

| Category | Title |
|------------------|----------------|
| General guidance | Uncertainties |
| | |
| Version | Guidebook 2023 |

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1 Overview

The 'Guidelines for Reporting Emissions and Projections Data under the Convention on Long-range Transboundary Air Pollution' (United Nations Economic Commission for Europe) (1) indicate that:

'Parties shall quantify uncertainties in their emission estimates using the most appropriate methodologies available, taking into account guidance provided in the EMEP/EEA Guidebook. Uncertainties should be described in the IIR'

This chapter provides guidance on the quantification of uncertainties in emissions inventories and is aligned with the '2019 Refinement to the 2006 IPCC Guidelines for National GHG Inventories' guidance (IPCC (2019). This chapter provides the user with a basic understanding of the issues of emission inventory uncertainty, with default values to be used in a first uncertainty analysis and describes the information on uncertainty that needs to be reported.

Uncertainty assessment is an important part of compiling an emissions inventory and to assess how uncertainties evolve over time. It is considered best practice that emissions inventories contain neither over- nor under-estimates as far as can be judged, and for which uncertainties are reduced as far as practicable.

Guidance on reducing uncertainties in emission inventories is not included in this chapter, but information can be taken from Section 3.1.6 Reducing Uncertainties of the 2019 Refinement to the 2006 IPCC Guidelines for National GHG Inventories (IPCC 2019).

It is impossible to eliminate uncertainty completely, leading to the conclusion that for every value reported in an inventory there will exist an associated uncertainty. Knowledge of this uncertainty is an integral part of the inventory compilation effort. Furthermore, as a priority, effort should focus on accuracy, ensuring that emissions are neither over- nor under-estimated i.e. bias should be eliminated as far as can be judged. While variability is a characteristic of the inventory compilation process and cannot be eliminated, uncertainty, which covers both random error and bias, can be broadly associated with lack of knowledge.

Uncertainty in emission estimates is a function of the uncertainty of input data i.e. activity or emission factors, used to compile the inventory. Hence, data collection and uncertainty evaluation are strongly linked, and all data contributing to the estimation of emissions should have an associated uncertainty assessment.

Finally, it is important to note that producing an uncertainty analysis for the inventory is not an independent goal in itself, but is an important tool in the process of improvement of the inventory. Together with the key category analysis, it helps the inventory compilers in prioritising the improvements in methodology development and data collection for the different source and sink categories.

The 'Uncertainties' chapter of the 2019 Refinement to the 2006 IPCC Guidelines (IPCC 2019) provides detailed background information on planning and undertaking an uncertainty analysis. The contents

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⁽¹) Guidelines for reporting emissions and projections data (ECE/EB.AIR/125). The Guidelines and annexes are available online from the CEIP website (www.ceip.at/)

of this chapter have been drafted to align with the information from the IPCC, so as to ensure consistency between the approaches used for GHG and air quality pollutant emission inventories.

The IPCC Guidance states that the process of producing an uncertainty analysis can pragmatically be divided into four parts:

- (1) the rigorous investigation of the likely causes of data uncertainty and quality;
- (2) the creation of quantitative uncertainty estimates and parameter correlations;
- (3) the mathematical combination of those estimates when used as inputs to a statistical model (e.g., first-order error propagation or Monte Carlo method); and
- (4) the selection of inventory improvement actions (improvement plan) to take in response to the results of the previous three parts.

The following sections summarise the approaches for each of these four steps. More detail on best practices can be found by referring to the IPCC guidance.

2 Quantifying uncertainty

2.1 Expressing uncertainty

An important aspect of an uncertainty analysis concerns the ways on how to express the uncertainties associated with individual estimates or the total inventory. It is recommended to use the same quantity to express uncertainty in a LRTAP Convention inventory as required in a greenhouse gas inventory, namely the 95 % confidence interval.

This 95 % confidence interval is specified by the confidence limits defined by the 2.5 percentile and 97.5 percentile of the cumulative distribution function of the estimated quantity. Put another way, it is good practice to express the range of an uncertain quantity within an inventory such that:

- there is a 95 % probability that the actual value of the quantity estimated is within the interval defined by the confidence limits; and
- it is equally likely that the actual value, should it be outside the range quoted, lies above or below it

In practical terms, the 95 % confidence interval for a normal distribution lies between \pm 2 standard deviations around the mean. Therefore, when uncertainties are not too large (standard deviations less than 30 % of the mean value), the (cumulative) distribution function of the estimated quantity might be assumed to be normal and the 95 % confidence can be estimated as being two times the standard deviation.

2.2 Variables and parameters

A significant portion of an emission inventory is compiled by collecting activity data and appropriate emission factors according to the Tier 1 default approach:

$$Emission_{pollutant} = \sum_{activities} Activity \ rate_{activity} \times Emission \ factor_{activity,pollutant}$$
 (1)

In cases where a Tier 2 or Tier 3 methodology is applied (best practice for all key categories), the equation to be used to estimate emissions is more complicated than a simple multiplication of a variable (*Activity rateactivity*) and a parameter (*Emission factoractivity,pollutant*). However, in this section we present for reasons of simplicity the quantification methods and principles using this simple equation. In case of a more complicated algorithm, the calculation becomes also more complicated but not essentially different.

2.3 Methods

Regardless of the methodology used to estimate emissions for a category, the uncertainty evaluation will be based on the underlying data. The overall uncertainty of the emissions will depend on the uncertainty associated with every piece of data that is used to inform the inventory. As such, uncertainty assessment begins with good practice in data collection. Uncertainty consideration needs to be an integral part of the data collection effort.

To enable a quantitative uncertainty analysis as proposed in this chapter, both the variables and parameters need quantitative uncertainty ranges. The following sections present some essential parts of the 2006 IPCC Guidelines on this issue.

2.3.1 Measurements

In some cases, periodic emission measurements may be available at a site. If these measurements can be linked to representative activity data, which of course is crucial, then it is possible to determine a site-specific emission factor, together with an associated probability density function to represent annual emissions.

This can be a complex task. To achieve representativeness, it may be necessary to partition (or stratify) the data to reflect typical operating conditions. For example:

- start-up and shut down can give different emission rates relative to activity data. In this case, it is good practice to partition the data with separate emission factors and probability density functions derived for steady state, start-up and shut down conditions;
- emission factors can depend on load. In this case, the total emissions estimation and uncertainty
 analysis may need to be stratified to take account of load expressed, for example, as percentage
 of full capacity. This could be done by regression analysis and scatter plots of the emission rate
 against likely controlling variables (e.g. emissions versus load) with load becoming part of the
 activity data needed;
- measurements taken for another purpose may not be representative. For example, methane
 measurements made for safety reasons at coalmines and landfills may not reflect total
 emissions. In such cases, it is good practice to estimate the ratio between the measured data
 and total emissions for the uncertainty analysis.

If the data sample size is large enough, standard statistical goodness-of-fit tests can be used in combination with expert judgement to help in deciding which probability density function to use for describing variability in the data (partitioned if necessary) and how to parameterise it. However, in many cases, the number of measurements from which to make an inference regarding uncertainty will be small. Typically, as long as there are three or more data points, and as long as the data are a random representative sample of the quantity of interest, it is possible to apply statistical techniques to estimate the values of the parameters of many two-parameter distributions (e.g. normal, lognormal) that can be used to describe variability in the data set. With small sample sizes, there will

be large uncertainties regarding the parameter estimates that should be reflected in the quantification of uncertainty for use in the emissions inventory. Furthermore, it is typically not possible to rely on statistical methods to differentiate goodness-of-fit of alternative parametric distributions when sample sizes are very small. Therefore, considerable judgement is required in selecting an appropriate parametric distribution to fit to a very small data set. In situations where the coefficient of variation is less than approximately 0.3, a normal distribution may be a reasonable assumption. When the coefficient of variation is large and the quantity is non-negative, then a positively skewed distribution such as a lognormal one may be appropriate. Guidance on the selection of distributions is provided in Appendix A, copied from subsection 3.2.2.4 of the Uncertainties Chapter of the General Guidance Volume of the 2006 IPCC Guidelines, Conceptual Basis for Uncertainty Analysis, and the use of expert judgements in this context is outlined below.

