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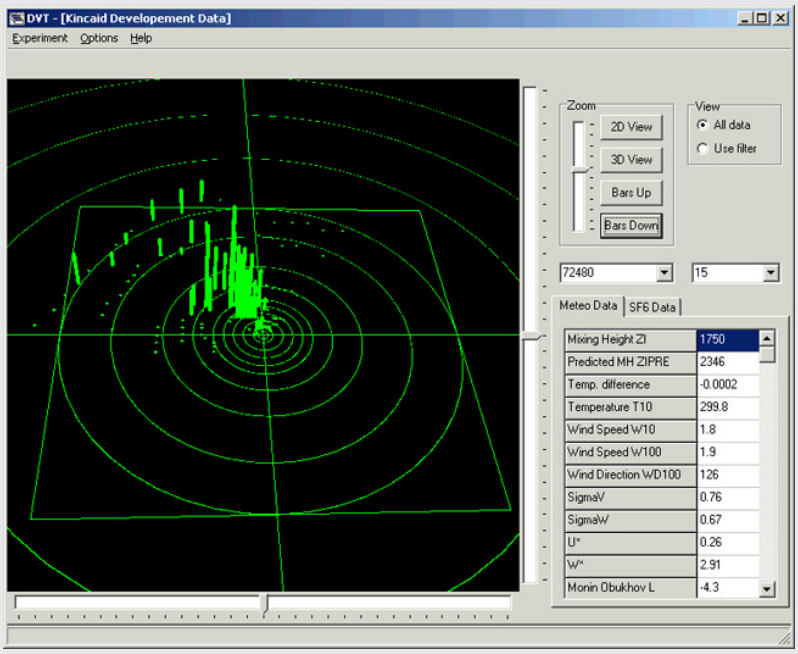
User's Guide to the Model Validation Kit

Research Notes from NERI No. 226



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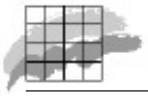

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Research Notes from NERI No. 226
2005

Helge Rørdam Olesen

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Abstract:	The so-called Model Validation Kit is a compilation of field data sets, software and documentation that provides a framework for evaluation of atmospheric dispersion models. The kit has been used extensively by a large number of research groups since it was first introduced in 1993. In particular, it has been used for a series of workshops and conferences on *Harmonisation within Atmospheric Dispersion Modelling for Regulatory purposes* (see www.harmo.org). The present report is a User's Guide to the kit, and provides an overview of the entire material. Besides data sets and software for model evaluation, the package also includes supplementary material, such as a data visualisation tool and video film from experiments. The Model Validation Kit has undergone a major revision to version 2.0 in autumn 2005. The package can be downloaded from the Internet at www.harmo.org/kit
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Summary

The so-called Model Validation Kit is a compilation of field data sets, software and documentation that provides a framework for evaluation of atmospheric dispersion models.

The kit has been used extensively by a large number of research groups since it was first introduced in 1993. In particular, it has been used for a series of workshops and conferences on *Harmonisation within Atmospheric Dispersion Modelling for Regulatory purposes* (see www.harmo.org).

The present report is a User's Guide to the kit, and provides an overview of the entire material. Besides data sets and software for model evaluation, the package also includes supplementary material, such as a data visualisation tool and video film from experiments.

In autumn 2005 the Model Validation Kit has undergone a major revision, resulting in version 2.0. The new version allows the same studies to be carried out as the previous version, but it has been revised in several respects. New software and computing environments have made it necessary to update the package. Furthermore, the documentation is significantly improved and brought up to date. The package can be downloaded from the Internet at www.harmo.org/kit

1 Introduction

The present report is a companion to a set of software and datasets for evaluation of atmospheric dispersion models. The entire material is known as the *Model Validation Kit*, and it can be found through the web page of the initiative on *Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes*, www.harmo.org.

Also, future updates to the material can be found can be found here, more specifically at www.harmo.org/kit.

The material has been compiled by Helge Rørdam Olesen of the National Environmental Research Institute in Denmark, but it is based on joint efforts by many persons – see Chapter 13 for Acknowledgements.

The recommended way to use the report is as follows.

Read the chapter ***Key to the Model Validation*** Kit in order to understand what the Model Validation Kit is and where you should look for the various types of information.

Further browse through the chapter ***Pitfalls and FAQ*** as it may save you work and trouble.

Finally, go on reading the remaining chapters according to your needs.

Note that the chapter ***Package contents*** gives an overview of the available material.

2 Key to the Model Validation Kit

The kit has been used at the Harmonisation conferences

The so-called *Model Validation Kit* has been used for a series of workshops and conferences on *Harmonisation within Atmospheric Dispersion Modelling for Regulatory purposes* (see www.harmo.org). During the series of Harmonisation conferences, many papers have used the Kit, which was introduced in 1993. The present Guide describes the material after a revision in autumn 2005.

This chapter serves as a key to the entire material. Its purpose is to give you a background, so you can assess how well the kit fulfils your needs, and give you a qualified background to decide which parts of the Kit you will work with.

2.1 Some basic recommendations

Exploratory data analysis is important!

It is recommended that any model evaluation exercise start with clear definitions of the evaluation goal and the variables to be considered, followed by exploratory data analysis as explained in Section 2.5, and then statistical performance evaluation. The implications of this are discussed more closely in the User's Guide to BOOT, which is part of the material at hand (Chang and Hanna, 2005).

Thus, statistical model performance evaluation should not be a stand-alone exercise. It is highly recommended to be coupled with exploratory data analysis, which can reveal model errors, and errors and inconsistencies in data. The Model Validation Kit offers tools for this.

2.2 The Model Validation Kit

A common frame of reference

The Model Validation Kit is intended to be used for evaluation of atmospheric dispersion models. It is a collection of four field data sets as well as software for model evaluation. The Kit is a practical tool intended to serve as a common frame of reference for model performance evaluation. It is, however, limited in scope, as described in subsequent discussions.

History

The Kit has been used for the series of Harmonisation workshops and conferences. A preliminary version of the Kit was used for the workshop in 1993, while a subsequent version was used essentially unchanged throughout the period 1994 - 2005 (in 1997, a supplement was added). It has been distributed in hardcopy (diskette/CD and paper) to more than 250 research groups during that period.

The package was updated to Version 2.0 in October 2005. The new version allows the same studies to be carried out as the previous version, but has been revised in several respects. New software and computing environments have made it necessary to update the package. Furthermore, the documentation is significantly improved and brought up to date. The package can be downloaded from the Internet at www.harmo.org/kit.

Elements of the package

The package contains the following main elements:

- Field data sets from Kincaid, Indianapolis, Copenhagen and Lillestrom;
- The BOOT statistical model evaluation software package;
- Tools for exploratory data analysis, useful for diagnostic model evaluation;
- A recommended procedure (protocol) for model performance evaluation. The approach is explained in the Chapter ***Step by step instructions***. This procedure is relatively simple and thus has some limitations.

For the Kincaid experiment there is also supporting material that can be useful (video clips and a *Dispersion Visualisation Tool*) – see Chapters 8 and 10.

Note that although the emphasis of the Model Validation Kit is on the protocol, some tools included in the Kit – in particular the BOOT software – are general and can be applied for problems beyond the scope of the protocol.

When the Model Validation Kit is distributed on CD, the material is organised in folders as described in Chapter 4 on *Package contents*. Here, in the documentation we use the folder names of the CD.

The material can also be downloaded from the Web in a number of packages (self-extracting zipped files).

2.3 Data sets

The Model Validation Kit addresses the classic problem of a single stack emitting a non-reactive gas. The Kit comprises data from the following four field experiments:

- The Kincaid experiment (1980-81) with tracer releases from a 187-m stack. There are 171 hours of tracer data from monitoring arcs at distances from 0.5 to 50 km. In the Model Validation Kit, the emphasis is on arc-wise maximum concentrations.
- Data from an experiment in Copenhagen, Denmark in 1978-79 with releases from a non-buoyant elevated source (115 m) in neutral and unstable conditions. Nine hours of tracer data are available on arcs from 2 to 6 km. Both arc-wise maxima and crosswind-integrated concentrations are considered reliable.
- Data from an experiment in Lillestrøm, Norway (1987) with tracer releases from a non-buoyant source at 36 m in stable (winter) conditions. Sampling took place during 8 15-minute periods, not during an entire hour. Therefore, when comparing observations with models yielding one-hour averages, crosswind integrated

concentrations can be compared without problems, whereas it is not straightforward to compare arc-wise maxima.

- The Indianapolis experiment (1985) with tracer releases from an 84-m power plant stack in the city of Indianapolis, USA. There are 170 hours of tracer data from monitoring arcs at distances from 0.25 to 12 km. The emphasis is on arc-wise maxima.

Quality indicator

One experience from the past work – an experience that has been repeatedly confirmed – is the usefulness of assigning a quality indicator to experimental data, indicating how reliable a particular set of observations is. Such a quality indicator can be assigned by subjective methods (e.g., inspection of graphs), or assigned by a computer code according to certain objective criteria. The use of a quality indicator is valuable, because subsets of data can be selected in a well-defined manner. This can be utilised to discard data that would have been misleading if they were blindly included in an analysis. For two of the experiments, Kincaid and Indianapolis, the tracer data have been flagged by a manually assigned quality indicator assessing the quality of arc-wise maximum concentrations.

