}$	Mass fluxes of pollutant i within j	Kg s <sup>-1</sup>	X	10 <sup>5</sup>
2	$M_{i,j}$	Mass of pollutant i within j	Kg	$\vartheta_1$	10 <sup>-2.91</sup>
3	$K_{adv,i,j}$	Advection removal rate for pollutant i within j	s <sup>-1</sup>	$artheta_2$	0.002
4	$E_{i,j}$	Emissions of pollutant i in medium j (assumed to be)	Kg day <sup>-1</sup>	$\vartheta_3$	0.003
5	$K_{i,air}$	Removal rate for pollutant i in medium air	day <sup>-1</sup>	$artheta_4$	18
6	$K_{i,part}$	Particle dry deposition	s <sup>-1</sup>	$artheta_5$	0.335
7	φ	Aerosol mass fraction of pollutant i	dimensionless	$\vartheta_6$	0.000004
8	$K_{i,gas}$	Gas absorption rate	s <sup>-1</sup>	$\vartheta_7$	0.000004
9	$K_{i,wet}$	Wet deposition rate	s <sup>-1</sup>	$\vartheta_8$	32
10	ABL	Atmospheric boundary layer height	m	$\vartheta_9$	0.285
11	$K_{i,deg}$	Degradation rate	s <sup>-1</sup>	$\vartheta_{10}$	0.036
12	$u_{10}$	Wind speed at 10m	m s <sup>-1</sup>	$\vartheta_{11}$	0.0078
14	$F_{OC}$	Deposition flux of atmospheric organic carbon	kg m <sup>-2</sup> s <sup>-1</sup>	$artheta_{12}$	0.045
15	ос	Concentration of particulate organic carbon	Kg m <sup>-3</sup>	$\vartheta_{13}$	300
17	$K_{OW}$	Octanol-water partitioning coefficient	dimensionless	$\vartheta_{14}$	0.0000123
18	$K_{AW}$	Air-water partitioning coefficient	dimensionless	$\vartheta_{15}$	18
19	$K_{AW_0}$	Air-water partitioning coefficient at reference temperature	dimensionless	S	2 10 <sup>5</sup>
21	$K_{deg0}$	Degradation rate at reference temperature	s <sup>-1</sup>		
22	$\gamma_1$	Temperature air-water partitioning coefficient	dimensionless		
23	$\gamma_2$	Temperature degradation coefficient	dimensionless		
22	T	Absolute temperature of air	°C		
23	$K_{GW}$	Absorption velocity on water	s <sup>-1</sup>		
24	w	Cell % of water surface	%		
25	Imp	Cell % of impervious surface cover	%		
26	Dec	Cell % of deciduous forest	%		
27	Eve	Cell % of evergreen forest	%		
28	$K_{GF}$	Absorption velocity on forest	s <sup>-1</sup>		
29	$K_{GS}$	Absorption velocity on soil	s <sup>-1</sup>		
		DICC I I II I	-1		

Chemical specific input

Environment specific input

Diffusion velocity on air

Molecular Weight

Total precipitation

Diffusion velocity on water

Cell % of broadleaved forest

Output

30

 $v_a$ 

 $\frac{v_w}{MW}$ 

Bro

Table 6. Inputs, outputs and parameter of MAPPE model. Distinction of environment and chemical specific input is reported. In MAPPE implementation  $E_{i,j}$  is supposed as constant and equal to 1kg.  $\gamma_1$  and  $\gamma_2$ , unless differently specified are set to 0, as no information on the two temperature degradation coefficients are available

m s<sup>-1</sup>

m s<sup>-1</sup>

MW

%

m day<sup>-1</sup>

# 5.2. Application

# 5.2.1. Fixed input data

Differently from car-following models, as we have seen in the previous section, the output of the MAPPE model is the total atmospheric removal rate for a given chemical (day<sup>-1</sup>) emitted in air. In reality, as pointed

out, the actual atmospheric removal rate should be expected between the formulations with and without the advection component (Pistocchi et al. 2011). For this reason we are considering two outputs (and thus we are performing two different sensitivity analyses): results of equation (28-29), namely the atmospheric removal rate with and without the advection component.

In the previous section we have listed all the inputs and parameters of the MAPPE models. Model parameters will be considered as fixed (as they were calibrated). The sensitivity analysis will therefore be focused on the inputs. This is a substantial difference with the application to traffic models. The reason for this is simple. In traffic models, the aim of the analysis was the selection of the parameters to calibrate. Here the objective is to individuate those input which deserve higher accuracy in their definition and those which can be neglected and kept as fixed to certain values.

As detailed in the previous section, the MAPPE model has two types of input factors: environment and chemical specific. A complete sensitivity analysis of the model would involve all the inputs together. The problem here is that some chemical specific inputs (in particular  $K_{OW}$  and  $K_{AW_0}$ ) are strongly. As pointed out in section 2.8, sensitivity analysis in the presence of correlated inputs is not a trivial task. In addition, differently from the case of the Gipps' car-following model, the correlation here is not introduced by a constraint, but is intrinsic of the chemical properties of the different substances.

For this reason we decide to perform two different sensitivity analyses:

- 1. sensitivity analysis of environment specific inputs. In this case, chemical-specific inputs were considered as fixed and assumed the values corresponding to three different chemicals: acephate,  $\gamma$ -HCH (Lindane) and phtalate, di(n-octyl). The selection of three chemicals, with very different physical-chemical properties<sup>7</sup>, allows in any case understanding the role played by the chemical properties.
- 2. sensitivity analysis of environment and chemical specific inputs. All the parameters are included explicitly or implicitly. In particular chemical specific input factors were only implicitly considered. More in details, the four chemical specific inputs have been substituted by just one dummy variable named chemical. The value assumed by this variable (in the range [0,1]), identifies a specific chemical (among those modelled in MAPPE) and, therefore, the value of its parameters. In this way we don't know how the different chemical specific input factors play on the model outputs, but at least are able to compare the impact of the chemical chosen with respect to the environment specific inputs.

# 5.2.2.Setting up the method for the MAPPE model

The approach presented for car-following models holds also in this case. In particular, also with the MAPPE model, we are using the variance-based sensitivity technique defined in section 2.7.1. For this reason both the

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<sup>&</sup>lt;sup>7</sup> In the chemical space defined by Kow and Kaw, acephate represents a hydrophilic chemical, whilst di(n.octyl)phatalate a hydrophobic one. Lindane, instead, is a multimedia chemicals, meaning that it represents those chemical that are close to equal affinity for air, soil and water

uncertainty propagation and the computation of sensitivity indices phases will follow the same approach adopted in the previous case-study.

