THE USE OF NATIONAL POLLUTANT INVENTORY DATA IN ATMOSPHERIC DISPERSION MODELLING

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Summary

Atmospheric dispersion modelling can be used to estimate the environmental impact of releases to air. The purpose of this paper is determine whether the National Pollutant Inventory (NPI), Australia's national database of pollutant releases, can be used for atmospheric dispersion modelling and, if so, the conditions that must be satisfied for it to be used effectively. The selection of emission estimation techniques (EETs) significantly affects the reliability of reported NPI emissions. The reliability of NPI data has improved as facilities gain a better understanding of the reporting process, as Industry Handbooks are reviewed and as facilities find beneficial uses for NPI data within their organisations. Although NPI data in isolation do not satisfy dispersion modelling requirements, it is likely that the necessary supporting information relating to variation in emissions and source characteristics will be obtained or calculated by industry as part of the NPI reporting process. Regulatory authorities may be able to obtain these data through other regulatory requirements. To lessen the burden on industry in collecting the necessary supporting information for regional dispersion modelling, environmental regulatory authorities could consider the coordinated collection, storage and updating of the necessary information. Dispersion modelling using NPI data may be associated with relatively large uncertainties. However, provided that the uncertainty in NPI emissions estimates is recognised and depending on the end use of the modelling, predictions based on these data could provide the basis for effective decision making.

Keywords: National Pollutant Inventory, Dispersion Modelling, Emissions Estimation.

1. Introduction

The National Pollutant Inventory (NPI) is Australia's national register of pollutant emissions. The NPI provides no direct measure of the impacts of these releases on the environment. Atmospheric dispersion modelling is required to estimate ambient concentrations, which provide the basis for assessing these impacts.

The purpose of this paper is to determine whether NPI data can be used for dispersion modelling, and if so, the conditions that must be satisfied for it to be used effectively. This paper explores the suitability of NPI data for use in dispersion modelling through:

- An analysis of the quality of data typically reported to the NPI;
- An outline of the data requirements for atmospheric dispersion modelling; and
- A comparison of these data requirements with those of the NPI.

2. The National Pollutant Inventory

The NPI has been operational since July 1998. Initially, industries which exceeded certain reporting thresholds were required to report emissions from a list of 36 substances. This list has now been extended to 90 substances. This list, while not comprehensive, and with the notable exception of greenhouse gases, is generally considered to currently reflect all significant pollutants of concern within Australia (Rae, 2002). It should be noted that industrial greenhouse emissions are considered under a number of other programs within Australia.

There are five reporting thresholds, as follows:

- If 10 tonnes or more of a Category 1 substance is used by a facility in a reporting year, emissions resulting from the use of that substance must be reported.
- If 25 tonnes or more of a Category 1a substance is used by a facility in a reporting year, emissions resulting from the use of that substance must be reported. For bulk storage facilities, the reporting threshold is only triggered if the design capacity of the facility exceeds 25 kilotonnes.

- If more than 400 tonnes of fuel or waste is burned in a reporting year, or 1 tonne or more of fuel or waste is burned in any hour in the reporting year, emissions of Category 2a substances must be reported.
- If more than 2,000 tonnes of fuel or waste is burned; or more than 60,000 megawatt-hours of energy is consumed in a reporting year; or if the maximum potential power consumption of the facility at any time is rated at 20 megawatt-hours or more, emissions of Category 2b substances must be reported, in addition to Category 2a substances.
- If releases to water, other than groundwater, exceed the specified amounts of total nitrogen or total phosphorous, releases of these Category 3 substances must be reported.

Facilities that have triggered a particular reporting threshold are required to report all emissions of that substance to the inventory as an annual aggregate emission from the facility (i.e., kg/year).

It should be noted that although most pollutants of concern are considered under the NPI, it is possible that in some cases emissions of pollutants of interest will not be collected as part of the NPI reporting process.

Under the NPI, releases to purpose built facilities such as sewers or landfill are classed as transfers and are not required to be reported (NEPC 2000).

It should also be noted that the estimation of aggregated emissions that have not triggered thresholds (i.e., sub-threshold emissions), mobile sources (e.g., on-road motor vehicles) or facilities specifically excluded from the NPI (e.g., service stations) is the responsibility of the governing State or Territory environmental regulatory authority. The focus of this paper is on the use of industrial emissions data. Clearly, for urban areas in particular, mobile and other smaller point and diffuse emission sources would need to be considered for a comprehensive assessment of ambient pollutant concentrations.