The quality index has values of 0, 1, 2 and 3, with 2 and 3 representing the most reliable data. Comparison studies of observed data with model results should in general be conducted with a quality indicator of 2 or 3.

The data sets are described in the chapter ***Field data***.

2.4 The BOOT software

BOOT is a general tool

The main tool for statistical performance evaluation is the BOOT software package. The BOOT program has been improved and is now available in version 2.0 with a comprehensive, rewritten User's Guide (Chang and Hanna, 2005). Besides detailed technical description of performance measures and the use of the software, the User's Guide also provides a discussion of model evaluation objectives and exploratory data analysis. The BOOT package is flexible and general in nature. Although it has been primarily used to evaluate the performance of air dispersion models, the same procedures and approaches implemented in BOOT also apply to other types of models.

Performance measures considered in BOOT

Compared to the previous version of BOOT, the program now includes some additional performance measures, and an implementation of the ASTM statistical model evaluation procedure (see later). The BOOT package is capable of computing performance measures such as the Fractional Bias (FB), the Normalised Mean Square Error (NMSE), the Geometric Mean Bias (MG), the Geometric Variance (VG), the fraction within a factor of 2 (FAC2), the Measure of Effectiveness (MOE), as well as several others. (FB and MOE are in fact closely related.) With the new software version, FB and MG can be separated into overpredicting and underpredicting components. Bootstrap resampling is used to estimate the confidence limits of a performance measure – hence the name BOOT of the package.

Files related to BOOT

On the distribution CD, the `BOOT` folder contains the BOOT program, a comprehensive User's Guide and various sample files. The `Tools` folder contains additional utilities for use in the present context, as described in Chapter 6 on ***Step by step instructions*** .

2.5 Tools for exploratory data analysis

When performing model evaluation, it is not sufficient to consider just statistical evaluation that produces some performance metrics. Rather, it is recommended that exploratory data analysis also be performed using graphical techniques.

The SIGPLOT graphical package: features and drawbacks

The Model Validation Kit includes some tools for such graphical analyses in the form of the SIGPLOT graphical package and the RESIDUAL utility. The SIGPLOT package is offered as an option that is specifically tailored for model performance evaluation. It must be mentioned that the SIGPLOT program, as well as a number of associated utility programs included in the Model Validation Kit only function in a DOS environment. The package can produce residual plots, where model residuals are depicted as a function of independent variables such as the downwind distance and time of day. Examples are shown in *Figure 7* (in Chapter 6).

It is recognised that the somewhat archaic SIGPLOT package is only one of the many ways of performing exploratory data analysis. More modern and interactive tools than the SIGPLOT package can certainly be used to achieve the same goals. For example, a potential alternative is to use Microsoft Excel for data handling and graphical analyses. Excel offers some very powerful tools for interactive data analysis. In particular, its *Autofilter* feature is useful for investigation of model behaviour. Nevertheless, Excel does not offer the specialised plots that SIGPLOT produces. The advantages of using SIGPLOT are that you will be able to produce residual and other types of specialised plots with data in a relatively standardised format, which has been used by others. Furthermore, the required utilities are already prepared, and the procedures for using the software are described in detail. The drawback is that you will have to work in a DOS environment (Section 6.2.5 provides some hints on this).

More details on Sigplot can be found in the chapter ***Step by step instructions*** as well as in the chapter ***SIGPLOT software***.

2.6 Limitations

It must be recognised that model evaluation studies performed on the basis of the Model Validation Kit are limited in scope. These limitations can be summarised as follows:

- Only four experimental data sets are considered.
- The emphasis is on operational short-range models.
- The problem of interest is relatively simple, namely a point source emitting a non-reactive gas over flat terrain, due to the fact that

this is the scenario represented by the four field experiments. On the other hand, much of the software included in the Kit is general and applicable to many different release scenarios.

- Further, the emphasis is primarily on a) *arc-wise maximum concentrations*, and to some extent b) *cross-wind integrated concentrations*.

- The Kit does not explicitly account for the stochastic nature of dispersion problems.

The tools in the Kit can be used to diagnose strengths and weaknesses of the models, but as a consequence of the above limitations, you should be careful in interpreting the results.

Quantile-quantile plots cannot be expected to show one-to-one correspondence

To further elaborate the last bullet in the above list, atmospheric dispersion processes are stochastic, whereas models in general predict only ensemble averages – not individual realisations. This means that there is a basic conceptual problem with the procedure of directly comparing model predictions to observations, as they cannot be expected to have the same statistical distribution. One consequence is that if the monitoring network is sufficiently dense and if the data represent a sufficient number of scenarios, then a "perfect model" is likely to underpredict the highest observed concentrations (this issue is elaborated by *Olesen*, 1997).

Note further that the so-called quantile-quantile plots from an entire experimental database should not stand alone as the result from a model evaluation. A very useful supplement is residual plots, which provide more insight into model behaviour.

Despite its limitations the Model Validation Kit has the advantage of being straightforward to apply and practically oriented. It also provides a common framework where the results of different studies can be intercompared.

2.7 An alternative: The ASTM methodology

A separate "ASTM package" exists

As noted, there is a concern that direct comparison of model predictions against observations could cause misleading results. Therefore, an alternative approach has been proposed by John Irwin, and has resulted in ASTM Standard Guide D6589. This procedure has also been incorporated in the latest version of the BOOT software as an option. The procedure is *not* treated in depth in the present compendium. However, there exists also a separate package (software and data sets), specifically devised as an implementation of the ASTM procedure – here referred to as the *ASTM package*. It was prepared by John Irwin and is available on the Internet (www.harmo.org/astm). This is not part of the Model Validation Kit, but it can be used as a supplement or an alternative to the Model Validation Kit.

The chapter ***Notes on the "ASTM package"*** of the present Compendium outlines the main principles of the ASTM

methodology. Further, it explains some features that distinguish the two packages and lists certain issues of concern.

2.8 Forum for compilation of experiences - a 'Wiki'

A 'Wiki' is a website that allows users to easily create web pages and edit pages others have created. Wiki's are excellent for collaboration. A Wiki on atmospheric dispersion modelling has recently been created, and this is a potential forum for reporting and retrieving experiences on use of the Model Validation Kit.

The address of the Wiki is
http://atmosphericdispersion.wikicities.com

There is also a link to the Wiki from the web site of the kit, www.harmo.org/kit.

2.9 Structure of the User's Guide

In order to become acquainted with the Model Validation Kit, the two subsequent chapters are recommended reading. They concern, respectively, ***Pitfalls and FAQ***, and ***Package contents***.

Then follows a long chapter on ***Field data***, yielding an overview of the four field experiments and of the data included in the kit.

Chapter 6 ***Step by step instructions*** explains in detail how the tools of the kit can be used. You may choose not to use all of the tools, as some of them – especially those related to the SIGPLOT package – may seem unfamiliar to today's computer users

After Chapter 6 several short chapters with optional information follow, concerning:

- The SIGPLOT software
- The Dispersion Visualisation Tool
- Tools for Grapher
- Video clips from Kincaid
- Notes on the "ASTM package"
- Changes since the previous version of the Model Validation Kit.

Details on the BOOT software are not included here, as there is a separate User's Guide in the `BOOT` folder of the CD. The User's Guide also contains a general discussion on model evaluation.

3 Pitfalls and FAQ

Pitfalls

Please browse through this chapter!

It gives an overview of pitfalls that you may run into when working with the Model Validation Kit. Although nearly all of these are mentioned elsewhere in the material, it may save you time and trouble to become acquainted with them as soon as you begin your work.

FAQ

Further, the chapter provides answers to some commonly asked questions.

3.1 Pitfalls

Should model predictions really fit observations?

It is a basic assumption that for a good model you expect model predictions to fit observed results. *This assumption may not always be warranted!* It is important to consider this question when interpreting results from model evaluation. Don't throw your results blindly into a statistical blackbox!

Some examples follow:

- Quantile-quantile plots should be interpreted with care because of the stochastic nature of atmospheric dispersion. A model typically predicts ensemble averages, so it must be expected that the very highest observed concentrations are larger than predictions.

- A plume may not be properly 'captured' by an arc of monitors. As a consequence, you may obtain misleading values for observed arc-wise maxima and/or crosswind integrated concentrations. This problem is attempted solved in the Model Validation Kit by means of quality indicator for arc-wise maxima for Kincaid and Indianapolis.
  Crosswind integrated concentrations from these two data sets are not included among the data, because no proper quality assurance has been undertaken.
  In the case of Copenhagen and Lillestrøm data, the coverage by monitoring arcs has been considered good enough for both arc-wise maxima and crosswind integrated concentration to be determined.

- Pay attention to averaging times. In the context of the Lillestrøm experiment, sampling took place during 15-minute periods. Such a plume should be expected to be narrower than a plume sampled over an entire hour, so if your model predicts one-hour averages, a comparison of arc-wise maxima may be well be misleading. A comparison of crosswind integrated concentrations will be more reasonable, as the effect of plume meandering is irrelevant in such a comparison.

- Other examples are (these examples are not relevant in the case of the Model Validation Kit): deposition may occur (a problem relevant for the Prairie Gras experiment); a comparison of observed *near-centreline* concentrations with predicted *centerline* concentrations will not be fair (a problem related to an implementation of the ASTM procedure).