The data assimilation phase for the MAPPE model is, on the contrary, totally different. In this case, in fact, the ranges for the different inputs are perfectly known (i.e. they are the values attained by the different inputs in the different 1x1° cells of the model representation of earth and the values of the inputs with respect to the different chemicals) and, therefore, the application of sensitivity analysis techniques is apparently more straightforward.

Table 7 reports on the input factors considered along with the space adopted for them in the analysis. The subscript 1 indicates the ranges adopted in the first experiment.

0	MAPPE model							
Parameter	LB <sub>1</sub>	$UB_1$	LB <sub>2</sub>	UB <sub>2</sub>	LB <sub>3</sub>	UB₃		
ABL	285	900	285	900	285	900		
U <sub>10</sub>	2	5.5	2	5.5	2	5.5		
foc	2.02e-19	2.06e-12	2.02e-19	2.06e-12	2.02e-19	2.06e-12		
ОС	3.98e-15	1e-8	3.98e-15	1e-8	3.98e-15	1e-8		
T	-10	30	-10	30	-10	30		
w	0	100						
Imp	0	50						
Dec	0	80						
Eve	0	100						
Bro	0	100						
P	8.97e-8	7.17e-3	8.97e-8	7.17e-3	8.97e-8	7.17e-3		
cov			0	1	0	1		
chemical					0	1		

Table 7. Input factors space adopted. Subscripts 1 and 2 refer to different sensitivity analysis performed (Source: Zulian et al., 2010)

As one can see from the table, 5 out of the 11 environment specific input factors are connected to the coverage of a given geographic cell (*Imp, Dec, Eve, Bro*). These five input factors are strongly correlated, as their combination must not exceed the 100% of the cell. For this reason we operated as for the Gipps' carfollowing model and imposed that, during the quasi-random number generation, input factor violating the following two constraints would have been discarded:

 $w+Imp+Dec+Eve \le 100$ 

*Bro≤Dec+Eve* 

Unfortunately, differently from the case of the Gipps' model, the adoption of these constraints introduced a problem in the computation of the Sobol sensitivity indices. This problem showed up as first order sensitivity indices of the five coverage types resulted greater than the correspondent total order indices (even with a very

large size of the Monte Carlo experiment<sup>8</sup>). From a theoretic point this is the proof that the correlated input

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<sup>&</sup>lt;sup>8</sup> It is worth remembering that equations (18) and (19) are approximated relationships to evaluate first order and total sensitivity indices. As a consequence, errors in the evaluation of the sensitivity may arise when the size of the Monte Carlo experiment is not sufficiently big. Typical errors are first order indices bigger than total order ones.

factors generate a distortion in the Sobol indices calculated with equation (18) and (19) (see Saltelli et al. 2004, Chapter 1). In practice Sobol sensitivity indices cannot be used to understand the relative role played by the different coverage related factors.

We, then, performed a second experiment in which the five coverage-related factors were substituted by a single "dummy" variable *cov* defined in the range [0,1]. The values attained by this dummy variable defined a specific combination of the five coverage factors, correspondent to a real combination of a cell in the MAPPE representation of the world. Since the MAPPE model considers 140x360 cells, the connection between the dummy variable and the cell combination of coverage factors would be computationally expensive. In addition, many cells have the same combination and thus there is an easier way to match them with the variable *cov*: defining the empirical cumulative probability distribution (Cdf) of the different combinations. Given that each combination will have a certain cumulative probability (in the range [0,1]), it is easy to link the value attained by the dummy variable with the combination of coverage values.

In this way about 1.400 combinations are representative of all the 50.400 cells of the model. Figure 8 shows the cumulative distribution function (Cdf) .

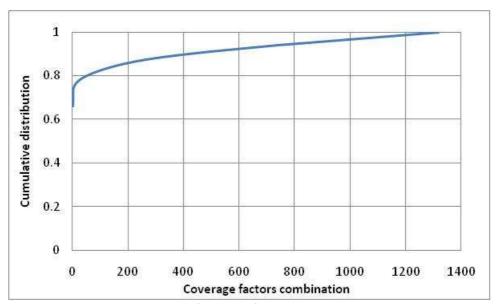


FIGURE 8. Cumulative probability distribution function of coverage combinations on earth in the MAPPE model

In Figure 8, it is possible to see that the first combination of natural coverage factors accounts for almost the 65% of the cells in MAPPE. This combination has w=100 and all the other factors equal to 0, namely it represents the cell in the oceans and seas. In order not do distort the analysis with this predominance of full water cells, we decided to perform two analysis: a first one with the Cdf of natural coverage as in Figure 8, and another one with the Cdf as in Figure 9, in which the full water cells have been removed from the sample.

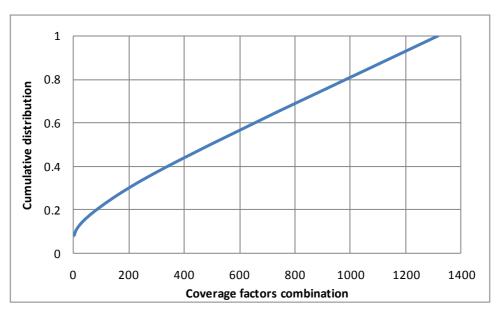


FIGURE 9. Cumulative probability distribution function of coverage combinations in the MAPPE model (without considering sea cells)

The same approach adopted for coverage combination has been adopted also to connect the dummy variable *chemical* to the different chemicals of the MAPPE model. In this case the Cdf function is a straight line, since any chemical has the same probability to be selected. In this case we selected the 34 chemicals listed in Table 3 of Pistocchi et al. (2011). As it will be described in the remainder, also in this case we performed two different analyses: one with the complete set of chemicals and another without a small group of chemicals (Acephate, Benomyl, Methomyl and Propoxur) with the biggest impact on the outputs of the model. Data used to characterize the different chemicals are retrieved from Pistocchi et al. (2011, Table 3).

## 5.2.3.Results - Environment specific inputs

What has been already described for the two car-following models, has been applied also here. In particular, we paid attention that all the sensitivity indices resulted stable at the end of the analysis. In all the experiments carried out we used a size of the Monte Carlo experiment N=20.000. Sobol indices proved to be stable with no less than 5.000 iterations (and therefore the MAPPE model resulted more instable that the two car-following models).

Further to what produced for the traffic models, in this application we also derived the scatter plots of each input factor per each output and the confidence interval of the Sobol indices calculated.