2.3.2 Literature and other documented data

When site-specific data are unavailable, good practice will usually be to develop emission estimates using average emission factors drawn from references consistent with this Guidebook. These factors will have been measured under particular circumstances that are judged to be typical. There will be uncertainties associated with the original measurements, as well as with the use of the factors in circumstances other than those associated with the original measurements.

It is a key function of good practice guidance for each source category to guide the choice of emission factors to minimise this second source of uncertainty to the extent possible. Where such emission factors are used, it is good practice to estimate the associated uncertainties from:

- original research including country-specific data: for measurement-based emission factors, the
 data from the original measurement programme may enable an assessment of the uncertainty
 and possibly the probability density function. Well-designed measurement programmes will
 provide sample data that cover the range of types of plants and their maintenance, size and age,
 so that the factors and their uncertainties can be used directly. In other cases, expert judgement
 will be needed to extrapolate from the measurements to the full population of plants in that
 particular source category;
- this Guidebook: the sectoral chapters provide emission factors for every NFR (Nomenclature for Reporting) code. All emission factors for use with Tier 1 and Tier 2 methodology have (an estimation of) the 95 % confidence interval listed in the same table.

Unless clear evidence to the contrary is available, the probability density functions are assumed to be normal. However, it is good practice that the inventory agency evaluates representativeness of the default for its own situation. If the default is judged to be unrepresentative and the source category is important to the inventory, it is good practice to develop improved assumptions based upon expert judgement.

2.3.3 Expert judgement

When empirical data are lacking, estimates of uncertainty in emission factors or direct emission measurements will need to be based on expert judgement.

It is important to select appropriate experts with respect to the emission of inventory inputs for which uncertainty estimates are needed.

The goal of expert judgement here is to develop a probability density function, taking into account relevant information such as:

- is the emission source similar to other sources? How is the uncertainty likely to compare?
- how well is the emission process understood? Have all possible emission sources been identified?
- are there physical limits on how much the emission factor can vary? Unless the process is reversible it cannot emit less than zero, and this may constrain a very wide uncertainty range.
 Mass balance considerations or other process data may place an upper limit on emissions;
- are the emissions consistent with atmospheric concentrations? Emissions are reflected in atmospheric concentrations at site-specific and larger scales and again this may limit the possible emission rates.

A degree of expert judgement is required even when applying classical statistical techniques to data sets, since one must judge whether the data are a representative random sample and, if so, what methods to use to analyse the data. This may require both technical and statistical judgement. Interpretation is especially needed for data sets that are small, highly skewed or censored. The formal methods for obtaining data from experts are known as expert elicitation.

The IPCC 2006 Guidelines propose a protocol for expert elicitation. The use of this protocol is strongly recommended to minimise misunderstandings between inventory compiler and the expert and to avoid unintentional bias.

2.4 Default uncertainty ranges

2.4.1 Activity data

Activity data are usually derived from (economic) statistics, including energy statistics and balances, economic production rates, population data, etc. It is possible that these agencies have already assessed the uncertainties associated with their data as part of their data collection procedures. These uncertainties can be used to construct probability density functions.

In some cases, uncertainty data for activity rates are not easily available. Since any uncertainty analysis needs quantitative input, quantitative uncertainty ranges are needed. **Error! Reference source not found.** proposes indicative ranges that could be applied in all cases where no independent data are available.

Table 2-1 Indicative error ranges in activity data for uncertainty analysis

| Data source | Error range | Remarks |
|--|------------------------------------|---|
| The national (official) statistics | 0-2 % | The official statistics of a country may be reported with an uncertainty range, although it is also common for the data to be assumed to be 'fixed', with no uncertainty. |
| | | In fact, however, for energy data an indication of the uncertainties could be derived from the entry under 'statistical differences', representing the mismatch between production and consumption. |
| An update of last year's statistics, using gross economic growth factors | 0-2 % | The economic system of a country will probably not shift more than a few per cent between successive years. Hence, if an update of last year's data is used, an uncertainty of a few per cent seems reasonable |
| IEA energy statistics/balances | OECD: 2-3 % non-OECD: 5-10 % | The International Energy Agency (IEA) publishes national energy statistics and balances for many countries. For the Organisation for Economic Co-operation and Development (OECD) countries these statistics will ideally be equal to the official energy statistics. For other countries the uncertainties could be expected to be in the order of 5 to 10 % (educated guess). |
| UN statistical databases | 5-10 % | These data might have a similar uncertainty as the ones provided by IEA. |
| Default values, other sectors and data sources | 30-100 % | |

Error! Reference source not found. proposes for the uncertainty range, when official statistics are used, a possible value of 0 %. This can, of course, not be a true uncertainty range. The value here is given to facilitate a selection of a certain range. It is recommended to always use experts' opinions to make the final selection.

2.4.2 Emission factors

In many cases uncertainty ranges for emission factors are rather difficult to obtain. **Error! Reference source not found.** represents an application of the concepts of qualitative data rating schemes for all pollutants of concern in the Guidebook. This table is organized by major NFR code groupings. It is important to note that any such qualitative summary is subjective and individual opinions will differ.

Definitions of the ratings used in **Error! Reference source not found.** are presented in **Error! Reference source not found.** This table also proposes default error ranges associated with each quality rating. The error ranges are obtained from the EU Guidance Report on Supplementary Assessment under EC Air Quality Directives, where they have been defined for application in air quality models.

In addition, each of the emission factors presented in the Tier 1 and Tier 2 approaches in the different sectoral chapters of this EMEP/EEA Guidebook each have a 95% confidence interval associated with them. It should be noted however that these upper and lower estimates are often based on either

expert judgement or on the translation of a rating such as presented in **Error! Reference source not found.**. They may also not take into account uncertainties associated with poor representativeness (see below).

Table 2-2 Rating definitions

| Rating | Definition | Typical error range |
|--------|---|-----------------------|
| A | An estimate based on a large number of measurements made at a large number of facilities or individual sources across a comprehensive range of operating conditions that fully represent the sector | 10 to 30 % |
| В | An estimate based on a large number of measurements made at a large number of facilities or individual sources across a range of operating conditions that represent a large part of the sector | 20 to 60 % |
| С | An estimate based on a number of measurements made at a small number of representative facilities or individual sources across a smaller range of operating conditions, or an engineering judgement based on a number of relevant facts. An estimate based on a large number of measurements across a range of conditions for a source which is complex and/or variable. | 50 to 200 % |
| D | An estimate based on single measurements, or an engineering calculation derived from a number of relevant facts An estimate based on a large number of measurements across a range of conditions for a source which is particularly complex and/or variable. | 100 to 300 % |
| Е | An estimate based on an engineering calculation derived from assumptions only An estimate based on a limited number of measurements for a source which is particularly complex and/or variable. | order of magnitude |