Kincaid

Pay attention to the following problems when using data from Kincaid:

- The derived meteorological parameters, u_*, w_*, L and h_{pred}, should be used with care or replaced.
- σ_w and σ_v are suspected to be unreliable.
- It is recommended to use data with a quality indicator of 2 or 3 when analyzing model behaviour. One point is important to be aware of: observations with QUAL=3 are biased in the sense that they are never zero.

Copenhagen

Pay attention to the following problems when using data from Copenhagen:

- The tracer monitoring arcs were in general placed at distances where the concentration was decreasing, i.e., the maximum was closer to the source than any of the arcs.
- It is observed (Gryning and Tassone, 1994) that measured values of σ_w are smaller than predictions by theory.
- The computed heat flux values may not be representative for a greater area.
- When using the enclosed tools, pay attention to the format used for time. E.g., 1417 means 14:17 – whereas Kincaid and Indianapolis data are given for integer values of hour.

Lillestrøm

Pay attention to the following problems when using data from Lillestrøm:

- The averaging period is only 15 minutes for the tracer data. Concentration averages taken over longer time will tend to be smaller than those registered, due to meandering.
- There was generally very light wind during the experiments.
- u_* was recorded as zero for the experiment with the highest concentrations.
- In the data set, stability category has been computed based upon the original method by Turner (1964). This is consistent with the method used for the other data sets, but it does not very well take account of Norwegian winter conditions with snow-covered ground.
- Pay attention to the time format, which is a four-digit format like that of Copenhagen (e.g. 1030 for 10:30).

Indianapolis

Pay attention to the following problems when using data from Indianapolis:

- There is a mixing height of 0 m for several night-time hours (September 21, 28 and 29). Rawinsonde showed a ground-based inversion on the hours in question.

3.2 Frequently Asked Questions

In the Kincaid data set, focus is on arc-wise concentrations. What should I do if I am interested in the entire data set?

If you wish to inspect the concentrations visually, then the Dispersion Visualisation Tool is an excellent option – see Chapter 8.

There is also an alternative, which requires the commercial software package Grapher, as described in Chapter 9.

The data are provided in the data set SF6_ALL.DAT. Note that *all* concentrations are included in SF6_ALL.DAT – also those considered outliers (details in the file OUTLIERS.TXT). Further note that the unit for concentrations in this file is ppt – contrary to other concentration data in the package.

As an alternative, you can find a version of the Kincaid data set in the ASTM package (see Chapter 11) prepared by John Irwin of the US EPA/NOAA. The package contains a file (KINReanArcs.DAT), where data have been organised in arcs. Note that in this version a few outliers are marked as negative concentration values (consult the documentation in the package for further details).

If you are interested in the entire data set from *Indianapolis*, you will find 170 files with data in the folder
`Field_data\Ind\XY_conc_standard`
As for Kincaid, you can find an alternative file in the ASTM package.

How can I create a Command Line environment (run DOS) on a PC with Windows XP/ Windows 2000?

See Section 6.2.5.

What has happened to outliers in the data sets?

For Kincaid, five values from the raw data set have been discarded. See the file OUTLIERS.TXT in the folder **`Field_data\Kin`** for details.

4 Package contents

When the Model Validation Kit is distributed on CD, the material is organised in folders as described below. The material can also be downloaded from the Web in a number of packages (self-extracting zipped files).

The CD with the complete Model Validation Kit contains the following elements

- This compendium where most of the documentation related to the kit is compiled. Resides in the root folder of the CD.
- Field data from Kincaid, Indianapolis, Copenhagen and Lillestrøm. Folder: **`Field_data`**
- Boot software package. The complete package is in folder **`BOOT`**, while a copy of the BOOT program itself is also included in the **`Tools`** folder.
- Sigplot software package. The complete package is in folder **`SIGPLOT`**, while a copy of the SIGPLOT program itself is also included in the **`Tools`** folder.
- Tools. Various software and template files designed to be helpful for model evaluation. Thoroughly explained in Chapter 6. Folder: **`Tools`**.
- Samples. The folder **`Samples`** contain some samples of files referring to Kincaid data. They illustrate the results of using BOOT, RESIDUAL and SIGPLOT as described in Chapter 6.
- The *Dispersion Visualisation Tool*, which is a utility for displaying observed concentration data. Described in Chapter 8. Folder: **`Visualisation`**.
- Tools for preparing concentration data from Kincaid and Indianapolis, so they can be plotted in a map-like fashion with the commercial plotting software Grapher. Described in Chapter 9. Folder: **`Grapher_tools`**
- Video films from Kincaid as described in Chapter 10. Folder: **`Kincaid_video`**

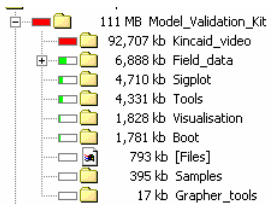


Figure 1 Space used by the various folders of the Model Validation Kit.

5 Field data

Please pay attention to the information given in the sections "Points to be noted" for each data set. In these sections, some potential pitfalls are pointed out.

Before using the data, also carefully inspect the files PAR_KIN.TXT, PAR_CPH.TXT, PAR_LIL.TXT and PAR_INDI.TXT which contain important notes.

One basic detail: The von Karman constant `K` has been assumed to have a value of 0.40 in the data presented.

5.1 Kincaid

The Kincaid-related files are located in the folder
`Field_data\Kin`

Note that there is video from the Kincaid experiment in the folder **`Kincaid_video`** (see Chapter 10), and that the Dispersion Visualisation Tool described in Chapter 8 can be used to visualise observed concentrations.

5.1.1 Experimental set-up

The Kincaid field experiment was performed as part of the EPRI Plume Model Validation and Development Project. A very comprehensive experimental campaign was conducted in 1980 and 1981. A large number of reports concerning the Kincaid experiment have been published by EPRI, including *Overview, Results, and Conclusions for the EPRI Plume Model Validation and development Project: Plains Site* (Bowne and Londergan, 1983) which gives a good overall description of the Kincaid experimental campaign.

Terrain

The Kincaid power plant is situated in Illinois, USA (39.59 °N, 89.49 °W) and is surrounded by flat farmland with some lakes. The UTM coordinates are 285.66 (Easting) and 4385.10 (Northing). The terrain is at an elevation of approximately 180 m a.m.s.l.

The roughness length is approximately 10 cm.

There is further information on geographical coordinates in the file geo_kin.txt

Source

The power plant has a 187 m stack with a diameter of 9 m. During the experiment, SF_6 was released from the stack. The tracer releases started some hours before the sampling.

There is a nearby building with a height of approximately 75 meter. It is rectangular – 25 m by 95 m – with the long side oriented east - west. The stack is 152 m south of the centre of the southern edge of the building, and 182 m south of the tallest part of the building, which has a maximum significant elevation of 74.4 m.

5.1.2 Meteorological data

The data that you receive have been supplied by the EPRI Air Quality Data Center operated by Earth Tech (formerly: Sigma Research Corporation). The meteorological parameters u_*, w_*, L and h_{pred} were derived by Earth Tech using pre-processing methods described in Hanna and Paine (1989). Steve Hanna (who was affiliated to Earth Tech when the data were prepared) warns that these parameters should be used with caution because his suggested boundary layer formulas have been slightly modified since 1989 (cf. the paper by Hanna and Chang, 1992). He recommends that modellers use their own pre-processing methods. Thus, the presence of these parameters in the data does not indicate a recommendation of their use.

Observed mixing heights were determined manually by interpretation of radiosonde data (there were on-site radio soundings several times a day).

We wish to warn you against using measured values of σ_w from the Kincaid study. According to Steve Hanna there were many, many problems with the Gill σ_w data, and he cautions anyone about using them. Also, there are indications that observed σ_v values are unreliable (this statement is based on experience with their use as discussed during the Manno workshop).

Most meteorological measurements (the 100-m and 10-m meteorological towers, solar and terrestrial radiation equipment) were taken from a "Central Site" located around 650 m east of the Kincaid plant.

This site was situated in fallow fields away from major obstacles.

The NWS data are from the National Weather Service station in Springfield, 30.6 km northwest of the source.

The radiosonde data supplied on diskette are routine data from the station Peoria, 120 km north of the source, 199 m above mean sea level.

5.1.3 Tracer data

Selection of data

There were approximately 350 hours of tracer experiments during the experimental campaign. When used by Hanna and Paine (1989), the data were divided (by day) into two parts – a developmental data base and an evaluation data base. The distinction between these two subsets of data has been maintained, and the data distributed here belong to the development data base. There is a total of 171 hours in the development data base distributed. For each hour, data are available from several crosswind arcs of monitors. Screening of data has led to the conclusion that a few observed values were unreliable (5 cases) and they have been removed (details in data set OUTLIERS.TXT). This has resulted in a total of 1284 arc-hours in the data set.

Warning: irregular concentration patterns

It is important to note that the concentration pattern is often irregular for the Kincaid experiment – high and low concentrations may occur intermittently along an arc. *Figure 2* shows an example. Therefore it is often difficult to determine a representative maximum concentration along a crosswind arc of monitors. Further, there may be gaps in the monitoring arcs. Therefore, a variable has been assigned to each monitoring arc, indicating *how reliable* the arc-wise maximum should be considered. This quality indicator has been assigned by Earth Tech on the basis of manual inspection of the geographical patterns of concentration distribution. The criteria for assigning the indicator are shown in Table 1.