Scatter plots can be very useful to understand if the first order effect of an input on the outputs is regular or, for example, is connected with just specific values of the inputs. It therefore represents an important tool to check about the robustness of the analysis and about the suitability of the ranges adopted to describe the inputs' variability.

Confidence intervals can be used to assess the robustness of the indices derived, to check their stability and also to rank the different inputs (in a factor prioritization setting). Confidence intervals have been numerically derived using the *bootstrapping* technique. In particular, let consider that the Sobol indices are

calculated on 1.024 model evaluations. To calculate the confidence intervals of these Sobol indices with bootstrapping, we need *M* vectors of model evaluations of the same size of that used to calculate the indices (in this case 1024) obtained by sampling the original vector with replacement. In this way we are able to evaluate M different values of the Sobol indices and use them to evaluate the confidence interval. For further details about the bootstrapping technique, please refer to Saltelli et al. (2008). In the present application the level of confidence adopted has been 0.9.

## 5.2.3.1. Acephate, gamma-HCH (Lindane) and Phtalate, di(n-octyl)

In the following figures, the results of the sensitivity analysis for the three chemicals are reported. As already pointed out in the previous section, we expect for the temperature not to have any effect on the outputs, as  $\gamma(1)=\gamma(3)=0$ .

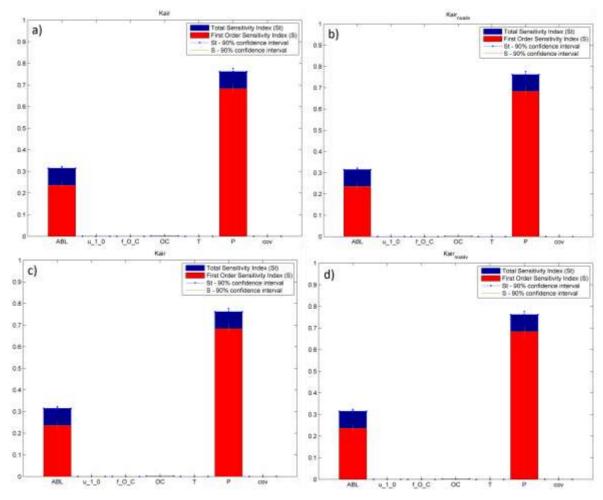


FIGURE 10. First order, total order sensitivity indices and their confidence interval for environment specific input factors of the MAPPE model with respect to the Acephate. Charts a) and c) refer to the total air removal rate, while b) and d) do not consider advection. Indices in charts a) and b) are calculated with the complete Cdf for coverage combinations, while c) and d) refer only to coverage combinations without sea cells

Figure 10 reports the results for the Acephate. The four charts give approximately the same figures and this means that neither the coverage combinations, nor the advection phenomenon exert any impact on the model outputs for this chemical. The air removal rate, in this case, is only affected by the value of the average precipitation in the cell and by the atmospheric boundary layer (both for their first order and

combined effects). This is reasonable as the Acephate is a highly hydrophilic chemical and also because, as it is well known in the literature, spatially resolute models usually overestimate the role of precipitation.

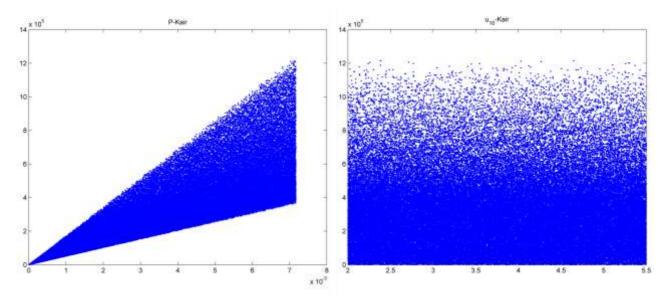


FIGURE 11. Scatter plots of the air removal rate K<sub>air</sub> (resulting from the MAPPE model) with respect to precipitation P and wind speed u<sub>10</sub> for the Acephate

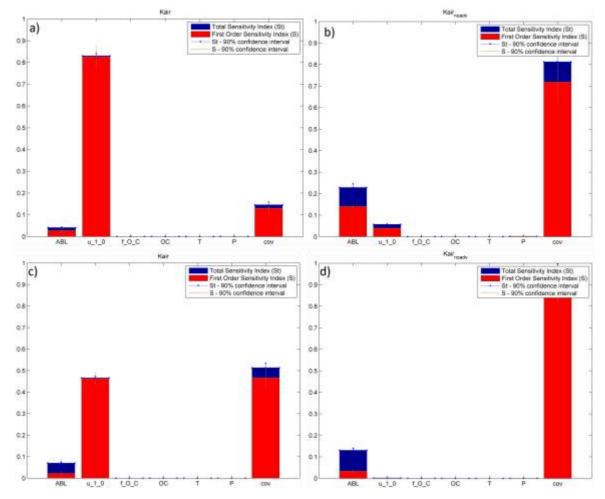


FIGURE 12. First order, total order sensitivity indices and their confidence interval for environment specific input factors of the MAPPE model with respect to the  $\gamma$ -HCH. Charts a) and c) refer to the total air removal rate, while b) and d) do not consider advection. Indices in charts a) and b) are calculated with the complete Cdf for coverage combinations, while c) and d) refer only to coverage combinations without sea cells

In all the charts, first order indices are lower than total order ones and confidence interval are quite small around the calculated values. These are both good indications about the reliability of the results achieved.

Just to understand the meaning for an input factor to be considered as sensitive, Figure 11 reports the scatter plots of the removal rate  $K_{air}$  with respect to the precipitation, P, and the wind speed  $u_{10}$ . It is evident as the shape of the scatter plot is heavily affected by the value of the precipitation input, while it is not by the value of the wind speed.

Figure 12 reports on the results of the sensitivity analysis for the MAPPE model with respect to the  $\gamma$ -HCH (Lindane). In this case both the coverage combinations and the advection have a significant impact on the results. On the contrary the precipitation has no influence on the outputs of the model. Comparing the chart in Figure 10 with those in Figure 12 it is possible to see that chemical specific factors have a significant effect on the model. For the Lindane the coverage combinations and the wind speed have the most important effects. This quantitatively varies if we consider sea cells or not (see the difference between Figure 12a and Figure 12c). Also in this case the atmospheric boundary layer has an effect on the model outputs, even if lower than in the case of the Acephate.

Also in this case, in all the charts, first order indices are lower than total order ones and confidence interval are quite small around the calculated values. Again, these are both good indications about the reliability of the results achieved.