Table 2-3 Main NFR source categories with applicable quality data ratings

| | | v | 7 | _ | | - | 70 | _ | |
|---------|--|-----------------|-----------------|-----|---|-----------------|----|----------------|--|
| NFR | SOURCE CATEGORY | SO ₂ | NO _x | VOC | 6 | NH ₃ | Š | HM/POP | |
| | | | | | | | | 7 | |
| 1.A.1 | Public power, cogeneration and district heating | Α | В | С | В | Е | С | D | |
| 1.A.2 | Industrial combustion | Α | В | С | В | E | С | D | |
| 1.A.3.b | Road transport | А | С | С | С | E | С | E ² | |
| 1.A.3.a | Other mobile sources and machinery | В | D | D | D | Е | D | Е | |
| 1.A.3.c | | | | | | | | | |
| 1.A.3.d | | | | | | | | | |
| 1.A.3.e | | | | | | | | | |
| 1.A.4 | Commercial, institutional and residential combustion | A | С | С | С | Е | D | E | |
| 1.B | Extraction and distribution of fossil fuels | С | С | С | С | | D | E | |
| 2 | Industrial processes | В | С | С | С | E | С | Е | |
| 3 | Solvent use | | | В | | | D | E ¹ | |
| 4 | Agriculture activities | | D | D | D | D | Е | Е | |
| 5.a | Waste treatment | В | В | В | С | | С | D | |
| 5.b | | | | | | | | | |
| 5.c | Waste disposal activities | С | С | С | С | Е | С | Е | |
| 11 | Nature ³ | D | D | D | E | Е | Е | E ³ | |

Notes:

The letter grade ratings are primarily applicable to the estimation approaches for emissions inventory preparation that rely on emission factors and estimates of activity indicators. In all cases, the application of more direct approaches based on measurement would receive higher quality ratings.

The application of these subjective ratings for the aggregated source category groupings represented by the major NFR-code groupings can be misleading in some specific cases. For example, the rating specified for heavy metals/persistent organic pollutants for road transport is

¹ In some cases, solvents may be toxic compounds.

² Rating representative of typical pollutant source category combination; some specific cases may have smaller error ranges.

³ Natural sources could be contributed from volcanoes and other geothermal events.

listed as E to apply in general to the understanding of the contribution of these pollutants from mobile sources. In fact, for the specific case of lead from mobile sources, the emission factors and emissions estimates are known with significantly more confidence. In such an analysis at that level of disaggregation, lead from mobile sources would receive a B rating. Also, at this level of aggregation, several source category pollutant combinations are irrelevant in that emissions of the pollutant from that source category are zero or so minimal as to be of little or no importance.

Uncertainty of Emission Factors and issues of 'applicability'

Emission factors included in the sectoral chapters of this Guidebook include estimates of the associated uncertainty ranges. However, caution should be adopted when using these uncertainty ranges.

Uncertainties in measurement data can be determined in different ways, for example based on known sources of error (such as instrumentation), or from the variance of a particular set of measurements. This provides a level of uncertainty that can be assigned to an emission factor. However, for many source and pollutant combinations presented in this Guidebook there are few or no measurements to draw on. To ensure that emission factors can be provided for all possible pollutant and source combination, emission factors are presented which may have been derived from measurement of similar but different sources. It is also possible that the measurements have been made in a specific country or region that may not be representative for all of Europe, or in previous years which are no longer representative of the emissions characteristics of current years. All of these issues can be considered as issues of 'applicability'.

It can therefore be the case that uncertainties derived from only the variance in measurement data, or the combination of known measurement errors, significantly underestimate the uncertainty of emission factors.

One solution to this issue could be to review the source of EFs in detail, and where possible amend quality data ratings outlined above to account for applicability issues. However, this has not yet been undertaken. Furthermore, methods to quantify the uncertainties associated with applicability have not yet been developed. As a result, the quantification of uncertainties using e.g. a propagation of errors, may well underestimate uncertainty if the uncertainties applied to the emission factors are not characterised sufficiently.

3 Aggregating uncertainties

Once the uncertainties in the source categories have been determined, they may be combined to provide uncertainty estimates for the entire inventory in any year and the uncertainty in the overall inventory trend over time.

The error propagation equation, as discussed more extensively in the Uncertainties Chapter of the General Guidance Volume of the 2006 IPCC Guidelines, yields two convenient rules for combining uncorrelated uncertainties under addition and multiplication:

1. *Rule A:* where uncertain quantities are to be combined by addition, the standard deviation of the sum will be the square root of the sum of the squares of the standard deviations of the quantities that are added with the standard deviations all expressed in absolute terms (this rule is exact for uncorrelated variables).

Using this interpretation, a simple equation can be derived for the uncertainty of the sum, that when expressed in percentage terms U (defined as the uncertainty divided by the quantity itself) becomes:

$$U_{\text{total}} = \frac{\sqrt{(U_1 \cdot x_1)^2 + (U_2 \cdot x_2)^2 + \dots + (U_n \cdot x_n)^2}}{x_1 + x_2 + \dots + x_n},$$
(2)

where

x_i are the quantities,

U_i are the uncertain quantities and the percentage uncertainties (half the 95 % confidence interval) associated with them, respectively,

U_{total} is the percentage uncertainty in the sum of the quantities (half the 95 % confidence interval divided by the total (i.e. mean) and expressed as a percentage);

2. *Rule B*: where uncertain quantities are to be combined by multiplication, the same rule applies except that the standard deviations must all be expressed as fractions of the appropriate mean values (this rule is approximate for all random variables).

A simple equation can also be derived for the uncertainty of the product, again expressed in percentage terms:

$$U_{\text{total}} = \sqrt{U_1^2 + U_2^2 + ... + U_n^2} , \tag{3}$$

where

U_i are the percentage uncertainties (half the 95 % confidence interval) associated with each of the quantities,

U_{total} is the percentage uncertainty in the product of the quantities (half the 95 % confidence interval divided by the total and expressed as a percentage).

The inventory is principally the sum of products of emission factors and activity data. Therefore, Rules A and B can be used repeatedly to estimate the uncertainty of the total inventory.

In practice however, uncertainties found in inventory source categories vary from a few per cent to orders of magnitude, and may be correlated. This is not consistent with the assumptions of Rules A and B that the variables are uncorrelated with a standard deviation of less than about 30 % of the mean, but under these circumstances, Rules A and B may still be used to obtain an approximate result. Alternatively, a stochastic simulation (the Monte Carlo method) can be used, that can combine uncertainties with any probability distribution, range, and correlation structure provided they have been suitably quantified. Thus, two approaches for uncertainty analysis are described below:

- Approach 1: estimation of uncertainties by source category using the error propagation
 equation via Rules A and B, and simple combination of uncertainties by source category to
 estimate overall uncertainty for one year and the uncertainty in the trend;
- Approach 2: estimation of uncertainties by source category and in the overall inventory by stochasticsimulation for one year and the uncertainty in the trend. More information with regard to this procedure is presented in IPCC (2006).

In many cases a quantitative indicator of inventory uncertainty will be sufficient, although the Monte Carlo approach will provide considerably more reliable results. Chapter 5 on Inventory management, improvement and QA/QC presents Approach 1 for LRTAP Convention pollutants in a simple calculation scheme.

The Approach 1 method does not account for correlation and dependency between source categories that may occur because the same activity data or emission factors may be used for multiple estimates. Correlation and dependency may be significant for fossil fuels because a given fuel is used with the same emission factor across several sub-categories. In addition, in many cases total consumption of a fuel may be better known than consumption disaggregated by source category, which implies that hidden dependencies will exist within the statistics because of the constraint provided by overall consumption. Dependency and correlation can be addressed by aggregating the source categories to the level of overall consumption of individual fuels before the uncertainties are combined. This entails some loss of detail in reporting on uncertainties but will deal with the dependencies where they are thought to be significant (e.g. where the uncertainties in fossil fuel emissions when aggregated from the source category level are greater than expected).

4 Uncertainties in trends

An emission factor that over- or underestimates emissions in the base year will probably do so in subsequent years. Therefore, uncertainties due to emission factors will tend to be correlated over time. The Approach 1 uncertainty aggregation method, as proposed by 2006 IPCC Guidelines, is in principle able to deal with this issue.