2.1 Factors Affecting Data Quality

The quality of the emissions estimates supplied to the NPI is a direct reflection of the suitability of a particular emission estimation technique (EET) to a particular situation. The level of uncertainty associated with a particular EET depends on the situation and is a reflection of how well a particular EET reflects the processes and emissions at a facility.

Facilities that report to the NPI use a number of different EETs to estimate their releases to the environment as follows:

- Continuous Emissions Monitoring (CEM): The collection of data using a permanently mounted gas or liquid collection system that directs sample streams to a reliable and stable analytical device with capabilities to record continuous measurements through electronic media.
- Predictive Emissions Monitoring (PEM): PEM (also known as parametric emissions monitoring) relates the release rate of a particular substance (or group of substances) to various operational parameters that are readily known and available to a facility. This is typically done through the development of a correlation between the operational parameters and the release rate.
- Source Testing: Source tests are short-term release measurements taken at a stack, vent or other release point.
- Material Balance: Releases are estimated based on the difference between material input and material output across a vessel, process or entire facility.
- Empirical or Physico-Chemical Relationships: Relationships are derived from the fundamentals of chemistry and physics. Empirical relationships are also physico-chemical relationships. However, they differ as they are developed through scientific observations in either the laboratory or industrial operations under simulated or actual processes.
- Emission Factors: A single number based on a unit of activity (eg. x kg carbon monoxide emitted per tonne of fuel burned). This is a value derived from measured source tests distilled into a single value through statistical analysis.
- Engineering Judgement: An engineering judgement is made when specific emission estimation techniques are not feasible to use. Such estimations are usually made by an engineer familiar with the specific process, and are based on whatever knowledge may be available.
- Models: Release models are software programs based on a combination of physico-chemical and empirical relationships.

It can be seen from this list that some EETs are likely to be more reliable than others. However, depending on the application, this is not always the case. In any given situation, there may be more than one suitable EET. For example, in some situations, CEM may be equally as reliable as emission factors. The selection of an EET is not just a matter of selecting the most accurate EET but involves trade offs between the desired accuracy and factors such as cost, data availability and the inventory goals/objectives. Figure 1 below illustrates the relationship between cost and reliability of different EETs and shows the potentially significant overlap in the reliability of EETs.

One of the important features of the NPI (with respect to data quality) is that companies are not expected to conduct source testing to meet their reporting requirements. Also, fugitive emissions (which by definition cannot be measured) are estimated using EETs of generally less reliability (usually emission factors). Therefore, when the NPI reporting and emissions estimation process was new, facilities tended to rely