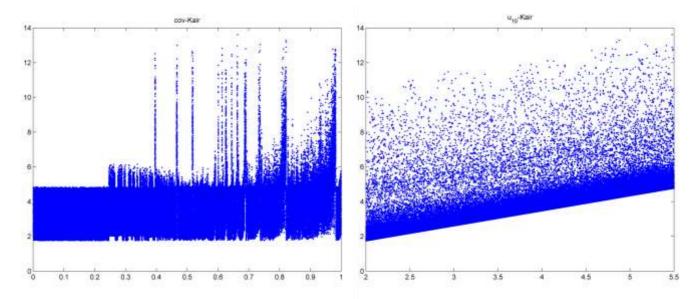


FIGURE 13. Scatter plots of the air removal rate K<sub>air</sub> (resulting from the MAPPE model) with respect to coverage combination cov and wind speed u<sub>10</sub> for the gamma-HCH chemical

Figure 13 shows the scatter plots of the removal rate  $K_{air}$  with respect to the coverage, cov, and the wind speed  $u_{10}$ . It is peculiar to see that some coverage combinations allow value of the removal rate much higher than others. The effect of the wind speed is instead to define a lower bound for the removal rate.

Differently from the other chemicals, with Lindane, we performed also an additional analysis since the parameters of the relation between both  $K_{aw}$  and  $K_{deg}$  and the temperature T are available. This relationship considers  $\gamma(1)=0.0783$  and  $\gamma(3)=0.0255$ . Results are reported in Figure 14.

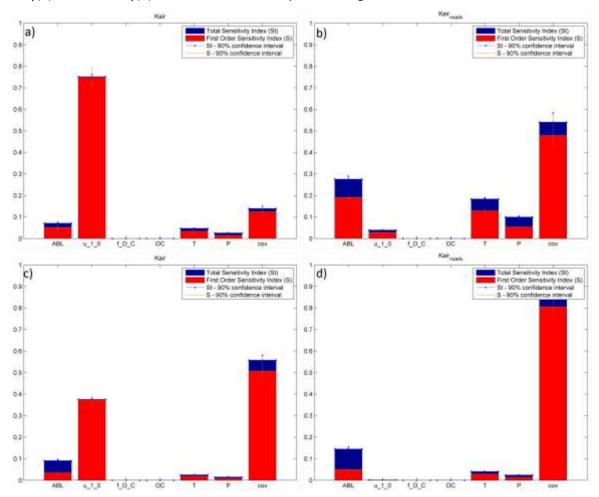


FIGURE 14. First order, total order sensitivity indices and their confidence interval for environment specific input factors of the MAPPE model with respect to the  $\gamma$ -HCH chemical with the influence of the temperature modelled. Charts a) and c) refer to the total air removal rate, while b) and d) do not consider advection. Indices in charts a) and b) are calculated with the complete Cdf for coverage combinations, while c) and d) refer only to coverage combinations without sea cells

Results are fairly different from the previous case. Apart from the organic carbon and its fluxes, all the inputs show an effect on the model outputs. This is particularly true considering sea cells without advection. Being a multimedia chemical, this behaviour for the Lindane was expected: the chemical does not show a clear preference toward a medium with respect to the others. For this reason, without an explicit link with the temperature we could conclude that the MAPPE model proves not to be sufficiently accurate to reproduce the behaviour of chemicals like Lindane.

Figure 15 shows the results of the model sensitivity analysis for the di(n octyl) phtalate.

Again the results are different from the other chemicals, and this further confirms what stated before. For the di(n octyl) phtalate, almost all the input factors have an effect on the model outputs (apart from the organic carbon fluxes and the temperature that, however, is not modelled for this chemical). The atmospheric boundary layer has still an important effect, even if most of the variance in the outputs is accounted by the

wind speed and the precipitation. Figure 16 shows the scatter plots of removal rate without advection with respect to the organic carbon OC and the atmospheric boundary layer ABL input factors.

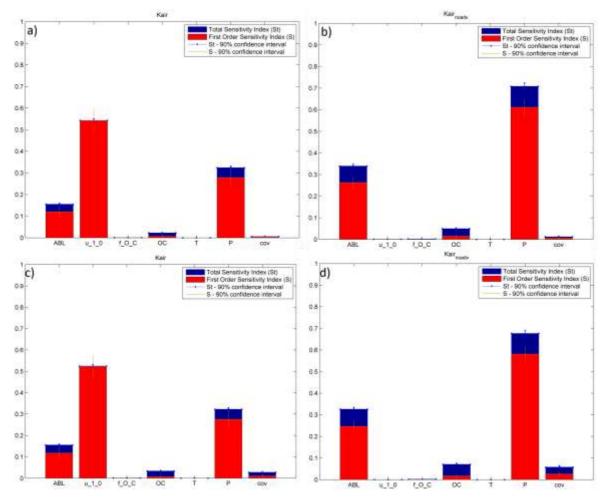


FIGURE 15. First order, total order sensitivity indices and their confidence interval for environment specific input factors of the MAPPE model with respect to the di(n octyl) phtalate. Charts a) and c) refer to the total air removal rate, while b) and d) do not consider advection. Indices in charts a) and b) are calculated with the complete Cdf for coverage combinations, while c) and d) refer only to coverage combinations without sea cells

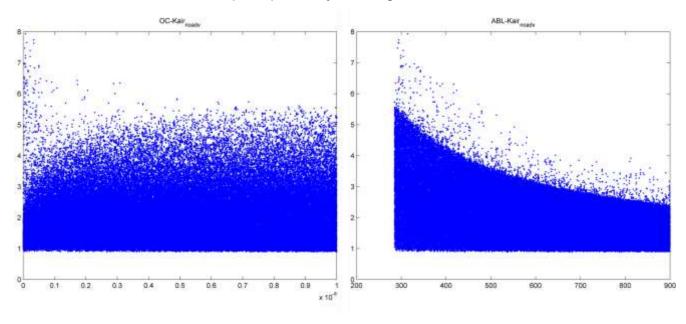


FIGURE 16. Scatter plots of the air removal rate (without advection) K<sub>air</sub> (resulting from the MAPPE model) with respect to organic carbon OC and atmospheric boundary layer ABL for the di(n octyl) phtalate

Before drawing any inference about the results of the sensitivity analysis for this chemical, it is worth showing that in absolute terms, the air removal rate for both Lindane and di(n octyl) phtalate are much lower that for the acephate. This means that, on average, Lindane and di(n octyl) phtalate are expected to stay much longer in the air compartment than the acephate. If this can be expected for the Lindane, this is probably not the case for the di(n octyl) phtalate, which has and extreme lipophilic character (even though this feature might be explained by the fact that the chemical remains in air associated with particulate matterers). For this reason the model behaviour should not be checked against the effects of the input factor, but, in this case, against the reliability of the output. In any case the fact that, differently from the other chemicals, the organic carbon has a certain effect on the model outputs should be seen as a proof that the MAPPE model is able, within certain limits, to mimic the mechanisms that lead a chemical to follow its natural pathway.