Trend uncertainties are estimated using two sensitivities:

- i. Type A sensitivity: the change in the difference in overall emissions between the base year and the current year, expressed as a percentage, resulting from a 1 % increase in emissions of a given source category and pollutant in both the base year and the current year;
- ii. Type B sensitivity: the change in the difference in overall emissions between the base year and the current year, expressed as a percentage, resulting from a 1 % increase in emissions of a given source category and pollutant in the current year only.

Conceptually, Type A sensitivity arises from uncertainties that affect emissions in the base year and the current year equally, whereas Type B sensitivity arises from uncertainties that affect emissions in the current year only. Uncertainties that are fully correlated between years will be associated with Type A sensitivities, and uncertainties that are not correlated between years will be associated with Type B sensitivities.

The 2006 IPCC Guidelines suggest that emission factor uncertainties will tend to have Type A sensitivities, and activity data uncertainties will tend to have Type B. However, this association will not always hold and it is possible to apply Type A sensitivities to activity data, and Type B sensitivities to emission factors to reflect particular national circumstances. Type A and Type B sensitivities are simplifications introduced for the analysis of correlation.

Once the uncertainties introduced into national emissions by Type A and Type B sensitivities have been calculated, they can be summed using the error propagation equation (Rule A) to give the overall uncertainty in the trend.

5 The Approach 1 uncertainty aggregation scheme

Table 5-1 shows the calculation scheme, which is an adaption of the spreadsheet scheme as presented in the 2006 IPCC Guidelines for National Greenhouse Gas Inventories (IPCC, 2006).

| Α | В | С | D | E | F | G | Н | ı | J | К | L | М | N | 0 | Р | Q |
|-----------------------|-----------|---------------------|------------------|---------------------------|-----------------------------|----------------------|---|---------------------|--------------------|--|--|---|-----------------------------------|---------------------------------|------------------------------------|---------------------------|
| NRF sector (and FUEL) | Pollutant | Base year emissions | Year t emissions | Activity data uncertainty | Emission factor uncertainty | Combined uncertainty | Combined uncertainty as % of total national emissions in year t | Type A sensitivity | Type B sensitivity | Uncertainty in trend in national emissions introduced by emission factor uncertainty | Uncertainty in trend in national emissions introduced by activity data uncertainty | Uncertainty introduced into the trend in total national emissions | Emission factor quality indicator | Activity data quality indicator | Expert judgement reference numbers | Footnote reference number |
| | | Input data | Input data | Input data | Input data | $\sqrt{E^2 + F^2}$ | $\frac{(G \cdot D)^2}{(\sum D)^2}$ | Note B ¹ | $\frac{D}{\sum C}$ | I • F Note C ¹ | $J \bullet E \bullet \sqrt{2}$ Note D ¹ | $K^2 + L^2$ | Note E 1 | Note E 1 | | |
| | | Mg | Mg | % | % | % | % | % | % | % | % | % | | | | |
| 1.A.1.a | | | | | | | | | | | | | | | | |
| 1.A.1.b | | | | | | | | | | | | | | | | |
| 1.A.1.c | | | | | | | | | | | | | | | | |
| etc. | | | | | | | | | | | | | | | | |
| Total | | ΣC | ΣD | | | | $\sqrt{\sum H}$ | | | | | $\sqrt{\sum M}$ | | | | |

⁽¹⁾ Notes are explained on the next page.

Note A:

If only total uncertainty is known for a source category (not for emission factor and activity data separately), then:

- (i) if uncertainty is correlated across years, enter the uncertainty into column F, and enter 0 in column E;
- (ii) if uncertainty is not correlated across years, enter the uncertainty into column E and enter 0 in column F.

NOTE B:

Absolute value of:

$$\frac{0.01 \bullet D_x + \sum D_i - (0.01 \bullet C_x + \sum C_i)}{(0.01 \bullet C_x + \sum C_i)} \bullet 100 - \frac{\sum D_i - \sum C_i}{\sum C_i} \bullet 100$$

NOTE C:

In the case where no correlation between emission factors is assumed, sensitivity B should be used and the result multiplied by $\sqrt{2}$:

$$K_x = J_x \bullet F_x \bullet \sqrt{2}$$

NOTE D:

In the case where correlation between activity data is assumed, sensitivity A should be used and the $\sqrt{2}$ is not required:

$$L_{x} = I_{x} \bullet E_{x}$$

Note E:

Please use the following abbreviations:

D - NFR source category default

M - measurement based

R – national referenced data

The columns of the table are labelled A to Q and contain the following information:

- columns A and B show the NFR source category and pollutant;
- columns C and D are the inventory estimates in the base year and the current year (2) respectively, for the source category and gas specified in columns A and B;
- columns E and F contain the uncertainties for the activity data and emission factors respectively, derived from a mixture of empirical data and expert judgement as previously described in this chapter, entered as half the 95 % confidence interval divided by the mean and expressed as a percentage. The reason for halving the 95 % confidence interval is that the value entered in columns E and F then corresponds to the familiar plus or minus value when uncertainties are loosely quoted as 'plus or minus x %', so expert judgements of this type can be directly entered

⁽²⁾ The current year is the most recent year for which inventory data are available.

- in the spreadsheet. If uncertainty is known to be highly asymmetrical, enter the larger percentage difference between the mean and the confidence limit;
- column G is the combined uncertainty by source category derived from the data in columns E and F using the error propagation equation (Rule B). The entry in column G is therefore the square root of the sum of the squares of the entries in columns E and F;
- column H shows the uncertainty in column G as a percentage of total national emissions in the current year. This is a measure of the degree of uncertainty introduced into the national emissions total by the source category in question. The entry in each row of column H is the entry in column G multiplied by the entry in column D squared, divided by the total at the foot of column D squared. The total at the foot of column H is an estimate of the percentage uncertainty in total national emissions in the current year, calculated from the entries above using Rule A. This total is obtained by summing all the entries in column H and taking the square
- column I shows how the percentage difference in emissions between the base year and the current year changes in response to a one per cent increase in source category emissions in both the base year and the current year. This shows the sensitivity of the trend in emissions to a systematic uncertainty in the emissions estimate (i.e. one that is correlated between the base year and the current year). This is the Type A sensitivity as defined above. Appendix 6A.1 of IPCC's Good Practice Guidance (IPCC, 2000) provides the derivation for the formula for the entries in column I;
- column J shows how the percentage difference in emissions between the base year and the current year changes in response to a one per cent increase in source category emissions in the current year only. This shows the sensitivity of the trend in emissions to random error in the emissions estimate (i.e. one, that is not correlated, between the base year and the current year). This is the Type B sensitivity as described above. The formula for the entries in column J is derived in Appendix 6A of IPCC's Good Practice Guidance (IPCC, 2000);
- column K uses the information in columns I and F to show the uncertainty introduced into the trend in emissions by emission factor uncertainty, under the assumption that uncertainty in emission factors is correlated between years. If the user decides that the emission factor uncertainties are not correlated between years then it is good practice to use the entry in column J in place of that in column I and the result multiplied by $\sqrt{2}$. The formula for the entries in column K is derived in Appendix 6A of IPCC's Good Practice Guidance (IPCC, 2000);
- column L uses the information in columns J and E to show the uncertainty introduced into the trend in emissions by activity data uncertainty, under the assumption that uncertainty in activity data is not correlated between years. If the user decides that the activity data uncertainties are correlated between years then it is good practice to use the entry in column I in place of that in column J and the $\sqrt{2}$ factor does not then apply. The formula for the entries in column L is derived in Appendix 6A of IPCC's Good Practice Guidance (IPCC, 2000);
- column M contains an estimate of the uncertainty introduced into the trend in national emissions by the source category in question. Under Approach 1, this is derived from the data in columns K and L. The entry in column M is therefore the sum of the squares of the entries in columns K and L. The total at the foot of this column is an estimate of the total uncertainty in the trend, calculated from the entries above using the error propagation equation. This total is obtained by summing all the entries in column M and taking the square root. The formula for

the entries in column M and the total at the foot of column M is shown in Appendix 6A of IPCC's Good Practice Guidance (IPCC, 2000);

- columns N to Q are used for indicators and cross referencing to footnotes:
 - o column N contains D, M or R, depending on whether the emission factor uncertainty range is based on default (D) information in source category guidance, measurements (M) made for the purpose or national referenced (R) information;
 - column O contains D, M or R, depending on whether the activity data uncertainty range is based on default information in sector guidance, measurements made for the purpose or national referenced information:
 - column P contains the reference numbers of any expert judgements used to estimate uncertainties in this source category;
 - o column Q contains the number of an explanatory footnote to go at bottom of table to identify documentary reference of uncertainty data (including measured data) or other comments relevant to the line.