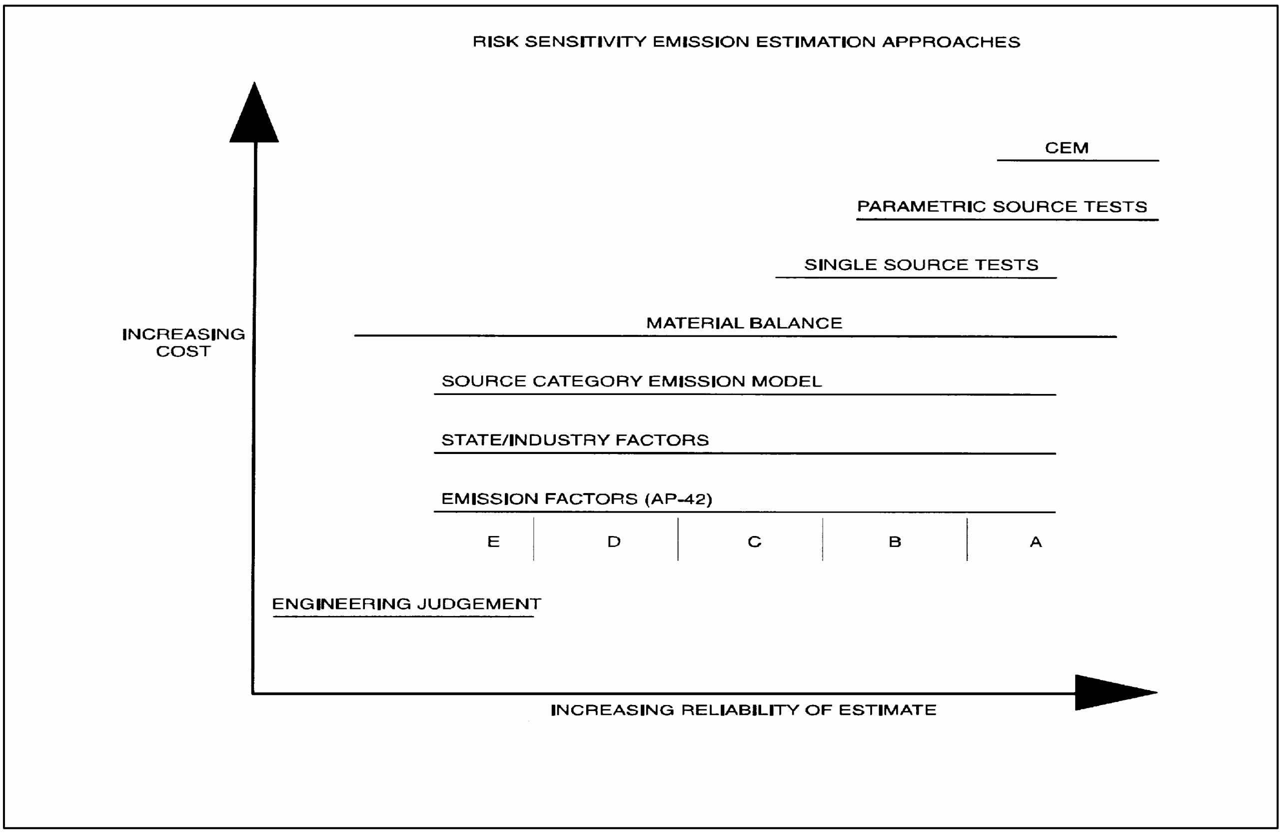

Figure 1. The relationship between the cost and reliability of EETs (adapted from USEPA (1997))

heavily on emission factors which are usually sourced from the US or Europe. The simplicity of emission factors enables facilities' emissions to be estimated without the need for monitoring. The disadvantages of published emission factors are that they can, in some cases, be very poor predictors of the performance of an individual facility (USEPA 1996) and that the uncertainty in emissions estimates is difficult to define.

However, it has also been shown that overseas emission factors can (provided that the validation of emission factors is performed to ensure reliability of emissions estimates) reasonably reflect emissions at individual facilities (Sullivan & Woods 2000).

At this stage, the publicly available NPI data requires the specification of the EET that has been used to estimate each reportable emission. However, each reportable emission may be the aggregate from a number of sources, which may have been estimated using different EETs. Therefore, in some cases, no inference can be drawn about the reliability of the emissions information reported to the NPI. It may be possible, in some cases, to infer that only one source constitutes a total reported emission (e.g., oxides of nitrogen from a coal-fired power station). However, even if it is known which EET has been used to estimate a particular emission, it is not possible to infer the suitability of this EET for each particular application from the information supplied in the NPI report.

In addition, the Industry Handbooks containing industry-specific guidance on the application of EETs are the subject of ongoing review. As part of this process, a number of industry associations have initiated and are coordinating the review of Industry Handbooks. The review process enables the Handbooks to better reflect the information requirements of particular industries with the inclusion of EETs more relevant to the Australian context.

As the NPI reporting process has developed, companies have also become aware of the potential uses of NPI data in other areas such as corporate environmental reporting, cleaner production and internal environmental benchmarking. As the need for more reliable data for these applications becomes apparent, facilities are tending to use more reliable EETs and are beginning to integrate reporting processes.

In addition, the quality of data reported to the NPI has improved as industry gains a better understanding of the emissions estimation process. As companies have become more experienced with the reporting process the tendency has been towards the use of more reliable techniques. Many industries have recently developed site-specific EETs that do provide reasonable characterisation of site-specific operations.

It is apparent that many questions exist regarding the reliability of NPI data and that emissions data from the NPI may be associated with relatively high levels of uncertainty. However, the NPI may still be the only source of emissions information for a large number of facilities. Section 3 below outlines the data requirements for atmospheric dispersion modelling and Section 4 discusses whether these requirements can be met by NPI data.