#### 5.2.4.Results – Environment and chemical specific inputs

As pointed out in the previous sections, in order to quantify the effects on the outputs of choosing a specific chemical and to compare such effects with those of the other environment specific compounds, an additional sensitivity analysis has been carried out. Results are shown in Figure 17.

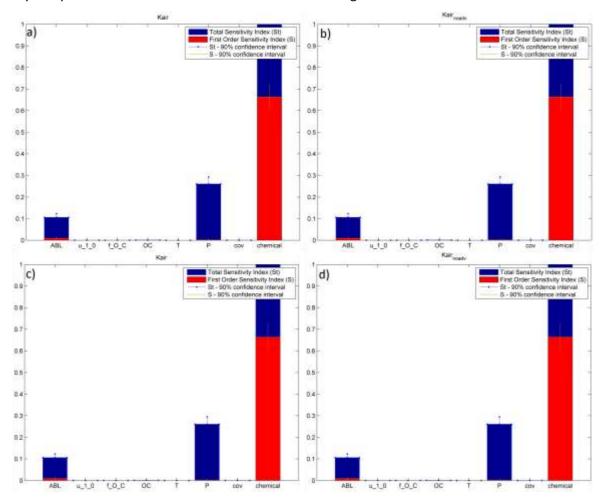


FIGURE 17. First order, total order sensitivity indices and their confidence interval for environment and chemical specific input factors of the MAPPE model. Charts a) and c) refer to the total air removal rate, while b) and d) do not consider advection. Indices in charts a) and b) are calculated with the complete Cdf for coverage combinations, while c) and d) refer only to coverage combinations without sea cells

From the analysis it is shown that the choice of the chemical, alone, accounts for approximately the 70% of the model output variance independently from all the other factors. Precipitation and the width of the atmospheric boundary layer have an effect only in combination between themselves and with the chemical. This is a clear indication that, once the properties of the chemical are known, precipitation and atmospheric boundary layer, alone, can provide a good indication of the time the compound will remain in the air compartment.

In Figure 18, scatter-plots of the air removal rate with respect to the chemical and the precipitation variables are shown.

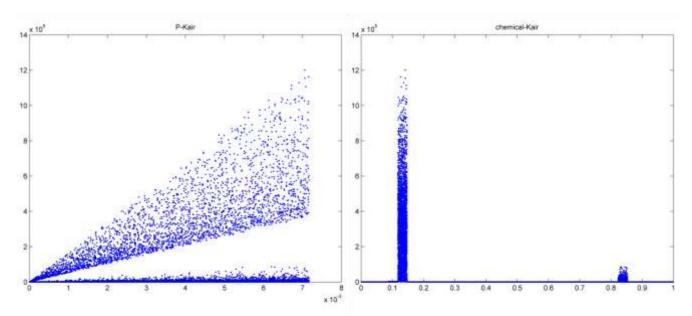


FIGURE 18. Scatter plots of the air removal rate (without advection) K<sub>air</sub> (resulting from the MAPPE model) with respect to precipitation P and chemical input factors

It is interesting to notice that both the charts clearly identify two (or even more) categories of chemicals: a category of chemicals with also very high removal rate and another category (including the vast majority of the compounds) with much lower removal rates. Since most of the variance in the outputs is owned by the first category, the scatter plots clearly explain why only ABL and P have showed up in the sensitivity analysis (confirming what stated for the acephate, which in fact is one of these high air removal rate chemical).

In order to get further insights into the model, also for the other chemicals, we performed an additional sensitivity analysis without considering the chemicals pertaining to the first category of compounds (namely Acephate, Benomyl, Methomyl and Propoxur).

Results are shown in Figure 19.

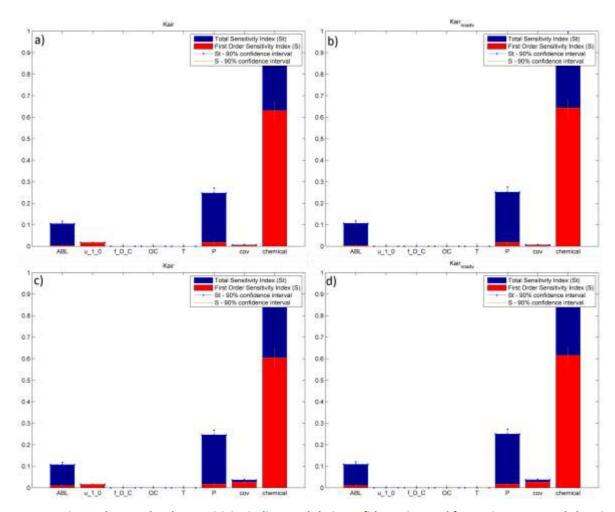


FIGURE 19. First order, total order sensitivity indices and their confidence interval for environment and chemical specific input factors of the MAPPE model (without considering Acephate, Benomyl, Methomyl and Propoxur among the chemicals). Charts a) and c) refer to the total air removal rate, while b) and d) do not consider advection. Indices in charts a) and b) are calculated with the complete Cdf for coverage combinations, while c) and d) refer only to coverage combinations without sea cells

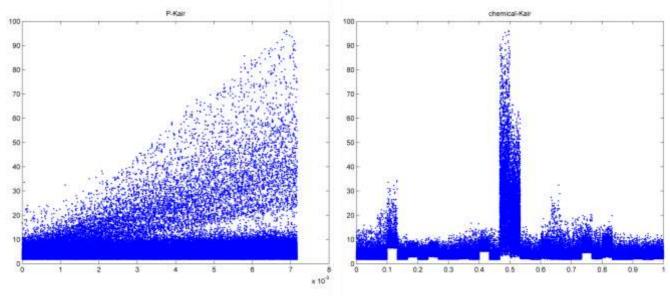


FIGURE 20. Scatter plots of the air removal rate (without advection) K<sub>air</sub> (resulting from the MAPPE model) with respect to precipitation P and chemical input factors

In this case more input factors appear exerting a certain impact on the outputs, even if the situation does not change considerably with chemical, P and ABL accounting the most of the variance in the model outputs. The main difference with the previous case is that the environment specific factor has an effect also by themselves and not only in combination with the other factors. One can conclude that, according to what foreseen by the MAPPE model, the magnitude of the air removal rate is totally defined once the chemical, the width of the atmospheric boundary layer and the amount of precipitations are defined. Then, the calculation can be refined by knowing also the average wind speed and the coverage combination. Scatter plots of Figure 20 do not add significant elements to this conclusion.