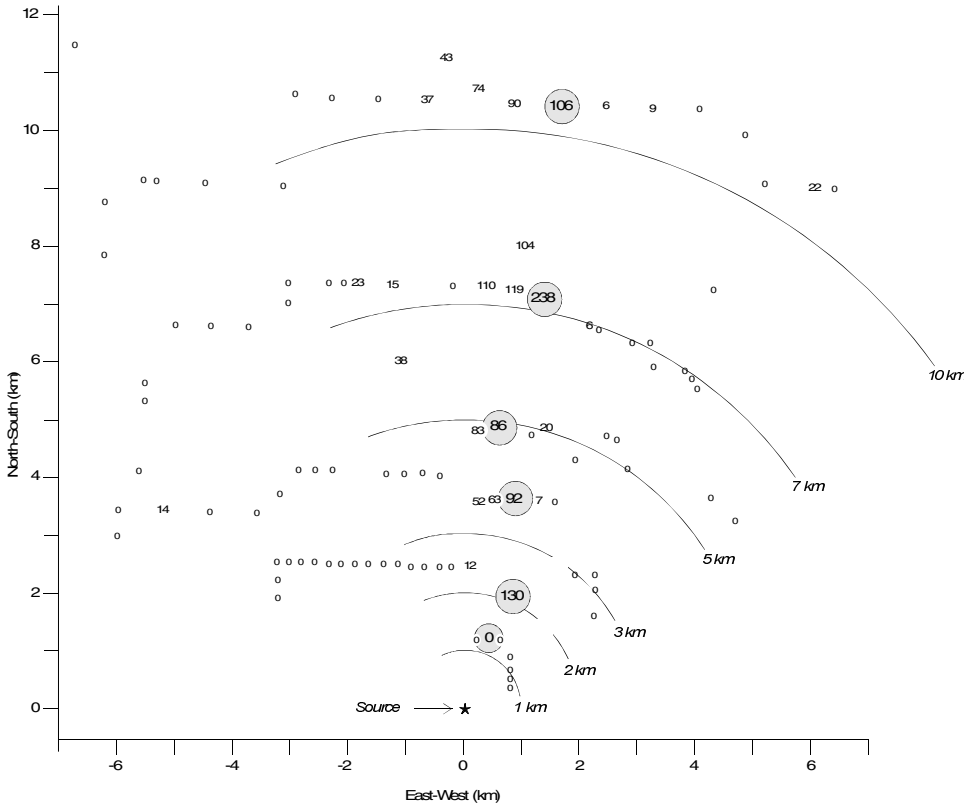


Figure 2 Geographical distribution of measured concentrations at Kincaid, 22 May 1981, 10-11 hours. Values are in ppt, and the arcwise maxima are enclosed in circles.

The complete set of tracer measurements at all monitors is distributed in the file SF6_ALL.DAT. The format of this file is a bit awkward, but in the folder **`Grapher_tools`** there is software capable of extracting information from it (See Chapter 9). An alternative is to use data in the ASTM package (see Section 3.2 with FAQ).

.

Table 1 The file QUAL.TXT contains the following explanation of quality indicator (QUAL) for Kincaid and Indianapolis.

```
The indicator variable has values from 0 to 3, indicating the following:

0      This value should clearly be disregarded (examples:  the plume obviously missed the monitors; the arc is
only a continuation of a neighbouring arc).

1      This value is most probably not the maximum value (examples:  there are gaps in the monitoring arc; the
observed maximum is isolated; there is no smooth variation from one arc to the next; the maximum is on the edge
of the arc).

2      A maximum is identified, but the true value may well be different (examples:  the concentration pattern is
irregular; there are only 2 or 3 monitors impacted; the plume is near the edge of the arc).
Note:  Also, arcs where the observed maximum is essentially zero, but where there is evidence that a plume is
present aloft, have been categorized in this group.

3      A relatively well-defined maximum is observed, which is continuous in space, is away from the edge of the
monitoring arc, and is not irregular or isolated.


It is recommended that you use data with a quality indicator of 2 or 3 in your analyses.  Note that observations
with QUAL=3 are biased in the sense that they are never zero.
```

5.1.4 Data files

"Hour" indicates "end of the hour" for time-averaged parameters. Thus, 10 means an average over the period between 9 and 10 Central Standard Time. CST is equivalent to GMT-6.
The following files are supplied in the **`Kincaid`** folder:

DISTM_K.DAT	Distances to arcs with values of max. conc.
EMISSION.DAT	Emission data for all hours, not just sampling hours.
GEO_KIN.TXT	Info on geographical coordinates.
MET_K1-L.DAT	Meteorological data; 'long' (continuous) period
MET_K1.DAT	Meteorological data; tracer hours
MET_K2-L.DAT	More met. parameters
MET_K2.DAT	-
MET_K3-L.DAT	-
MET_K3.DAT	-
MISC_KIN.DAT	Miscellaneous data
OUTLIERS.TXT	Information on outliers (changes to original data)
PAR_KIN.TXT	Overview of parameters and missing data.
QUAL.TXT	Explanation of quality indicator
RAWIN.DAT	Routine radiosonde data
SF6_ALL.DAT	SF_6 data, all monitors
SF6_KIN.DAT	SF_6 data, arc-wise maxima

There are corresponding pairs of files such as MET_K1.DAT and MET_K1-L.DAT. The 'L' files are 'long', and include meteorological information for the hours between tracer experiments. They have been included to permit modellers to run met preprocessor requiring continuous periods of data.
The tables on the next pages yield an overview of the variables contained in the data sets.

5.1.5 Points to be noted

A summary of some potential pitfalls when using data is given below:

- The derived meteorological parameters, u_*, w_*, L and h_{pred}, should be used with care or replaced.
- σ_w and σ_v are suspected to be unreliable. According to Steve Hanna, there were *many* problems with Gill σ_w data, and use of them may severely degenerate modelling results.
  Also, according to results for one specific model shown at the workshop in Manno, the effect of choosing observed values of σ_v – as opposed to computed values – resulted in predictions of the

maximum concentration for the entire data set which were factor of three larger than otherwise.

- It is recommended to use data with a quality indicator of 2 or 3 when analyzing model behaviour. One point is important to be aware of: observations with QUAL=3 are biased in the sense that they are never zero.

5.1.6 Additional information

The data distributed constitute only a small fraction of the wide variety of variables collected during the campaign. A large number of reports concerning the Kincaid experiment have been published by EPRI. Therefore, if you wish to analyze certain questions in further detail, you may want to request some of these reports from EPRI (see the list of addresses at the end of the chapter with references..

Also, please note that a piece of recommended reading concerning the Kincaid experiment is the paper *Hybrid Plume Dispersion Model (HPDM) Development and Evaluation* by Hanna and Paine (1989). It gives a brief description of the layout of the Kincaid experimental campaign.

See the list of references and the list of addresses in the back for details.