3. Atmospheric Dispersion Modelling

Atmospheric dispersion modelling is used to estimate the state of the atmospheric environment. In general, the data required to operate a dispersion model are as follows:

- For stack sources: the stack diameter, exit velocity, exit temperature, and emission rate of pollutant.
- For volume and area sources: the dimensions of the source and the emission rate of pollutant.
- The variation in emission rates (e.g., diurnal, seasonal).
- The location of the source.
- The dimensions of nearby buildings which may cause turbulent effects due to building wakes.
- Information relating to particle size for dust deposition modelling.
- Meteorological data from the local area or region.
- Information relating to the geography of the area (e.g., elevation, land use).

The specific format of the data listed above varies depending on the model used. The selection of an appropriate dispersion model depends on the application for which it is to be used and on the terrain and meteorology of the area to be assessed. The selection of dispersion models does not greatly affect the general data requirements listed above and will not be discussed further here.

Atmospheric dispersion modelling is usually performed on either a local or regional scale and is performed by industry, for industry (e.g., consultants) or by regulatory authorities. Local scale modelling is used to assess the impacts of individual facilities within the local area, usually no further than the nearest sensitive receptors. Effects from nearby facilities are often not considered explicitly. Regional-scale modelling is usually concerned with the impacts over a particular airshed containing multiple emission sources.

The quality of data available for dispersion modelling depends on the situation. Modelling performed by industry or by consultants for industry on a local scale is usually based on relatively accurate emissions data for the facility in question. Existing industrial facilities are usually able to characterise their emissions to a suitable level of accuracy for the purposes of local dispersion modelling.

However, if emissions from other sources are required (e.g., for regional scale modelling) then, depending on the project, site-specific emissions data may be made available from the facility in question or may have to be estimated using non-site-specific techniques such as emission factors. Screening studies (performed by/for industrial facilities or regulatory authorities) for local scale modelling are also often performed using emission factors as the basis for emission rates. If predicted ground level concentrations are within levels of concern, more reliable data may be required.

Regional-scale modelling is often performed by, or on behalf of, environmental regulatory authorities to aid in air quality policy development. In this case, facility-specific information is usually obtained through the use of a questionnaire which is sent to all facilities within the airshed that are likely to contribute significantly to regional impacts. One of the major problems with this approach is the low return rate of the questionnaires. This may be due to the resources required to obtain the necessary information and the reluctance by individual facilities to release site-specific information on a voluntary basis. Also, in our experience, industries are reluctant to forward information which has already been forwarded to regulatory authorities for other purposes.

Increasingly, authorities are requiring that cumulative impacts be considered when dealing with the impacts of specific industrial facilities, e.g., in EIS and licensing applications. Explicit modelling of cumulative impacts then necessitates the use of regional or sub-regional emissions data by the private sector.

For local scale modelling, it is important that the impacts close to the source are adequately characterised. Therefore, it is extremely important that information which affects these impacts is appropriately specified. Information important for the assessment of local impacts includes nearby building dimensions for stack sources, localised terrain and meteorology. Regulatory authorities may not have detailed information and may have to make assumptions regarding emissions (e.g., using emission factors) or source characteristics (e.g., using licence limits, previous modelling studies, engineering judgement).

For regional scale modelling, ideally, all sources within the airshed (industrial, area-based and mobile sources) are characterised to predict pollutant concentrations within the region. Due to the large scale nature of the modelling, the following simplifying assumptions are often made in regional dispersion modelling:

- Stack sources below a certain height (say 30 m) are lumped into aggregated area sources (e.g., at a grid spacing of 1 km);
- Terrain is on a coarser resolution than for local scale modelling; and
- Smaller sources are lumped into aggregated area sources.

Both local and regional scale modelling applications require information relating to the variation in emission rate (e.g., by hour of the day, season, weekend/weekday).

It should also be noted that the cost of emissions data may also be a limiting factor. Facilities will generally use the cheapest method of estimating emissions that satisfies regulatory requirements. Depending on the application, the cheapest method for estimating emissions for the purposes of the NPI may not be appropriate for dispersion modelling.

3.1.1 Uncertainty in Dispersion Modelling

As with any mathematical abstraction of the real environment, atmospheric dispersion modelling represents a simplification of the many complex processes involved in determining ground level concentrations of pollutants. Uncertainty associated with dispersion models arises from both errors in measured and assumed parameters used as input, and from inherent uncertainty in the behaviour of the atmosphere, especially on shorter time scales, due to the effects of apparently random turbulence.