#### 5.3. Discussion

In this study, variance based sensitivity analysis techniques have been used to shed light on the properties of the Multimedia assessment of pollutant pathways in the environment (MAPPE) model. The output considered in the analysis has been the air removal rate with and without considering the advection component (the inverse of the resident time of a chemical in a specific compartment).

Two different types of analysis have been carried out. In the first only environmental inputs were considered, while in the second both environmental and chemical specific inputs are considered. As a first outcome of the study, results confirm the conclusions of Hollander et al. (2009) concerning the predominance of the chemical properties in the quantification of the removal rate. However, once defined the specific chemical (or at least the specific archetype the chemical pertains to), the definition of the more influential environmental parameters has a total novel character. A summary of the results is provided in Table 8.

Chemical Archetype	Key parameters for archetypes
Hydrophilic	Precipitation, ABL
Lipofilic	Wind, Precipitation, ABL, OC, Coverage
High volatility	Wind, Coverage, ABL
Multimedia	Wind, Coverage, ABL

Table 8. Results' summary: key environmental parameters for different chemical archetypes as resulting from the sensitivity analysis of the MAPPE model

Results highlights the following issues:

- the Atmospheric Boundary Layer (ABL) parameter has always a certain effect on the model outputs (though it is never the most influential parameter) independently from the chemical;
- the wind speed (the main driver of the advection process) has an effect on most of the chemicals and therefore the advection is really the uppermost process of removal from air only for certain chemicals;
- land coverage and the forest have a significant effect on the model outputs, especially for multi-media chemicals and especially when assessing removal from land surface (see Figure 11);
- the role of precipitation, especially for hydrophilic substances, is significant. However, as already pointed out by Jolliet and Hauschild (2005) this is probably due to the assumption of continuous

(versus intermittent) rain that produce an overestimation that has to be further explored and adjusted in multimedia models.

Furthermore, the results achieved suggest the development of chemical specific and landscape specific archetypes that might be based on climatic zones (usually based on wind, precipitation and coverage as in Masson et al. 2003).

As a further development, the analysis may lead to the definition of robust archetypes of emission, in order to build realistic scenarios of distribution of chemical in the environment, reducing the computational burden related to complex and at high resolution multimedia models.

## 6. Example of application of uncertainty analysis in sustainability assessment

As pointed out in section 1 and 2, the report is mainly focused on sensitivity analysis techniques. However, an introduction to the techniques to perform uncertainty analysis has been provided in section 3. In the present section our intention is to report on the approach followed in Dorini et al. (2011) as a typical case study for uncertainty analysis in sustainability assessment.

The case study in Dorin et al. (2011) regards the necessity to satisfy the demand for electricity of a certain Region with a new additional power plant with an installed power of 40MW. Objective of the assessment is to understand whether is better to produce the required power with a coal or a bio-mass power plant. The assessment follows the PUrE sustainability decision support framework (Azapagic and Perdan 2005, <a href="http://www.pureframework.org/">http://www.pureframework.org/</a>) and concerns the evaluation of 22 different criteria (13 environmental and 9 socio-economic ones). Basing on the criteria a Multi Criteria Decision Analysis (MCDA) has been performed using the opinion of 6 experts.

In particular, the experts were asked:

- to select the most suitable sub-set of criteria for the evaluation;
- to define a vector of weights  $\mathbf{w} = (w_1, ..., w_N)$  for the N criteria (according to the MCDA logic)
- to define vectors of upper  $\mathbf{ub} = (ub_1,...,ub_N)$  and lower bounds  $\mathbf{lb} = (lb_1,...,lb_N)$  for the criteria.

In this way the best option is that satisfying the following condition:

$$\min_{j} \quad \sum_{i=1}^{N} \frac{q_{i,j} - lb_i}{ub_i - lb_i} w_i \tag{41}$$

where  $q_{i,j}$  is the estimated value for the criterium i attained by the alternative j (in this case i=22 and j=2).

Please consider that this is true if we consider the criteria as impacts (so we have to minimize the overall impact). In the case the criteria are benefits, equation (41) has to be seen in a maximization framework.

The method involves two sources of uncertainty:

- 1. uncertainties in  $q_{i,j}$  (expert judgement independent);
- 2. uncertainties in  $w_i$  (expert judgement dependent);

In Dorini et al. (2011) the two sources of uncertainties have been progressively added in the analysis (namely, they first perform MCDA without uncertainty, then with the first source only and finally with all the two sources). A Monte Carlo-based approach was used for this purpose.

## 6.1. MCDA without uncertainty

In the first analysis, results from the PRuE framework were considered for both the power plants and the multi criteria indicator was evaluated using as weights the mean of the weights provided by the experts. Using this approach, the Biomass option resulted to be preferred.

## 6.2. MCDA with uncertainty in models

As clearly pointed out in section 1, each model is only a coarse representation of the reality, with its outputs usually affected by the value assigned to its parameters. A perfect knowledge of such values is usually

unknown. More easily the analyst has an estimate of the range in which they can vary. A Monte Carlo framework for the uncertainty analysis tries to resemble the distribution of the model outputs by evaluating the model many times in different points of the domain of the parameters. In Dorini et al. (2011) the authors adopted this approach. Again the weights were considered as the average values of the weights proposed by the experts.

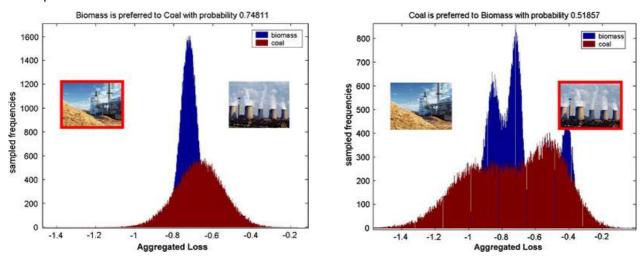


FIGURE 21. Results of the uncertainty analysis presented in Dorini et al. (2011) concerning the sustainability assessment of two alternative electricity power plants. Picture on the left refers to the case of uncertainties in models only, while the picture on the right refers to the case of uncertainty in both models and experts preferences. (source Dorini et al. 2011)

Using this approach, the authors were able to assess that the Biomass plant is the best option with the 75% of confidence (which is a completely different answer, since, on average, in 25 cases out of 100 it can the opposite).