Table 2 Contents of the file PAR_KIN.TXT

```
                    Parameters supplied in the distributed files from Kincaid
                    =========================================================

                                                                  FILE NAMES

                         3 files with each 2040 obs.:          MET_K1-L.DAT        MET_K3-L.DAT
                                                                  MET_K2-L.DAT

                         4 files with each 171 obs.:  MISC_KIN.DAT MET_K1.DAT MET_K2.DAT MET_K3.DAT

                         1 file with 1284 obs.:                                                SF6_KIN.DAT

Basic parameters:

   YR       Year                                          +         +            +         +       +
   MO       Month                                         +         +            +         +       +
   DY       Day                                           +         +            +         +       +
   HR       Hour  (end of hour; GMT-6)                    +         +            +         +       +

Observed meteorological parameters:

   PRES     Pressure (mb)                                           +
   NET      Net radiation (W/m2)                                    +
   TOT      Total radiation (W/m2)                                  +
   DP100    Dew-point temperature at 100 m (K)                      +
   T100     Temperature at 100 m (K)                                +
   T50      Temperature at  50 m (K)                                +
   T10      Temperature at  10 m (K)                      +(*1)     +
   ZI       Mixing height, observed (m)                   +         +
   DTHDZ    Pot. temp. grad. between 100-50 m (K/m)       +         +

   WS100    Wind speed at 100 m (m/s)                     +                      +
   WS50     Wind speed at  50 m (m/s)                                            +
   WS30     Wind speed at  30 m (m/s)                                            +
   WS10     Wind speed at  10 m (m/s)                     +(*1)                  +
   WD100    Wind direction at 100 m (deg.)                +(*1)                  +
   WD50     Wind direction at  50 m (deg.)                                       +
   WD30     Wind direction at  30 m (deg.)                                       +
   WD10     Wind direction at  10 m (deg.)                                       +
   SWD100   Sigma WD100 (deg.)                                                   +
   SWD50    Sigma WD50  (deg.)                                                   +
   SWD30    Sigma WD30  (deg.)                                                   +
   SWD10    Sigma WD10  (deg.)                                                   +
   SIGW     Sigma of vertical velocity at 100 m (m/s)     +                      +
   SIGV     Sigma of cross-wind speed at 100 m (m/s)      +                      +
   FLAG     (*2)                                          +

   CEILNWS  Ceiling (100's of feet); -1=unlimited                                          +
   DPNWS    Dew-point temp. (F)                                                            +
   WDNWS    Wind direction (deg.)                                                          +
   WSNWS    Wind speed (knots)                                                             +
   PNWS     Pressure (inch. Hg)                                                            +
   TNWS     Temperature (F)                                                                +
   NNWS     Cloud cover (1/10)                                                             +
   PRECNWS  Precipitation (mm)                                                             +

Derived parameters:

   ZIPRE    Predicted mixing height (m)                   +
   UST      Friction velocity (m/s)                       +
   WST      Convective velocity (m/s)                     +
   L        Monin-Obukhov length (m)                      +
   TURNER   Turner stability class (based on NWS data)    +

Tracer parameters:

   Q        Emission rate (g/s)                           +                                       +
   TQ       Gas temp. (K)                                 +
   VSQ      Gas exit velocity (m/s)                       +

   ARCMAX   Max. conc. (ug/m3) at DIST (*3)                                                        +
   DIST     Distance (km) to arc of monitors                                                       +
   AZMAX    Direction (deg.) to ARCMAX                                                             +
   ARCMAX/Q Conc normalized by emission, times 10**9 (s/m3 10**(-9))                               +
   QUAL     Quality indicator for ARCMAX                                                           +

(*1): 5-6 observations are substituted with converted NWS observations.)
(*2): Value of flag describes which of the parameters T10, WS10 or WD100 are substituted.
      For each of the substitutions FLAG is added the value 1, 2 resp. 4 (no subs. FLAG=0).)
(*3): Converted from ppt by multiplying with 1.758*p/T)

The file DISTM_K.DAT is meant as a help for deciding at which distances computations
should be performed (where SF6 was measured). 12 different distance values appear in
the data set.

      Parametre          Units
                                                          DISTM_K
      YR       Year                                             +
      MO       Month                                            +
      DY       Day                                              +
      HR       Hour, (GMT-6)                                    +

      NUARCM   Number of arcs with values of max. conc. ARCMAX  +
      DM1        Distances (km) to arcs with                    +
      DM2           values of ARCMAX                            +
      ... DM12                                                  +
```

Table 3 Contents of the file PAR_KIN.TXT (continued)

Number of missing parameters and their dummy values in the distributed files from Kincaid.

Para-meters	Dummy value	FILE NAMES: MISC_KIN.DAT	MET_K1.DAT	MET_K1-L.DAT	MET_K2.DAT	MET_K2-L.DAT	MET_K3.DAT	MET_K3-L.DAT	SF6_KIN.DAT
YR	-	0	0	0	0	0	0	0	0
MO	-	0	0	0	0	0	0	0	0
DY	-	0	0	0	0	0	0	0	0
HR	-	0	0	0	0	0	0	0	0
PRES	-999		5	62					
NET	-999		8	202					
TOT	-999		8	379					
DP100	-999		52	370					
T100	-999		8	205					
T50	-999		8	205					
T10	-999	0	5	37					
ZI	-999	6	6	906					
DTHDZ	-9.9999	8	8	239					
WS100	-999	6			6	112			
WS50	-999				9	206			
WS30	-999				6	40			
WS10	-999	0			6	42			
WD100	-999	0			5	44			
WD50	-999				8	207			
WD30	-999				8	208			
WD10	-999				5	40			
SWD100	-999				6	190			
SWD50	-999				6	189			
SWD30	-999				6	189			
SWD10	-999				6	189			
SIGW	-9.99	18			18	461			
SIGV	-9.99	9			9	885			
FLAG	-								
CEILNWS	-						0	0	
DPNWS	-						0	0	
WDNWS	-						0	0	
WSNWS	-						0	0	
PNWS	-						0	0	
TNWS	-						0	0	
NNWS	-						0	0	
PRECNWS	-						0	0	
ZIPRE	-	0							
UST	-	0							
WST	-	0							
L	-	0							
TURNER	-	0							
Q	-	0							0
TQ	-	0							
VSQ	-	0							
DIST	-								0
ARCMAX	-								0
AZMAX	-999								355
ARCMAX/Q	-								0
QUAL	-								0

Notes on parameters:

The derived meteorological parameters have been included for reference.
They are computed using one of many possible methods and their inclusion
in the data set does not indicate a recommendation of their use.
It is recommended that modellers use their own processing methods.

Measured values of SIGW and SIGV are not to be considered reliable.

The Turner stability class has been computed based on NWS data. It is
included for reference; it is computed according to the original paper by
Turner: J. Appl. Met., (1964) 3., p.83 (this is the case also for
Copenhagen and Lillestrom data).

Be careful about units when using NWS data - they differ from the
European units!

The frequency distribution of the quality index for tracer arc-hours is as follows

QUAL	Frequency
0	442
1	256
2	248
3	338
All:	1284

Table 4 Samples of the most important data files from Kincaid.

MISC_KIN.DAT

YR	MO	DY	HR	ZI	ZIPRE	DTHDZ	T10	WS10	WS100	WD100	SIGV	SIGW	UST	WST	L	TURNER	Q	TQ	VSQ	FLAG
80	4	20	14	2076	2288	-9.9999	298.4	2.7	5.8	281	-9.99	-9.99	0.30	2.65	-8.6	4	10.2	416.0	14.6	0
80	4	20	15	2092	2313	-9.9999	298.4	2.9	5.8	302	-9.99	-9.99	0.31	2.53	-11.2	4	8.2	416.0	14.6	0
80	4	20	16	2104	2333	-9.9999	298.4	2.5	6.3	308	-9.99	-9.99	0.28	2.31	-9.9	4	8.4	416.0	15.0	0
80	4	25	12	893	1156	-0.0022	284.2	2.0	2.3	57	1.35	0.84	0.22	1.95	-3.9	2	11.2	432.0	29.6	0
80	4	25	13	1032	1332	-0.0022	285.2	2.1	2.3	52	0.49	0.90	0.22	1.95	-4.8	1	11.2	432.0	29.2	0
80	4	25	14	1175	1575	-0.0022	286.2	3.0	3.3	53	1.11	0.77	0.28	2.05	-10.4	3	11.3	432.0	29.6	0
80	4	25	15	1355	1753	-0.0022	286.6	2.1	2.4	29	1.23	0.71	0.25	2.19	-6.3	3	11.1	432.0	29.9	0
80	4	25	16	1539	1768	-0.0022	287.3	5.1	-999.0	42	-9.99	0.80	0.51	1.92	-84.7	3	11.3	432.0	30.0	2
80	4	25	17	1545	1774	-0.0022	287.7	2.3	2.8	31	0.53	0.62	0.23	1.39	-20.9	4	10.7	432.0	30.3	0
80	5	1	16	1300	1932	-0.0002	290.8	3.5	3.9	15	1.01	0.74	0.37	2.17	-23.5	3	11.5	441.0	27.9	0

MET_K1.DAT

YR	MO	DY	HR	PRES	NET	TOT	DP100	T100	T50	T10	ZI	DTHDZ
80	4	20	14	1000.0	-999.0	-999.00	279.5	-999.0	-999.0	298.4	2076	-9.9999
80	4	20	15	999.7	-999.0	-999.00	278.8	-999.0	-999.0	298.4	2092	-9.9999
80	4	20	16	999.7	-999.0	-999.00	278.8	-999.0	-999.0	298.4	2104	-9.9999
80	4	25	12	995.4	503.8	773.84	271.6	283.0	283.6	284.2	893	-0.0022
80	4	25	13	995.0	439.0	662.27	272.0	284.0	284.6	285.2	1032	-0.0022
80	4	25	14	994.7	432.9	685.54	272.3	284.8	285.4	286.2	1175	-0.0022
80	4	25	15	994.0	368.0	572.16	272.6	285.5	286.1	286.6	1355	-0.0022
80	4	25	16	993.5	250.7	415.56	272.5	286.2	286.8	287.3	1539	-0.0022
80	4	25	17	993.2	94.3	214.55	272.6	286.6	287.2	287.7	1545	-0.0022
80	5	1	16	994.5	331.3	545.19	278.6	289.7	290.2	290.8	1300	-0.0002
80	5	1	17	994.3	152.7	280.01	278.2	290.3	290.8	291.3	1743	-0.0002
80	5	1	18	994.2	60.5	179.78	278.1	290.5	291.0	291.6	1840	-0.0002