The Approach 2 Monte-Carlo 6 **Simulation**

A Monte Carlo analysis is suitable for detailed category-by-category assessment of uncertainty, particularly where uncertainties are large, distribution is non-normal, the emission estimation algorithms are complex functions and/or there are correlations between some of the activity sets, emission factors, or both. In Monte Carlo simulation, pseudo-random samples of model inputs are generated according to the probability density functions (PDFs) specified for each input. If the model has two or more inputs, then random samples are generated from the PDFs for each of the inputs, and one random value for each input is entered into the model to arrive at one estimate of the model output. This process is repeated over a desired number of iterations to arrive at multiple estimates of the model output. The multiple estimates are sample values of the PDF of the model output. By analysing the samples of the PDF for the model output, the mean, standard deviation, 95 percent confidence interval, and other properties of the output PDF can be inferred. Monte Carlo simulation is a numerical method, and therefore the precision of the results typically improves as the number of iterations is increased.

6.1 **Key assumptions**

Under the Monte Carlo approach, the simplifying assumptions required for the error propagation can be relaxed. Thus, numerical statistical techniques, particularly the Monte Carlo technique, as they can be generally applied, are more appropriate than Approach 1 for estimating uncertainty in emissions (from uncertainties in activity measures and emission factors/estimation parameters) when:

- uncertainties are large
- their distribution are non-Gaussian
- algorithms are complex functions
- correlations occur between some of the activity data sets, emission factors, or both
- uncertainties are different for different years of the inventory.

6.2 **Key requirements**

Monte Carlo simulation requires the analyst to specify PDFs that reasonably represent each model input for which the uncertainty is quantified (see Annex 1). The PDFs may be obtained by a variety of methods, including statistical analysis of data or expert elicitation. A key consideration is to develop the distributions for the input variables to the emission/removal calculation model so that they are based upon consistent underlying assumptions regarding averaging time, location, and other conditioning factors relevant to the particular assessment (e.g., climatic conditions influencing agricultural emissions of ammonia (NH₃). Monte Carlo analysis can include probability density functions of any physically possible shape and width, as well as varying degrees of correlation (both in time and between source categories). Monte Carlo analysis can deal with simple models (e.g., emission inventories that are the sum of sources and sinks, each of which is estimated using multiplicative factors) as well as more complex models.

6.3 **Monte Carlo procedures**

The principle of Monte Carlo analysis is to select random values of emission factor, activity data and other estimation parameters from within their individual probability density functions, and to calculate the corresponding emission values. This procedure is repeated many times and the results of each calculation contribute to an overall emission probability density function. Monte Carlo analysis can be performed at the category level, for aggregations of categories or for the inventory as a whole. Statistical software packages are readily available - some of which include Monte Carlo algorithms that are very user-friendly.

Like all methods, Monte Carlo analysis only provides satisfactory results if it is properly implemented. This requires the analyst to have scientific and technical understanding of the inventory. Of course, the results will only be valid to the extent that the input data, including any expert judgements, are sound.

Good practice guidance on selecting PDFs for different sources is included in Appendix A.

Reporting uncertainties 7

The LRTAP Convention Guidelines for reporting emissions and projections data (ECE/EB.AIR/125) request that (para 31):

Parties shall quantify uncertainties in their emission estimates using the most appropriate methodologies available, taking into account guidance provided in the EMEP/EEA Guidebook. Uncertainties should be described in the IIR.'

The reporting guidelines do not include detailed specifications on the format of reporting. However, it is sensible to align with approaches used for GHG emissions inventories, and therefore it is recommended to report uncertainty data in a table analogous to the one given in Section 5, Inventory management, improvement and QA/QC.

Glossary 8

Note: Definitions copied from the glossary to the General Guidance Volume of the 2006 IPCC Guidelines.

| Confidence interval | The value of the quantity for which the interval is to be estimated is a fixed but unknown constant, such as the annual total emissions in a given year for a given country. The confidence interval is a range that encloses the true value of an unknown fixed quantity with a specified confidence (probability). Typically, a 95 per cent confidence interval is assumed. From a traditional statistical perspective, the 95 per cent confidence interval has a 95 per cent probability of enclosing the true but unknown value of the quantity. An alternative interpretation is that the confidence interval is a range that may safely be declared to be consistent with observed data or information. The 95 per cent confidence interval is enclosed by the 2.5th and 97.5th percentiles of the Probability Density Function (PDF). |
|-------------------------|---|
| Correlation | Mutual dependence between two quantities. See correlation coefficient. |
| Correlation coefficient | A number lying between –1 and +1, which measures the mutual dependence between two variables that are observed together. A value of +1 means that the variables have a perfect linear relationship; a value of –1 means that there is a perfect inverse linear relation; and a value of 0 means that there is no straight line relation. It is defined as the covariance of the two variables divided by the product of their standard deviations. |
| Distribution function | A distribution function or cumulative distribution function $F(x)$ for a random variable X specifies the probability $P(X \le x)$ that X is less than or equal to x. |
| Expert judgement | A carefully considered, well-documented qualitative or quantitative judgement made in the absence of unequivocal observational evidence by a person or persons who have a demonstrable expertise in the given field. |
| Monte Carlo method | In these guidelines a Monte Carlo method is recommended to analyse the uncertainty of the inventory. The principle of Monte Carlo analysis is to perform the inventory calculation many times by computer, each time with the uncertain emission factors or model parameters and activity data chosen randomly (by the computer) within the distribution on uncertainties specified initially by the user. Uncertainties in emission factors and/or activity data are often large and may not have normal distributions. In this case the conventional statistical rules for combining uncertainties become very approximate. Monte Carlo analysis can deal with this situation by generating an uncertainty distribution for the inventory estimate that is consistent with the input uncertainty distributions on the emission factors, model parameters and activity data. |
| Normal distribution | The normal (or Gaussian) distribution has the PDF given in the following equation and is defined by two parameters (the mean μ and the standard σ deviation). $f(x) = \frac{1}{\sigma\sqrt{2\pi}}e^{-\frac{(x-\mu)^2}{2\sigma^2}} \text{, for } -\infty \leq x \leq \infty$ |