## 6.3. MCDA with uncertainty in models and experts preferences

Further than on the models, uncertainty analysis can be also applied to the experts' preferences. Indeed the choice of using the average value of the weights has no reason to represent the best choice. Making different trials with different model parameters and different weights, the results of the MCDA may also result very different. As a matter of fact the uncertainty analysis allowed the analysts concluding that there is no actual preference between the two options (the coal plant resulted the best option with a 52% level of confidence). From Figure 21 it is clear that, even though the most probable value for the Biomass plant has a lower MCDA indicator that the corresponding value of the Coal plants, the cumulative probability function shows that the two options have almost the same probability to result in the best option.

This example clearly shows the usefulness of uncertainty analysis in checking the robustness of the results of an impact/sustainability assessment. It is also important to prevent falsifications due, for example, to inappropriate weights provided by potentially interested experts. It is clear that, for a decision maker, the two answers "this is the best option" and "this is the best option with the 75% of confidence" may sound very differently. Further information may also arise from the analysis of the parameters/inputs/weights that have generated the unexpected tail in the cumulative probability distributions (with respect to the described case

study, for example, this may mean analyzing in which, operational/technical/causality conditions the coal plan
resulted the best option).

## 7. Dealing with fuzzy logic

In section 1 we have briefly described the difference between uncertain and fuzzy values. Aim of the present section is to provide further details about this difference and to briefly introduce the reader to the fuzzy set theory, which can be fruitfully applied to sustainability assessment.

Fuzzy logic originated from recognizing that the accuracy of many system analysis theories and techniques goes beyond the levels required in common real applications. L.A. Zadeh was the first to translate this concept into a new theory (just the fuzzy logic) in the early sixties in the U.S (Zadeh, 1065). From that moment on, fuzzy set theory has found several applications, especially in Japan, China and Europe.

Fuzzy set theory is basically an extension of the classical set theory in which the two Aristotelic principles of exclusions and of the "tertium non datur" are no longer valid. In practice it is allowed for something to pertain to a certain class A and contemporary to the class non-A (in contrast with the principle of exclusion) but with different degrees of membership (in the range [0,1]).

The concept of "degrees of membership" has opened the debate concerning the relationship between fuzzy logic and the probability theory. Both the theories deal with uncertainty, but from totally different perspectives: in probability theory, the uncertainty is connected to our incapability to foresee a certain event due to our ignorance on the phenomena that drive the event itself. Let consider the following example. I am not able to foresee the height of my daughter when she will be 18 years old. However, when my daughter will be 18 years old I will be able to measure her height (with the precision allowed by the device that I will use) and therefore the uncertain event will become certain (unless the uncertainty connected with the device's accuracy). This is the perspective of probability theory. What I can do now is to define a probability distribution of the height of my daughter basing on my current knowledge. In fuzzy logic the perspective is completely different. The previous example can be posed in this other way: I am not able to say if my daughter will be "tall" or not when she will be 18 years old. However, when she will be 18 years old, I will hardly be able to say if she is "tall" with absolute certainty, as "tall" is a subjective (thus "fuzzy") concept. What "tall" means for me can be very different from what it means for a basketball player. In this case, then, the uncertainty is intrinsic of the definition. With the fuzzy logic, however I will be able to say that my daughter is "tall" with a certain degree of membership. This means that fuzzy logic allows providing a concrete answer (also referred to as crisp) to a subjective problem.

Just in order to be more operational, fuzzy set theory applied to the previous problem would work in the following way. We need an automatic methodology to classify people as "Tall", "Short" or "Medium" height. These are fuzzy attributes that, however, in our mind have a numeric meaning. The first step of the process is the fuzzification, that is to say that we have to assign to the numerical values we have in mind a linguistic rule. So we call "Short" the people less than 140cm tall, "Tall" those more than 180cm tall and "Medium" those who are in the range 160-170 cm tall (in Figure 21 these ranges have degree of membership 1). Of course, in our mind we know that this classification has no reason to be universal and therefore we fuzzify the concept introducing level of membership in the range [0,1] for the three categories (which reflects

our difficulty in defining a person 155 tall as "Short" or "Medium"). This process produces the membership functions reported in Figure 22. Now we are ready to proceed with the classification and a person 175cm tall will be classified as "Medium" with membership 0.5 and "Tall" with membership 0.5. This classification has very little of linguistic and fuzzy. In truth it is a crisp classification which, however, reflects our intrinsic incapability of classification (not our ignorance). The process which has led to the classification is referred to as defuzzification. Fuzzification and defuzzifications are the two crucial steps of the fuzzy set approach. Between them, many operational treatments can be carried out by means of logical operators. In this way it is possible to deal with very complex analysis without a detailed mathematical description of the problem.

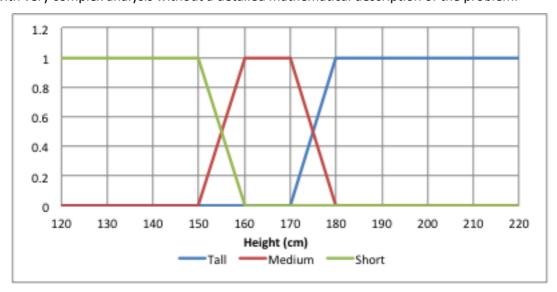


FIGURE 22. Fuzzification and membership functions for the Height attribute

This simple example is also able to show how the fuzzy logic is able to deal with subjective judgements and preferences and therefore that it can represent a suitable tool for social sciences. This is an important feature for sustainability assessment, as many targets may be posed by policy makers only in qualitative terms (even because, as already pointed out before, the concept of sustainability hardly leads to the definition of measurable yardsticks against which to assess practical policies, Phillis and Andriantiatsaholiniaina 2001).

In the following we will provide the reader with a brief literature review of the application of fuzzy set theory to sustainability appraisal applications.

Fuzzy logic and theory have been applied to sustainability assessment a few years later the introduction of the sustainable development concept by the Bruntland report (WCDE 1987). Marks et al. (1995) and Shrestha et al. (1996) respectively applied fuzzy logic for the sustainability assessment of the agriculture system (in combination with multi-criteria decision making) and of reservoir operations. The motivation was methodological rather than conceptual. Palmer et al. (1996) defined the terms sustainability and sustainable development as "fuzzy buzzwords", namely "terms that appear to encapsulate a discrete notion but which actually have multiple interpretations", and inspired subsequent studies to deal with sustainability assessment using the fuzzy logic.