MET_K1-L.DAT

YR	MO	DY	HR	PRES	NET	TOT	DP100	T100	T50	T10	ZI	DTHDZ
80	4	14	1	988.1	-999.0	-999.00	271.5	-999.0	-999.0	272.8	154	-9.9999
80	4	14	2	984.8	-999.0	-999.00	269.1	-999.0	-999.0	272.8	-999	-9.9999
80	4	14	3	982.7	-999.0	-999.00	270.8	-999.0	-999.0	273.5	-999	-9.9999
80	4	14	4	981.4	-999.0	-999.00	273.5	-999.0	-999.0	274.4	-999	-9.9999
80	4	14	5	980.0	-999.0	-999.00	272.8	-999.0	-999.0	274.4	-999	-9.9999
80	4	14	6	979.3	-999.0	-999.00	272.4	-999.0	-999.0	273.5	-999	-9.9999
80	4	14	7	978.7	-999.0	-999.00	272.4	-999.0	-999.0	273.5	-999	-9.9999
80	4	14	8	977.3	-999.0	-999.00	272.4	-999.0	-999.0	273.5	-999	-9.9999
80	4	14	9	976.0	-999.0	-999.00	272.4	-999.0	-999.0	273.5	-999	-9.9999
80	4	14	10	975.3	-999.0	-999.00	271.9	-999.0	-999.0	273.5	-999	-9.9999
80	4	14	11	975.3	-999.0	-999.00	271.5	-999.0	-999.0	273.5	-999	-9.9999
80	4	14	12	976.0	-999.0	-999.00	271.5	-999.0	-999.0	273.5	-999	-9.9999
80	4	14	13	976.6	-999.0	-999.00	271.5	-999.0	-999.0	273.5	-999	-9.9999
80	4	14	14	978.0	-999.0	-999.00	271.5	-999.0	-999.0	272.8	-999	-9.9999
80	4	14	15	978.0	-999.0	-999.00	271.1	-999.0	-999.0	272.8	-999	-9.9999
80	4	14	16	980.0	-999.0	-999.00	271.1	-999.0	-999.0	272.8	-999	-9.9999
80	4	14	17	980.7	-999.0	-999.00	271.1	-999.0	-999.0	272.8	-999	-9.9999
80	4	14	18	981.4	-999.0	-999.00	271.1	-999.0	-999.0	272.8	-999	-9.9999
80	4	14	19	982.7	-999.0	-999.00	271.1	-999.0	-999.0	272.8	-999	-9.9999
80	4	14	20	983.4	-999.0	-999.00	271.5	-999.0	-999.0	272.8	-999	-9.9999
80	4	14	21	984.1	-999.0	-999.00	271.5	-999.0	-999.0	272.8	-999	-9.9999
80	4	14	22	984.1	-999.0	-999.00	271.5	-999.0	-999.0	272.8	-999	-9.9999
80	4	14	23	984.8	-999.0	-999.00	271.5	-999.0	-999.0	272.8	-999	-9.9999
80	4	14	24	984.8	-999.0	-999.00	271.5	-999.0	-999.0	272.8	-999	-9.9999
80	4	15	1	984.8	-999.0	-999.00	271.5	-999.0	-999.0	273.5	-999	-9.9999
80	4	15	2	984.8	-999.0	-999.00	272.4	-999.0	-999.0	272.8	-999	-9.9999

MET_K2.DAT

YR	MO	DY	HR	WS100	WS50	WS30	WS10	WD100	WD50	WD30	WD10	SWD100	SWD50	SWD30	SWD10	SIGW	SIGV
80	4	20	14	5.8	-999.0	5.8	2.7	281	-999	-999	302	-999.00	-999.00	-999.00	-999.00	-9.99	-9.99
80	4	20	15	5.8	-999.0	6.3	2.9	302	-999	-999	319	-999.00	-999.00	-999.00	-999.00	-9.99	-9.99
80	4	20	16	6.3	-999.0	6.3	2.5	308	-999	-999	313	-999.00	-999.00	-999.00	-999.00	-9.99	-9.99
80	4	25	12	2.3	2.2	2.2	2.0	57	49	46	29	47.11	59.17	65.37	70.49	0.84	1.35
80	4	25	13	2.3	2.4	2.3	2.1	52	54	53	46	12.42	14.81	15.91	27.52	0.90	0.49
80	4	25	14	3.3	3.3	3.3	3.0	53	55	58	53	20.39	22.98	22.65	32.17	0.77	1.11
80	4	25	15	2.4	2.4	2.3	2.1	29	27	34	20	35.22	47.36	55.78	65.40	0.71	1.23
80	4	25	16	-999.0	-999.0	-999.0	-999.0	42	40	41	34	33.53	31.72	32.16	40.79	0.80	-9.99
80	4	25	17	2.8	2.6	2.5	2.3	31	27	26	16	11.02	21.18	26.15	29.04	0.62	0.53
80	5	1	16	3.9	4.1	4.0	3.5	15	16	16	7	15.29	15.41	16.36	16.56	0.74	1.01
80	5	1	17	4.0	4.0	3.9	3.4	21	21	19	11	8.61	7.26	8.21	7.59	0.53	0.59
80	5	1	18	3.8	3.7	3.5	3.0	33	34	33	25	11.97	10.94	11.67	12.03	0.45	0.78
80	5	1	19	4.0	3.8	3.4	2.8	47	46	44	36	3.69	3.73	3.71	4.33	0.22	0.26
80	5	1	20	3.2	2.7	2.2	1.4	67	63	64	60	14.20	12.31	13.28	20.20	0.13	0.77
80	5	1	21	2.4	2.2	1.9	0.9	133	137	133	147	14.92	18.86	23.32	28.54	0.09	0.60
80	5	4	7	4.9	2.9	1.7	1.0	323	333	339	326	5.40	3.18	3.71	21.19	0.06	0.46
80	5	4	8	4.6	2.3	2.0	1.7	331	337	337	336	1.38	3.20	2.92	8.01	0.19	0.11
80	5	4	9	3.0	2.8	2.8	2.5	340	343	342	337	3.86	3.57	4.40	4.86	0.37	0.20

MET_K3.DAT

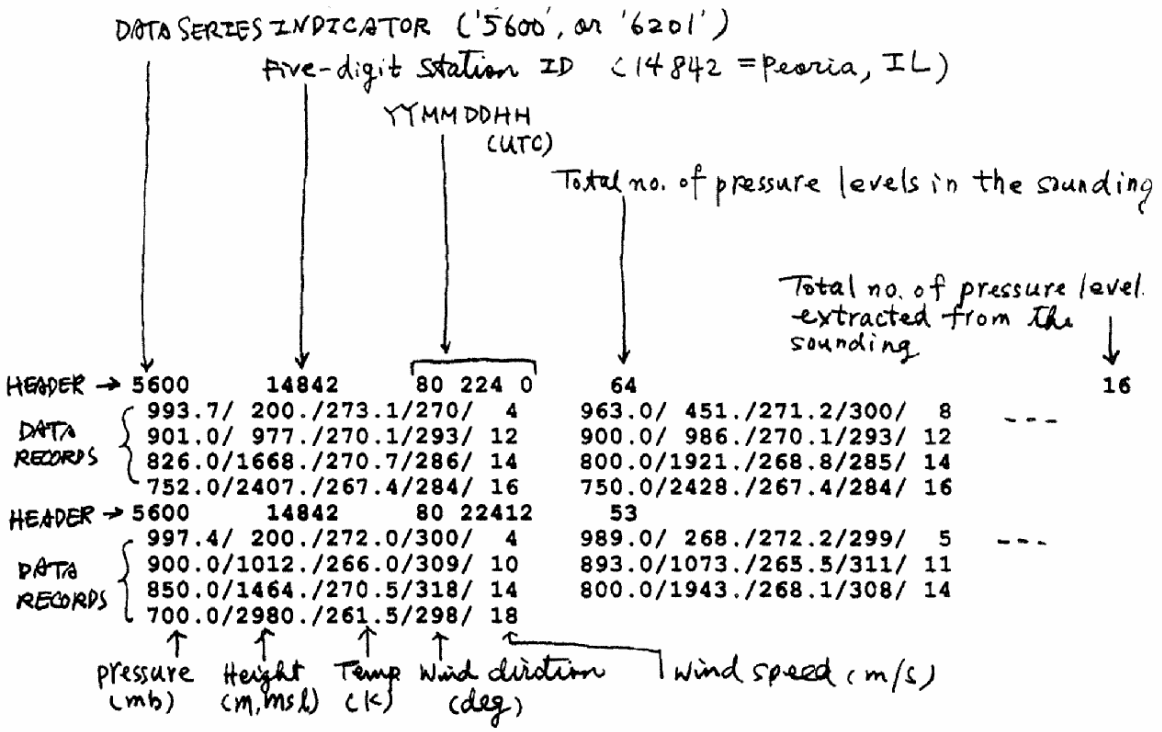
YR	MO	DY	HR	CEILNWS	DPNWS	WDNWS	WSNWS	PNWS	TNWS	NNWS	PRECNWS
80	4	20	14	-1	55	29	12	29.97	80	2	0.0
80	4	20	15	-1	52	29	14	29.97	81	3	0.0
80	4	20	16	-1	51	32	12	29.94	80	2	0.0
80	4	25	12	-1	35	30	6	29.97	57	3	0.0
80	4	25	13	-1	39	20	4	29.94	59	2	0.0
80	4	25	14	-1	41	1	8	29.94	60	3	0.0
80	4	25	15	-1	41	31	10	29.91	62	3	0.0
80	4	25	16	-1	41	1	10	29.91	61	3	0.0
80	4	25	17	-1	40	3	10	29.91	60	2	0.0
80	5	1	16	-1	50	4	8	29.94	68	3	0.0
80	5	1	17	-1	50	3	8	29.94	68	3	0.0

SF6_KIN.DAT

YR	MO	DY	HR	ARCMAX	DIST	AZMAX	Q	ARCMAX/Q	QUAL
80	4	20	14	0.748	3.0	92	10.2	73.4	3
80	4	20	14	0.218	5.0	117	10.2	21.4	1
80	4	20	14	0.216	7.0	94	10.2	21.2	1
80	4	20	14	0.138	10.0	95	10.2	13.6	1
80	4	20	14	0.210	15.0	131	10.2	20.6	1
80	4	20	14	0.084	20.0	57	10.2	8.3	1
80	4	20	15	0.442	3.0	83	8.2	53.9	3
80	4	20	15	0.249	5.0	120	8.2	30.3	3

Table 5 Format of RAWIN.DAT (radiosonde data).