| Probability | A probability is a real number in the scale 0 to 1 attached to a random event. There are different ways in which probability can be interpreted. One interpretation considers a probability as having the nature of a relative frequency (i.e., the proportion of all outcomes corresponding to an event), whilst another interpretation regards a probability as being a measure of degree of belief. |
|---------------------------------------|---|
| Probability density function (PDF) | The Probability Density Function describes the range and relative likelihood of possible values. The PDF can be used to describe uncertainty in the estimate of a quantity that is a fixed constant whose value is not exactly known, or it can be used to describe inherent variability. The purpose of the uncertainty analysis for the emission inventory is to quantify uncertainty in the unknown fixed value of total emissions as well as emissions and activity pertaining to specific categories. Thus, throughout these guidelines it is presumed that the PDF is used to estimate uncertainty, and not variability, unless otherwise stated. |
| Probability distribution | Statistical definition: a function giving the probability that a random variable takes any given value or belongs to a given set of values. The probability on the whole set of values of the random variable equals 1. |
| Standard deviation | The population standard deviation is the positive square root of the variance. It is estimated by the sample standard deviation that is the positive square root of the sample variance. |
| Uncertainty | Lack of knowledge of the true value of a variable that can be described as a probability density function characterizing the range and likelihood of possible values. Uncertainty depends on the analyst's state of knowledge, which in turn depends on the quality and quantity of applicable data as well as knowledge of underlying processes and inference methods. |
| Uncertainty analysis | An uncertainty analysis of a model aims to provide quantitative measures of the uncertainty of output values caused by uncertainties in the model itself and in its input values, and to examine the relative importance of these factors. |

References 9

IPCC (2006), 2006 IPCC Guidelines for National Greenhouse Gas Inventories, Volume 1 — General Guidance and Reporting (www.ipcc-nggip.iges.or.jp/public/2006gl/vol1.htm).

IPCC (2000), IPCC Good Practice Guidance, Penman J., Kruger D., Galbally I., Hiraishi T., Nyenzi B., Emmanul S., Buendia L., Hoppaus R., Martinsen T., Meijer J., Miwa K. and Tanabe K. (eds.) (2000), Good Practice Guidance and Uncertainty Management in National Greenhouse Gas Inventories, NGGIP Publications, IPCC National Greenhouse Gas Inventories Programme, Institute for Global Environmental Strategies, Japan, ISBN 4-88788-000-6.

IPCC (2019) 2019 Refinement to the 2006 IPCC Guidelines for National Greenhouse Gas Inventories (https://www.ipcc-nggip.iges.or.jp/public/2019rf/index.html), accessed 15 August 2019.

10 Point of enquiry

Enquiries concerning this chapter should be directed to the co-chairs of the Task Force on Emission Inventories and Projections (TFEIP). Please refer to the TFEIP website (www.tfeip-secretariat.org/) for the contact details of the current co-chairs.

Appendix A Good practice guidance for selecting probability density functions

Prior to selecting a probability density function (PDF) (3), it is good practice to account for biases in the data to the fullest extent possible. As noted previously, data collection and QA/QC procedures can assist in preventing or correcting biases. For example, if national statistics on timber harvest exist, but it is also suggested that these statistics have a bias of 5 per cent, then the mean estimate can be adjusted by 5 per cent prior to estimating the random component of the uncertainty. It is good practice that adjustments for bias should be done in developing the point estimate emission inventory. Another consideration is that the amount of bias can change over time as data measurement or collection procedures change, or as the geographic and temporal scope of data collection changes. Thus, the bias corrections may be different for different years.

However, to the extent that biases are believed or known to exist in data even after QA/QC procedures have been applied, then either empirical or judgment based techniques can be applied to account for the bias. Apparent biases can arise in probabilistic analysis for at least two reasons: (1) a fitted distribution may have a mean that is different from the most likely value used in the point estimate of the inventory (e.g. a skewed triangular distribution based on expert judgment); and (2) the mean value of a prediction from a nonlinear model that has uncertain inputs can be different from the point estimate obtained from the same model if only point estimates of the mean values of the inputs are used. Thus, there are some types of biases that may be revealed only after an uncertainty analysis has been done.

Types of Probability Density Functions 1.

There are many Probability Density Functions (PDFs) outlined in the statistical literature that often represent particular real situations. The choice of a particular type of PDF depends, at least in part, on the domain of the function (e.g. can it have both positive or negative values, or only non-negative values), the range of the function (e.g. is the range narrow or does it cover orders-of-magnitude), the shape (e.g. symmetry), and processes that generated the data (e.g. additive, multiplicative). These considerations are elaborated below in a brief discussion of many commonly used distributions of practical importance. Examples of such functions and the situations they represent are given below (4).

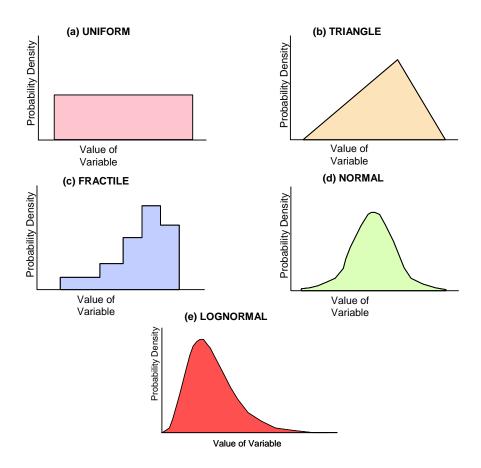
The normal distribution is most appropriate when the range of uncertainty is small, and symmetric relative to the mean. The normal distribution arises in situations where many individual inputs contribute to an overall uncertainty, and in which none of the individual uncertainties dominates the total uncertainty. Similarly, if an inventory is the sum of uncertainties of many individual categories, however, none of which dominates the total uncertainty, then the overall uncertainty is likely to be normal. A normality assumption is often

⁽³⁾ Note this section is copied from subsection 3.2.2.4 of the Uncertainties Chapter of the General Guidance Volume of the 2006 IPCC Guidelines.

⁽⁴⁾ Further information on methods for developing distributions based upon statistical analysis of data are described and illustrated by Cullen and Frey (1999). Other useful references include Hahn and Shapiro (1967), Ang and Tang (1975) D'Agostino and Stephens (1986), Morgan and Henrion (1990), and U.S.EPA (1996, 1997, 1999). Some examples of probabilistic analyses applied to emission inventories are given by Frey and Zheng (2002) and Frey and Zhao (2004).

- appropriate for many categories for which the relative range of uncertainty is small, e.g. fossil fuel emission factors and activity data.
- The lognormal distribution may be appropriate when uncertainties are large for a non-negative variable and known to be positively skewed. The emission factor for nitrous oxide from fertiliser applied to soil provides a typical inventory example. If many uncertain variables are multiplied, the product asymptotically approaches log normality. Because concentrations are the result of mixing processes, which are in turn multiplicative, concentration data tend to be distributed similar to a lognormal. However, real-world data may not be as tail-heavy as a lognormal distribution. The Weibull and Gamma distributions have approximately similar properties to the lognormal but are less tail-heavy and, therefore, are sometimes a better fit to data than the lognormal.
- Uniform distribution describes an equal likelihood of obtaining any value within a range. Sometimes the uniform distribution is useful for representing physically-bounded quantities (e.g. a fraction that must vary between 0 and 1) or for representing expert judgement when an expert is able to specify an upper and lower bound. The uniform distribution is a special case of the Beta distribution.
- The triangular distribution is appropriate where upper and lower limits and a preferred value are provided by experts but there is no other information about the PDF. The triangular distribution can be asymmetrical.
- Fractile distribution is a type of empirical distribution in which judgements are made regarding the relative likelihood of different ranges of values for a variable, such as illustrated in Figure A-1. This type of distribution is sometimes useful in representing expert judgement regarding uncertainty.