With good quality input data, modelled 1-hour average concentrations typically fall within a factor of two of the measured value when data are paired in time and space. Longer-term averages are typically within ±40% of the true value, provided that good quality data are used (USEPA, 2001). The main specific sources of uncertainty in dispersion models and their effects are summarised below:

Oversimplification of Physics in Model Code

The uncertainty associated with simplification of physical processes varies depending on the sophistication of the model being used. This simplification can lead to both underprediction and overprediction. Errors tend to be greater in simple models (e.g., Gaussian plume models), which do not include the effects of non-steady-state meteorology (i.e., spatially- and temporally-varying meteorology) than in non-steady-state models.

Errors in Emissions Data

Ground level concentrations are proportional to emission rate. Therefore, any uncertainty in emission rate is directly reflected in predictions of ground level concentrations, particularly if there is a bias in the estimates.

Errors in Meteorology

Wind direction affects direction of plume travel. Wind speed affects plume rise and dilution of plume, resulting in potential errors in distance of plume impact from source, and magnitude of impact.

Gaussian plume models use estimates of stability class, and three-dimensional models use explicit vertical profiles of temperature and wind. In either case errors in these parameters can cause either underprediction or overprediction of ground level concentrations.

Usually the effects of errors in temperature are relatively small, but temperature affects plume buoyancy, with potential errors in distance of plume impact from source, and magnitude of impact.

Inherent Uncertainty

Models predict 'ensemble mean' concentrations for any specific set of input data (say on a 1-hour basis), i.e., they predict the mean concentrations that would result from a large set of observations under the specific conditions being modelled. However, for any specific hour with those exact mean hourly conditions, the predicted ground level concentrations will never exactly match the actual pattern of ground level concentrations, due to the effects of random turbulent motions and random fluctuations in other factors such as temperature. In other words, the "inherent" uncertainty is a reflection of the stochastic nature of atmospheric turbulence, (Venkatram & Wyngaard 1988).

The United States Environmental Protection Agency states that the inherent uncertainty (i.e., before uncertainty in model inputs are taken into account) can be as much as 50% (USEPA 2001). Another study estimated the inherent uncertainty at between 50-75% for a 1-hour average simulation (Stein & Wyngaard, 2001).

Summary

Clearly, the uncertainty associated with dispersion modelling predictions can be relatively large and may become much larger depending on the reliability of emissions estimates. The question then becomes whether these relatively large uncertainties can still provide an effective basis for decision making.

4. Suitability of NPI Data in Atmospheric Dispersion Modelling

The suitability of NPI data for dispersion modelling is not dependant on some absolute measure of reliability. To determine the suitability of NPI data for use in dispersion modelling, the following questions should be answered:

- What are the end user requirements of the modelling?
- What assumptions are required relating to information requirements not satisfied by NPI data?
- Are these assumptions acceptable?

End User Requirements

The end-user requirements will define the emissions data requirements for dispersion modelling. For example, an industrial facility may require a screening study to determine whether more detailed modelling of local impacts is required. In this case, a relatively crude characterisation of emissions (e.g., based on overseas emission factors) is acceptable as further studies (with more accurate data) will be performed if predictions are within a range that may present an issue in terms of air quality.

In addition, assessments of relative impacts (e.g., using emissions estimates from the same facility using the same EETs for different years) are not as sensitive to the absolute accuracy of the emissions estimate. NPI data would often be suitable in this case.

Also, if modelling is required to assess impacts that occur at certain times of the day (e.g., due to afternoon sea breezes or stable early morning conditions) then a well-defined characterisation of variation in emissions is required. This can often be obtained from NPI data with appropriate knowledge of the process and/or facility in question.

Regional dispersion modelling generally requires the characterisation of all emission sources within an airshed. In general, the magnitude and variation in emissions of significant sources within the airshed should be specified using site-specific data, with smaller sources being specified using industry-wide emission factors.

The end-use requirements should be well defined before assessing the suitability of NPI data.

Information Requirements

After the end-use of the modelling predictions has been defined, the information requirements for the modelling should then be assessed.

The NPI provides information on total annual emissions of specific pollutants from individual pollutants. Dispersion modelling requires information characterising the variation in emissions in addition to information characterising the source (e.g., stack height, stack temperature, stack exit velocity, stack diameter, source dimensions for area and volume sources) and the surrounding environment (e.g., topography and meteorology). It is clear that the NPI can only provide information relating to the average emissions from a facility and all other information must be obtained elsewhere.