Format of RAWIN.DAT




```
***   I/O statement used to write the header records
      write(irawin,6200) stnid,year,month,day,hour,nlev,istop
6200  format(3x,'6201',5x,a5,5x,4i2,5x,i2,t69,i2), or
6200  format(3x,'5600',5x,a5,5x,4i2,5x,i2,t69,i2)


***   I/O statement used to write the data records
      write(irawin,6210) (pres(i),height(i),temp(i),wd(i),ws(i),
     1 i=1,istop)
6210  format(4(3x,f6.1,'/',f5.0,'/',f5.1,'/',i3,'/',i3))
```

5.2 Copenhagen

5.2.1 Experimental set-up

The experiments in question took place in the Northern part of Copenhagen in 1978-79. A full description can be found in Gryning (1981; available on request). A shorter description is found in a paper by Gryning and Lyck (1984; available from Helge Rørdam Olesen on request). A comprehensive data report is available electronically (Gryning and Lyck, 2002).

The dispersion experiments were carried out under neutral and unstable conditions. The tracer (SF_6) was released without buoyancy from a tower at a height of 115 m, and collected at ground-level positions in up to three crosswind series of tracer sampling units, positioned 2-6 km from the point of release. The site was mainly residential having a roughness length of 0.6 m.

For all runs during the experiment, the crosswind profiles of tracer concentrations were well determined, thus making a relatively accurate estimate of crosswind integrated concentration possible. The maximum concentrations given in the data set is the highest observed concentration along each arc.

The release took place in the suburb of Gladsaxe, latitude 55.735 N, longitude 12.494 E; the height of terrain is 49 m a.m.s.l. The tracer sampling units were mounted at lampposts at a height of 2-3 meters above the ground.

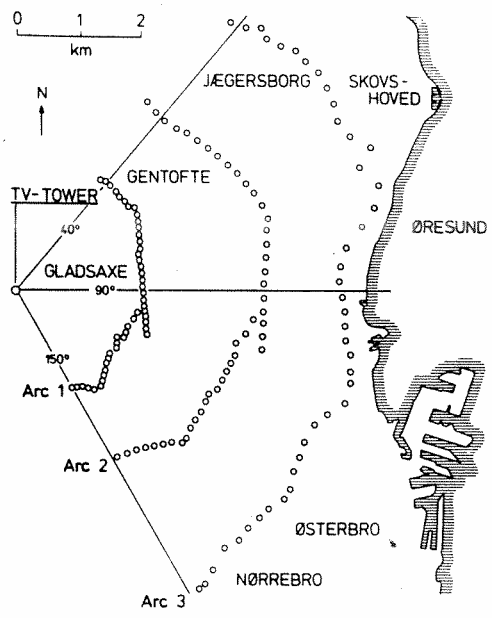


Figure 3 The experimental site in Copenhagen. A thick line indicates the coast of the straight of Øresund. Tracer sampling unit positions available for the experiments are indicated by circles. Not all positions were used for an experiment. Typically, 20 sampling units were used in each arc, and the units were deployed according to meteorological conditions.

5.2.2 Meteorological data

The meteorological measurements performed during the experiments included three-dimensional wind velocity fluctuations at the height of release. Much emphasis was put into the measurements at the release height (Gryning and Thomson, 1979). These measurements comprised u, σ_v and σ_w. It is recommended to make use of these measurements (cf. Gryning and Tassone, 1994). The temperature and wind speed profile along the mast was taken from routine measurements. The mixing height was determined from the daily radio sounding at Copenhagen, which was carried out around the time of tracer sampling.

In the revised data set, the values of u_*, L and heat flux have been determined using a standard meteorological preprocessor (in an implementation described by Sozzi and Fraternali, 1994). Two levels of temperature and one level of wind speed were used (not research-grade data). The computed heat fluxes etc. may be influenced by very local effects; in one case in particular, the heat flux was much larger than expected.

5.2.3 Points to be noted

The tracer monitoring arcs were in general placed at distances where the concentration was decreasing, i.e., the maximum was closer to the source than any of the arcs.
It is observed (Gryning and Tassone, 1994) that measured values of σ_w are smaller than predictions by theory.
The computed heat flux values may not be representative for a greater area.

5.2.4 Additional information

It is possible upon request to obtain supplementary meteorological data for the time before the measuring periods.
Please note that a comprehensive data report on the Copenhagen data set is available through the Web (Gryning and Lyck, 2002) .

Table 6 Contents of the file PAR_CPH.TXT

```
      Parameters supplied in the distributed files from Copenhagen
      ============================================================

Basic parameters:
      YR      Year
      MO      Month
      DY      Day
      HRS     Time start of period, (GMT+1). Example: 1317 means 13.17
      HRE     Time end of period, (GMT+1)

Observed meteorological parameters:
      W10     Wind speed at  10 m (m/s)
      W60     Wind speed at  60 m (m/s)
      W115    Wind speed at  115 m (m/s)
      T2      Temperature at  2 m  (deg. K)
      T40     Temperature at 40 m  (deg. K)
      T120    Temperature at 120 m (deg. K)
      SIGV    Sigma of cross-wind speed at 115 m (m/s)
      SIGW    Sigma of vertical velocity at 115 m(m/s)
      ZI      Mixing height, observed (m)
      NCLD    Fractional cloud cover (EIGHTS!)
      CEIL    Height to lowest cloud (m)

Derived meteorological parameters:
      UST     Friction velocity from profile (m/s)
      L       Monin-Obukhov length (m)
      HF      Heat flux  (W/m2)
      TURNER  Turner stability class according to Turner (1964)

Tracer release parameters:
      DIST     Distance (km) to arc of monitors
      Q        Emission rate (g/s)
      SIGY     Sigma-y (m) at DIST
      CY       Cross-wind integ. conc. (ug/m2) at DIST
      CY/Q     CY normalized by emission, times 10**6 (s/m2 10**(-6))
      ARCMAX   Max. conc. (ug/m3) at DIST
      ARCMAX/Q Conc normalized by emission, times 10**9 (s/m3 10**(-9))
      HS       Tracer release height (m)
      NUARC    Number of arcs for an experiment
      D1-D3    Distance (km) to arcs for an experiment


Notes on parameters:
--------------------
Measured values of SIGV and SIGW are considered more reliable than those
deduced from profile measurements.

The values of T2, W10 etc. have been formed as the average of 6 10-minute
averages.

HF, UST and L have been determined using measurements from a met tower
(two levels of temperature, one level of wind speed: T2, T40 and W10).
A roughness length of 0.6 m has been assumed.
For the processing, the subroutine PBL_1 of the software library
PBL_MET (described by Sozzi and Fraternali, 1994) has been used.

Turner stability class is computed according to the original paper by Turner:
J. Appl. Met., (1964) 3., 83.


Changes compared to the data set distributed for the Manno workshop:
--------------------------------------------------------------------
The following parameters have been included:
W60, T120, NCLD, CEIL, CY/Q, ARCMAX/Q

The parameter P (Pasquill class) has been omitted, and instead a Turner
stability class has been included.

The derived values of UST, L and HF have been determined using a standard
preprocessor, whereas they were formerly determined by a manual method.
```

Table 7 The full contents of files from Copenhagen.

MET_CPH.DAT

Revised data set for Copenhagen. Version from May 94, based on 6 10-min values.