Many other applications have followed, purposefully using fuzzy set theory for its methodological soundness to deal with qualitative and not well defined inputs/targets. These involve, the sustainability assessment of energy systems (Ludwig 1997), sustainable water/coastal management (Simonovic 1997, Hogarth and McGlade 1997), sustainability of projects (Carter et al. 1997). Other studies have then followed, exploiting the use of fuzzy logic to the definition itself of the sustainable development, rather than on its attributes. Application fields, in this case, have been forest management (Ducey and Larson 1999) and rural planning (Bosshal 2000). Main limitation of these and others works on the topic of that period is the fact that all of them looked at the sustainability problem from their own, field related perspective. The first example of fuzzy logic applied to sustainability assessment with an ecological economic perspective can be found in Phillis and Andriantiatsaholiniaina (2001). The authors also provide a thorough introduction to fuzzy set theory and the details of its application to sustainability assessment applications (see also Andriantiatsaholiniaina et al. 2004). In the last years, fuzzy logic has seen its application in hundreds of sustainability assessment studies. The interested reader can for example refer to the following interesting examples, Cornelissen et al. (2001), Opricovic and Tzeng (2002), Prato (2005), Zavadskas and Antucheviciene (2007), Erol et al. (2011).

## 8. Conclusions

Dealing with uncertainty is a big issue especially for policy makers. It can confuse them, but it can be made policy relevant if results are translated into the likelihood that policy targets will be met. Policy makers, then, have the choice to either accept the risks, or to take actions that increase the certainty that targets will be met. Basically there are two types of policy risks, i) doing too much (and spoil public money) or, ii) doing too little (and be confronted with irreversible environmental problems later). The acceptance of the different types of policy risks will depend on the preference of the chosen politicians and the priorities they will give to environmental, social and economic stakes. The careful politician will easily realize that policies can be made more robust when risks are acknowledged and adaptations are made to minimize the risks (or to define a strategy on how to respond when risks would really occur).

In this light, the role of the analysts is to provide the politicians with as much information as possible in order to facilitate their decision process. In particular, providing a robust estimation of the level of confidence of the results achieved may represent an invaluable contribution for a robust policy making.

In this report we have analysed some of the sources of uncertainty connected to the sustainability assessment practice and have provided a conceptual framework in order to deal with them. The conceptual framework is centred on the phases of sensitivity and uncertainty analysis. Different techniques can be used to carry out both the analyses and some of them have been discussed here. In particular, in the report we suggest the adoption of a Monte Carlo framework in both the cases, which should allow for a more effective exploration of the inputs' space. This framework has been applied to field specific simulation models in order to highlight the added value of their applications in the models' comprehensions.

Results of the application of sensitivity and uncertainty analysis to the different case studies also provide some interesting properties of the different models considered, as well as they may represent a useful guide through the application of the two different techniques.

The report ends with a brief presentation of the fuzzy-logic concept. The reason for this is twofold. On the one hand we want to clarify the differences between the concepts of uncertainty and fuzziness, which are frequently confused. On the other hand we claim that the fuzzy logic should be more and more applied in the sustainability assessment, given the fuzzy nature of the sustainability concept itself.

# Acknowledgements

Authors are mostly grateful to Stefano Tarantola, from the Joint Research Centre of the European Commission, and to Sergei Kucherenko, from the Imperial College of London, for their precious methodological suggestions in the set-up of the sensitivity analysis technique implemented in the report and for the comments on the report itself. Authors are also grateful to Marcello Montanino, from the University of Napoli "Federico II", for the help provided in part of the calculations and for the several discussions on the two car-following models. In addition authors are grateful Dimitar Marinov and Marco Trombetti for their support in the use of the MAPPE model and for their useful comments to this report. Finally authors are very grateful to Rob Maas, from the Dutch National Institute for Public Health and the Environment, for his precious comments on the scope and the structure of the report. Their contributions have significantly improved the contents of this report.

Part of the research contained within this report benefited from the participation in EU COST Action TU0903 MULTITUDE – Methods and tools for supporting the Use, calibration and validaTion of Traffic simulation models.

Part of the research contained within this report benefited from the participation to the LC-IMPACT project, cofunded by the European Commission under the 7th framework program on environment; ENV.2009.3.3.2.1: LC-IMPACT – Improved Life Cycle Impact Assessment methods (LCIA) for better sustainability assessment of technologies; Grant agreement n° 243827.

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European Commission

EUR 25166 - Joint Research Centre - Institute for Environment and Sustainability

Title: Dealing with uncertainty in sustainability assessment

Author(s): Biagio Ciuffo, Apollonia Miola, Vincenzo Punzo, Serenella Sala

Cover photo courtesy of Daniela Carrion and Mauro Tominetti

Luxembourg: Publications Office of the European Union

2012 - 82 pp. - 21.0 x 29.7 cm

EUR - Scientific and Technical Research series - ISSN 1831-9424 (online), ISSN 1018-5593 (print)

ISBN 978-92-79-22726-4 (PDF)

ISBN 978-92-79-22725-7 (print)

doi:10.2788/57452

#### Abstract

Assessing sustainability is more and more becoming a common practice in products, policies and institution appraisals. However, increasing concern has been recognized in the scientific community regarding whether the various available examples of sustainability assessment are really comprehensive and able to judge in a robust and reliable way if new developments to "meet the needs of the present without compromising the ability of future generations to meet their own needs". It is possible to identify three main sources of uncertainty: i) the "sustainable development" concept and the definition of boundaries (physical, economic and social) to assess it, ii) the intrinsic subjectivity of many assessment tools, iii) the incapability of many available modelling activities to mimic our world.

This report tries to define a conceptual framework in order to deal with the uncertainty within a sustainability assessment describing some statistical techniques that can be fruitfully applied for this purpose. The conceptual framework proposed is centred on sensitivity and uncertainty analysis. A Monte Carlo framework is suggested in both the cases, and examples of its application to field specific models are provided. Results clearly show the powerfulness of such techniques in providing the analyst with useful information to manage the uncertainties hidden behind any assessment exercise.

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Key policy areas include: environment and climate change; energy and transport; agriculture and food security; health and consumer protection; information society and digital agenda; safety and security including nuclear; all supported through a cross-cutting and multi-disciplinary approach.