Examples of some commonly used probability density function models Figure A-1 (e.g. based on Frey and Rubin, 1991)



Issues to consider when developing the Probability Density 2. **Function**

The following describes how inventory compilers can satisfy the principles of comparability, consistency and transparency in emissions inventories when selecting a PDF:

- where empirical data are available, it is good practice to first consider whether a normal distribution would be appropriate as a representation of uncertainty. If the variable must be non-negative, then it is good practice for the standard deviation of the normal distribution not to exceed 30 per cent of the mean value to avoid an unacceptably high probability of erroneously predicting negative values. Generally, it is good practice to avoid truncation of the lower tail of the normal distribution, because it changes the mean and other statistics of the distribution. Typically, a better alternative to truncation is to find a more appropriate distribution that is a better fit to the data. For example, for positively skewed data that must be non-negative, lognormal, Weibull, or Gamma distributions often can provide an acceptable fit; however, an empirical distribution of the data can also be used;
- where expert judgement is used, the distribution function adopted might typically be normal or lognormal, supplemented by uniform, triangular, or fractile distributions as appropriate;

other distributions may be used where there are compelling reasons, either from empirical observations or from expert judgement supported by theoretical argument.

The issue of identifying which function best fits a set of data can be difficult. One approach is to use the square of the skewness and the kurtosis to look for functional forms that can fit the data (Cullen and Frey, 1999). It is good practice to apply kurtosis and skewness only if there are sufficient data from which to estimate these values. The function is then fitted to the data by least squares fit or other means. Tests are available to assess the goodness-of-fit, including the chi-squared test and others (Cullen and Frey, 1999). In many cases, several functions will fit the data satisfactorily within a given probability limit. These different functions can have radically different distributions at the extremes where there are few or no data to constrain them, and the choice of one function over another can systematically change the outcome of an uncertainty analysis. Cullen and Frey (1999) reiterate the advice of previous authors in these cases that it must be knowledge of the underlying physical processes that governs the choice of a probability function. What the tests provide, in the light of this physical knowledge, is guidance on whether this function does or does not satisfactorily fit the data.

In order to use empirical data as a basis for developing PDFs, the first critical step is to determine if the data are a random, representative sample, in the case of a sample from a population. Some key questions to ask regarding the data include:

- are the data representative of the conditions pertaining to the emission or activity factors specific to national circumstances?
- are the data a random sample?
- what is the averaging time associated with the data set, and is it the same as for the assessment (which will be for annual emissions in a given year)? For example, emissions data might be measured during a short time period and not for an entire year. Thus, expert judgment may be required in order to extrapolate short-term data to a longer-term basis.

If the data are a random, representative sample, then the distribution can be established directly using classical statistical techniques, even if the sample size is small. Ideally the available data will represent an annual average but may be necessary to convert data using an appropriate averaging time. For normal distributions the 95 per cent confidence interval would be plus or minus twice the estimated standard deviation of the population. In other cases, the data may represent an exhaustive census of the sum of all activity (e.g. total energy use for a particular fuel). In this case, information regarding errors in the measurements or survey instruments would form a basis for assessing uncertainty. The range of uncertainty of activity data might be bounded by using independent methods or consistency checks. For example, fuel consumption data can be compared with estimates of production, including estimates of production via different methods.

There is a distinction between uncertainty in the mean and variability in the data for situations in which the data represent intra-country variability within a category. Since the goal is to estimate annual average emissions at the level of an individual country, it is good practice to average data that represent intra-country variability over the entire geographic area of the country, assess uncertainty in this average and use it as the basis for the inventory. Conversely, if international data are available at an aggregate level, without supporting details as to how such data can be disaggregated by country, there is a mismatch in scale that is more difficult to correct. Typically, in this case, the uncertainty will tend to increase as the geographic scope decreases, i.e. if the number of categories included decreases and if site-specific emissions data are not available. Thus, uncertainty ranges that are developed for aggregated international data may have to be widened for applicability to individual countries. In the absence of any empirical basis for estimating the relative range of uncertainty at the country level versus the aggregated international level, expert judgement can be used.

For a sample of an underlying population, the need is to evaluate whether the data are random and representative of the population. If so, classical statistical methods can be used to define the distribution. If not, then some combination of data analysis and elicitation of expert judgement regarding distributions will be required. In the former case, Cullen and Frey (1999) suggest exploration of the data set using summary statistics and graphics to evaluate essential features (e.g. central tendency, range of variation, skewness). It is good practice to consider the insights obtained by examining the data, combined with knowledge of the processes that generated the data, when selecting a mathematical or numerical representation of the distribution.

If a parametric distribution is selected as a candidate for fitting to the data set, techniques such as 'maximum likelihood estimation (5)' or the 'method of matching moments (6)' can be used to estimate the parameters of the distribution. The goodness-of-fit of the distribution can be evaluated in numerous ways, including comparison of the fitted cumulative distribution function (CDF) with the original data set, probability plots, and goodness-of-fit tests (e.g. Cullen and Frey, 1999). It is important that the selection of a parametric distribution to represent a data set should be based not solely upon goodness-of-fit tests, but upon similarities in processes that generated the data versus the theoretical basis for a distribution (e.g. Hahn and Shapiro, 1967).

If the data are averaged over less than one year, it may be necessary to extrapolate the uncertainty over the year. Consider an example in which the data set represents variability in daily average emissions measurements for a particular category. One approach, described in detail by Frey and Rhodes (1996), is to fit a parametric distribution to the data set for daily variability, use a numerical technique known as bootstrap simulation to estimate uncertainty in the parameters of the distribution, and use Monte Carlo simulation to simulate randomised annual averages of the emission factor. Using bootstrap simulation, the uncertainty in the sampling distribution for the parameters of the fitted distribution can be simulated (e.g. Efron and Tibshirani, 1993; Frey and Rhodes, 1996; Frey and Bammi, 2002).

Dependence and correlation among inputs 3.

This section provides a brief overview of issues pertaining to dependence and correlation among inputs. More details on this topic can be found in Morgan and Henrion (1990), Cullen and Frey (1999), and Smith et al. (1992).

When setting up a probabilistic analysis it is preferable to define the model so that the inputs are as statistically independent as possible. For example, rather than to try to estimate activity data for many subcategories for which data are derived at least in part by differences, it may be better to assign uncertainties to better known aggregate measures of activity. For example, residential fuel use might be estimated as the difference between total consumption and usage in the

⁽⁵⁾ The method of maximum likelihood selects as estimates the values of the parameters that maximise the likelihood of the observed sample (e.g. Holland and Fitz-Simons, 1982).

⁽⁶⁾ The method of moments finds estimators of unknown parameters by equating corresponding sample and population moments. The method is easy to employ and provides consistent estimators. In many cases, the method of moments estimators are biased (Wackerly, Mendenhall III and Scheaffer, 1996, pp. 395-397).

transportation, industrial, and commercial sectors. In this case, the estimate of uncertainty in residential fuel use is negatively correlated with the uncertainties in fuel use in the other subcategories, and may even be very large compared to the uncertainty in total consumption. Therefore, rather than trying to estimate uncertainties separately for each subcategory, it may be more practical to estimate uncertainty for aggregated categories, for which good estimates and cross-checks may be available.

Dependencies, if they exist, may not always be important to the assessment of uncertainties. Dependencies among inputs will matter only if the dependencies exist between two inputs to which the uncertainty in the inventory is sensitive and if the dependencies are sufficiently strong. In contrast, weak dependencies among inputs, or strong dependencies among inputs to which the uncertainty in the inventory is insensitive, will be of relatively little consequence to the analysis. Of course, some interdependencies are important and failure to account for those relationships can lead to misleading results. Positive correlations between inputs tend to increase the range of uncertainty in the output, whereas negative correlations tend to decrease the range of uncertainty in the output. However, positive correlations in uncertainties when comparing two years as part of trend analysis will decrease uncertainty in the trend.