Assuming that information not related to the emission source (e.g., topography and meteorology) can be obtained elsewhere, local scale modelling requires information characterising the sources (source dimensions, emission physical characteristics, building dimensions) at a particular facility. This information must be obtained from the facility. However, it is likely that, in the process of estimating emissions for the NPI, a large amount of the information required for dispersion modelling will be collected. For example stack test reports often contain information such as stack temperature, volumetric flowrate (which, using stack diameter, can be used to calculate exit velocity). Facilities wishing to perform dispersion modelling should be aware that much of the information required will be collected in the NPI reporting process.

The NPI provides information relating to total annual emissions. Industrial facilities wishing to use NPI data as a source of emissions data in dispersion modelling should note that the NPI data does not provide any information relating to variation in emissions or the contribution of different sources within a facility to total emissions. However, if a typical variation profile is known, and the relative contribution of each source to the total emissions is known then this information can be applied to the NPI value from year to year to obtain an emission profile suitable for dispersion modelling. This approach assumes that the characteristics of the sources do not vary from year to year. However, if this assumption is valid, then the assessment of air quality impacts on an annual basis would require minimal variation from year to year based on NPI reports.

Regional scale modelling requires the same emissions data as local scale modelling. However, the aggregation of sources simplifies the process. This is balanced by the fact that information is required from a relatively large number of sources.

Depending on who is performing the modelling, certain necessary information may not be available. Regulatory authorities may not be able to obtain information which characterises the emission sources (e.g., stack height, temperature, diameter and exit velocity and variation in emissions). Industrial facilities will have access to this information for their own facilities. However, if information is required on other facilities within the airshed, NPI data may be the only available source of data.

The necessary supporting data for dispersion modelling within an airshed is often obtained through the use of surveys sent to industrial facilities. Information may also be available through other regulatory requirements such as environmental licences. At this stage, no centralised source of site-specific modelling data is known to exist.

Acceptability of Assumptions

The acceptability of assumptions used to satisfy information requirements will be dependent on the end-use requirements of the modelling predictions (see above). In most cases, provided that the uncertainty in assumptions is recognised, appropriate decisions can be made based on modelling predictions. In some cases, modelling results may indicate that further, more reliable information input information is required. NPI data will in almost all cases form a useful first step in the impact assessment process.

5. Conclusions and Recommendations

The NPI provides no direct measure of the impacts of releases to the environment. Dispersion modelling is a tool, which given information relating to meteorology, geography and emissions sources can provide a measure of the impacts of NPI-reportable releases.

Industrial facilities use a number of different techniques to estimate their releases to the environment. In any given situation there may be more than one suitable EET and the selection of EETs is not just a matter of selecting the most reliable EET but involves a trade-off between the desired accuracy and factors such as cost, data availability and inventory goals and objectives.

Initially, the NPI was heavily reliant on overseas emission factors but as facilities become more experienced with the NPI reporting process and as facilities find other uses for NPI data within their organisations, the quality of data reported to the NPI has improved. The quality of EETs has also improved as a result of the ongoing review of Industry Handbooks, which in some cases, has been driven by industry.

It is important that dispersion modellers understand the relatively high levels of uncertainty often associated the NPI data and the characteristics of reliability associated with NPI data.

The specific data requirements for dispersion modelling depend on the end-use requirements of the modelling predictions, but generally include a characterisation of variation in emissions and supporting information relating to the source such as stack temperatures, diameters, exit velocities and heights.

If a typical variation profile is known, and the relative contribution of each source to the total emissions is known then this information can be applied to the NPI value from year to year to obtain an emission profile suitable for dispersion modelling.

Often, the necessary information is collected as part of the NPI reporting process. Regulatory authorities will, in some cases, have access to this information through the results of surveys and other regulatory requirements such as environmental licences. At this stage, no regulatory authority within Australia keeps the necessary supporting information for modelling in a centralised manner. It would be beneficial for the modelling process if regulatory authorities were to keep a database of modelling information for facilities within their jurisdiction, available on request, to those performing the modelling. This would streamline and standardise the information gathering process, reducing the burden on industry, especially for airshed modelling exercises.

The uncertainty associated with dispersion modelling predictions is, in absolute terms, quite large. However, depending on the end-use requirements of the modelling, even accounting for these uncertainties, dispersion modelling can provide a sound basis for decision making. Once the end-use requirements of the modelling have been well defined an assessment can then be made as to whether assumptions relating to information requirements (additional to those supplied by the NPI) are acceptable. The NPI, does in many cases, provide a useful resource for dispersion modelling.

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