Techniques can be considered for incorporating dependencies into the analysis including:

- stratifying or aggregating the categories to minimise the effect of the dependencies;
- modelling the dependence explicitly;
- simulating correlation using restricted pairing methods (that are included in many software packages);
- use of resampling techniques in cases where multivariate datasets are available;
- considering bounding or sensitivity cases (e.g. one case assuming independence and another case assuming complete positive correlation); and
- time series techniques can be used to analyse or simulate temporal autocorrelation.

As a simple example, Zhao and Frey (2004) evaluated the implications of whether or not emission factor uncertainty estimates for different categories obtained from the same data source should be considered as dependent or independent among the categories, and found that it did not matter to the overall inventory uncertainty. Of course, this result is specific to the particular case studies and it is good practice to test this in other applications. As a more complex example, given in Box 3.1, Ogle et al. (2003) accounted for dependencies in tillage management factors, which were estimated from a common set of data in a single regression-type model, by determining the covariance (7) between factors for reduced tillage and no-till management, and then using that information to generate tillage factor values with appropriate correlation during a Monte Carlo simulation (8). One should consider the potential for correlations among input variables and focus on those that would be likely to have the largest dependencies (e.g. applying management factors for the same practice

⁽⁷⁾ The covariance between two variables (x and y) measures the mutual dependence between them. The covariance of a sample consisting of n pairs of values is the total of the products of the deviation of individual xvalues from the mean x value times the deviation of the corresponding individual y value from the mean of the y values, divided by (n-1).

⁽⁸⁾ More discussion and examples of these types of methods are given in Cullen and Frey (1999), Morgan and Henrion (1990), and US EPA (1996). These documents also contain reference lists with citations to relevant literature.

in different years of an inventory, or correlations among management activities from one year to the next).

Box 3.1 Example of Monte Carlo uncertainty assessment dealing with correlations

Ogle et al. (2003) performed a Monte Carlo analysis to assess uncertainty in a source using a Tier 2 methodology, more specifically the changes in soil C attributed to land use and management of agricultural lands in the United States. Management factors were estimated from about 75 published studies using linear mixed effect models. PDFs were derived for the management effect at a depth of 30 cm following 20 years after its implementation. Reference stocks were estimated using a National Soil Survey Characterisation Database, which contained pedon data collected by United States Department of Agriculture (USDA). PDFs were based on the mean and variance from about 3 700 pedons, taking into account the spatial autocorrelation of pedon locations due to clumped distribution patterns. The land use and management activity data were recorded in the USDA National Resources Inventory, which tracks agricultural land management at more than 400 000 point locations in the United States, along with supplemental data on tillage practices provided by the Conservation Technology and Information Center (CTIC). The Monte Carlo analysis was implemented using a commercially available software package and code developed by U.S. analysts. Their analysis accounted for dependencies between estimation parameters that were derived from common datasets. For example, factors for set-aside lands and land use change between cultivated and uncultivated conditions were derived from a single regression analysis using an indicator variable for set-asides, and hence were interdependent. Their analysis also accounted for dependencies in the land use and management activity data. When simulating input values, factors were considered completely dependent from the base and current year in the inventory because the relative influence of management on soil C was assumed to be the same regardless of the year when a practice was implemented. As such, factors were simulated with identical random seed values. In contrast, reference carbon stocks for the various soil types in each climate region were simulated independently, with different random seeds, because stocks for each region were constructed from separate independent sets of data. U.S. analysts chose to use 50 000 iterations for their Monte Carlo analysis. This was satisfactory because they were only reporting one digit after the decimal, and simulation results were considered relatively stable at that level of significance. Ogle et al. (2003) estimated that mineral soils gained an average of 10.8 Tg C yr⁻¹ between 1982 and 1997, with a 95 per cent confidence interval ranging from 6.5 to 15.3 Tg C yr⁻¹. In contrast, managed organic soils lost an average of 9.4 Tg C yr⁻¹, ranging from 6.4 to 13.3 Tg C yr⁻¹. Further, Ogle et al. (2003) found that the variability in management factors contributed 90 per cent of the overall uncertainty for the final estimates of soil carbon change.

References to Appendix 1 4.

Ang, A. H-S., and Tang, W.H., (1984), Probability Concepts in Engineering Planning and Design, Volume 2 — Decision, Risk, and Reliability, John Wiley and Sons, New York.

Cullen, A.C. and Frey, H.C. (1999), Probabilistic Techniques in Exposure Assessment: A Handbook for Dealing with Variability and Uncertainty in Models and Inputs, Plenum, New York.

D'Agostino, R.B. and Stephens, M.A. (eds.) (1986), Goodness-of-Fit Techniques, Marcel Dekker, New York.

Efron, B. and Tibshirani, R.J. (1993), An Introduction to the Bootstrap, Chapman and Hall, New York.

Frey, H.C. and Bammi, S. (2002), 'Quantification of Variability and Uncertainty in Lawn and Garden Equipment NO_x and Total Hydrocarbon Emission Factors', J. Air & Waste Manage. Assoc., 52(4), pp. 435-448.

Frey, H.C. and Rhodes, D.S. (1996), 'Characterizing, Simulating, and Analyzing Variability and Uncertainty: An Illustration of Methods Using an Air Toxics Emissions Example', Human and Ecological Risk Assessment: An International Journal, 2(4), pp. 762–797, December 1996.

Frey, H.C. and Rubin, E.S. (1991), Development and Application of a Probabilistic Evaluation Method for Advanced Process Technologies, Final Report, DOE/MC/24248-3015, NTIS DE91002095, Prepared by Carnegie-Mellon University for the U.S. Department of Energy, Morgantown, West Virginia, April 1991, p. 364.

Frey, H.C. and Zheng, J. (2002), 'Probabilistic Analysis of Driving Cycle-Based Highway Vehicle Emission Factors', Environmental Science and Technology, 36(23), pp. 5184–5191, December 2002.

Hahn, G.J., and Shapiro, S.S. (1967), Statistical Models in Engineering, Wiley Classics Library, John Wiley and Sons, New York.

Holland, D.M and Fitz-Simons, T. (1982), 'Fitting statistical distributions to air quality data by the maximum likelihood method', Atmospheric Environment, 16(5), pp. 1071–1076.

Morgan, M.G., and Henrion, M. (1990), Uncertainty: A Guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis, Cambridge University Press, New York.

Ogle, S.M., Breidt, F.J., Eve, M.D. and Paustian, K. (2003), 'Uncertainty in estimating land use and management impacts on soil organic carbon storage for U.S. agricultural lands between 1982 and 1997', Global Change Biology 9, pp. 1521–1542.

Smith, A.E, Ryan, P.B. and Evans J.S. (1992), 'The effect of neglecting correlations when propagating uncertainty and estimating the population distribution of risk', Risk Analysis, 12, pp. 467–474.

US EPA (1996), Summary Report for the Workshop on Monte Carlo Analysis, EPA/630/R-96/010, Risk Assessment Forum, U.S. Environmental Protection Agency, Washington, DC.

US EPA (1997), Guiding Principles for Monte Carlo Analysis, EPA/630/R-97/001, Risk Assessment Forum, U.S. Environmental Protection Agency, Washington, DC.

US EPA (1999), Report of the Workshop on Selecting Input Distributions for Probabilistic Assessments, EPA/630/R-98/004, U.S. Environmental Protection Agency, Washington, DC, January 1999 (www.epa.gov/ncea/input.htm).

Wackerly, D.D., Mendenhall III, W. and Scheaffer, R.L. (1996), Mathematical Statistics with Applications, Duxbury Press, USA.

Zhao, Y. and Frey, H.C. (2004), 'Development of Probabilistic Emission Inventory for Air Toxic Emissions for Jacksonville, Florida', Journal of the Air & Waste Management Association, 54(11), pp. 1405-1421.