YR	MO	DY	HRS	HRE	W10	W60	W115	T2	T40	T120	SIGV	SIGW	ZI	NCLD	CEIL	UST	L	HF	TURNER
78	09	20	1317	1417	2.1	999.0	3.4	285.5	284.2	283.4	0.98	0.83	1980	7	7500	.36	-37	116.	3
78	09	26	1140	1240	4.9	999.0	10.6	288.7	287.5	286.6	1.39	1.07	1920	6	6000	.73	-292	120.	4
78	10	19	1213	1313	2.3	999.0	5.0	285.6	284.6	283.9	0.85	0.68	1120	5	480	.38	-71	69.	4
78	11	03	1320	1420	2.5	999.0	4.6	284.8	284.0	283.3	0.47	0.47	390	4	3600	.38	-133	39.	3
78	11	09	1330	1430	3.1	999.0	6.7	285.5	284.9	284.2	0.77	0.71	820	7	750	.45	-444	19.	4
79	04	30	1302	1402	7.2	11.7	13.2	280.1	278.6	277.6	2.26	1.33	1300	5	750	1.05	-432	242.	4
79	06	27	1245	1345	4.1	7.2	7.6	292.2	290.4	289.5	1.61	0.87	1850	6	2400	.64	-104	227.	3
79	07	06	1250	1350	4.2	10.6	9.4	293.8	290.9	289.9	1.35	0.72	810	5	6000	.69	-56	530.	3
79	07	19	1215	1315	5.1	9.0	10.5	289.8	288.5	287.5	1.71	0.98	2090	6	600	.75	-289	134.	4

SF6_CPH.DAT

YR	MO	DY	HRS	HRE	DIST	Q	SIGY	CY	CY/Q	ARCMAX	ARCMAX/Q	HS
78	09	20	1317	1417	1.90	3.2	254	2074	648.	3.360	1050.0	115
78	09	20	1317	1417	3.70	3.2	444	739	231.	0.685	214.1	115
78	09	26	1140	1240	2.10	3.2	329	1722	538.	3.152	985.0	115
78	09	26	1140	1240	4.20	3.2	438	944	295.	0.906	283.1	115
78	10	19	1213	1313	1.90	3.2	184	2624	820.	5.226	1633.1	115
78	10	19	1213	1313	3.70	3.2	283	1990	622.	2.544	795.0	115
78	10	19	1213	1313	5.40	3.2	404	1376	430.	1.203	375.9	115
78	11	03	1320	1420	4.00	2.3	301	2682	1166.	3.613	1570.9	115
78	11	09	1330	1430	2.10	3.2	185	2150	672.	3.875	1210.9	115
78	11	09	1330	1430	4.20	3.2	279	1869	584.	2.317	724.1	115
78	11	09	1330	1430	6.10	3.2	376	1590	497.	1.520	475.0	115
79	04	30	1302	1342	2.00	3.1	-999	1228	396.	2.306	743.9	115
79	04	30	1302	1342	4.20	3.1	-999	688	222.	1.045	337.1	115
79	04	30	1302	1342	5.90	3.1	-999	567	183.	0.539	173.9	115
79	06	27	1245	1345	2.00	2.4	290	1608	670.	2.275	947.9	115
79	06	27	1245	1345	4.10	2.4	595	780	325.	0.629	262.1	115
79	06	27	1245	1345	5.30	2.4	786	535	223.	0.276	115.0	115
79	07	06	1250	1350	1.90	3.0	190	1248	416.	2.928	976.0	115
79	07	06	1250	1350	3.60	3.0	402	606	202.	0.792	264.0	115
79	07	06	1250	1350	5.30	3.0	580	456	152.	0.294	98.0	115
79	07	19	1215	1318	2.10	3.3	236	1511	458.	2.812	852.1	115
79	07	19	1215	1318	4.20	3.3	460	1026	311.	0.878	266.1	115
79	07	19	1215	1318	6.00	3.3	623	855	259.	0.653	197.9	115

DIST_C.DAT

YR	MO	DY	HRE	NUARC	D1	D2	D3
78	09	20	1417	2	1.90	3.70	
78	09	26	1240	2	2.10	4.20	
78	10	19	1313	3	1.90	3.70	5.40
78	11	03	1420	1	4.00		
78	11	09	1430	3	2.10	4.20	6.10
79	04	30	1402	3	2.00	4.20	5.90
79	06	27	1345	3	2.00	4.10	5.30
79	07	06	1350	3	1.90	3.60	5.30
79	07	19	1318	3	2.10	4.20	6.00

5.3 Lillestrøm data

5.3.1 Experimental set-up

The tracer experiments of concern here took place in the town of Lillestrøm (near Oslo), Norway in 1987. They were performed by the Norwegian Institute of Air Research (NILU) which has put the data at our disposal.
A detailed description is given by Haugsbakk and Tønnesen (1989; available on request). A shorter description is found in the paper by Grønskei (1990).

Release from a 36 m mast. 15-minute sampling

The experiments were carried out in a flat residential area with 6-10 m high buildings and trees. A tracer system was used in which SF_6 was released from a mast 36 m above the ground. Each experiment consisted of two sequential 15-min periods. Thus, the sampling period is shorter than for the other experiments considered at the workshop.

The meteorological measurements were carried out along the 36 m high mast.

Sonic anemometer measurements were processed to give 10 min average values for wind speed and wind directions at the 10 m level. Further, covariances were determined between velocity components, and between velocity components and temperature fluctuations.

Norwegian winter: Snow-covered ground, low sun

The temperature during the tracer experiments was low ($\approx$ - 20° Celsius), and the ground was snow-covered. The sun was above the horizon, but at a very low angle. The surface roughness was about 0.5 m.

Generally, the vertical temperature profiles in the lowest 100 m showed an inversion (Haugsbakk and Tønnesen, 1989).

For all runs during the experimental campaign, the crosswind profiles of tracer concentrations were well determined, thus making a relatively accurate estimate of crosswind integrated concentration possible. The maximum concentrations given in the data set is the highest observed concentration along each arc.

Geographical coordinates for the position of release are: latitude 59.889 N, longitude 11.051 E; the height of terrain is 110 m a.m.s.l.

5.3.2 Points to be noted

Note that for Lillestrøm data, the averaging period is only 15 minutes for the tracer data. Concentration averages taken over longer time will tend to be smaller than those registered, due to meandering.

There was generally very light wind during the experiments.

u_* was recorded as zero for the experiment with the highest concentrations.

In the data set, stability category has been computed based upon the original method by Turner (1964). This is consistent with the method used for the other data sets, but it does not very well take account of Norwegian winter conditions with snow-covered ground.

Table 8 Contents of the file PAR_LIL.TXT

```
      Parameters supplied in the distributed files from Lillestrom
      ============================================================

   Note: the last observation in the data set was performed in
   conditions with VERY low wind speed (0.2 m/s at a height of 36 m).
   L was not determined.


Basic parameters:
      YR      Year
      MO      Month
      DY      Day
      HRS     Time start of period, (GMT+1). Example: 1317 means 13.17
      HRE     Time end of period, (GMT+1)

Observed meteorological parameters:
      WS10    Wind speed at  10 m sonic-anemometer (m/s)
      WS36    Wind speed at  36 m cup-anemometer (m/s); four values are missing, i.e. -99.9
      T10     Temperature at  10 m (deg. K)
      DT      Temperature difference 36-10 m (deg. K)
      SIGV    Sigma of cross-wind speed at 10 m, sonic-anemometer (m/s)
      SIGW    Sigma of vertical velocity at 10 m, sonic-anemometer (m/s)
      ZI      Mixing height  -  missing, i.e. -999
      NCLD    Fractional cloud cover (EIGHTS!)
      CEIL    Height to lowest cloud (m); -1=unlimited
      UST     Friction velocity at 10 m, sonic anemometer (m/s)
      L       Monin-Obukhov length, sonic anemometer (m)

Derived meteorological parameters:

      TURNER  Turner stability class according to Turner (1964)

Tracer release parameters:
      DIST    Distance (km) to arc of monitors
      Q       Emission rate (g/s)
      SIGY    Sigma-y (m) at DIST
      CY      Cross-wind integ. conc. (ug/m2) at DIST
      CY/Q    CY normalized by emission, times 10**6 (s/m2 10**(-6))
      ARCMAX  Max. conc. (ug/m3) at DIST
      ARCMAX/Q Conc normalized by emission, times 10**9 (s/m3 10**(-9))
      HS      Tracer release height (m)
      NUARC   Number of arcs for an experiment
      D1-D3   Distance (km) to arcs for an experiment


Notes on parameters:
--------------------
Turner stability class is computed according to the original paper by Turner:
J. Appl. Met., (1964) 3., 83 (thus, there is no provision for the snow
cover on the ground).


Changes compared to the data set distributed for the Manno workshop:
--------------------------------------------------------------------
The following parameters have been included:
NCLD, CEIL, CY/Q, ARCMAX/Q, DT

The parameter P (Pasquill class) has been omitted, and instead a Turner
stability class has been included.

Four values of W36 are now considered missing.
```

Table 9 The full contents of data files from Lillestrøm.

MET_LIL.DAT

YR	MO	DY	HRS	HRE	W10	W36	T10	DT	SIGV	SIGW	ZI	NCLD	CEIL	UST	L	TURNER
87	01	10	930	945	2.1	4.4	247.7	-0.1	0.62	0.47	-999	0	-1	0.374	235	4
87	01	10	945	1000	1.7	3.6	247.7	-0.2	0.54	0.42	-999	0	-1	0.283	130	3
87	01	12	930	945	1.7	3.0	252.7	1.3	0.32	0.22	-999	0	-1	0.173	27	3
87	01	12	945	1000	1.6	3.1	252.7	1.3	0.32	0.22	-999	0	-1	0.173	41	3
87	01	17	1000	1015	0.9	-99.9	252.0	1.5	0.24	0.10	-999	0	-1	0.224	-1601	3
87	01	17	1015	1030	0.5	-99.9	252.0	1.3	0.17	0.10	-999	0	-1	0.100	188	3
87	02	09	1000	1015	0.5	-99.9	260.4	0.2	0.17	0.17	-999	4	3050	0.100	-8.1	3
87	02	09	1015	1030	0.4	-99.9	260.4	0.5	0.22	0.14	-999	4	3050	0.000	-9999	3

SF6_LIL.DAT

YR	MO	DY	HRS	HRE	DIST	Q	SIGY	CY	CY/Q	ARCMAX	ARCMAX/Q	HS
87	01	10	930	945	0.160	0.102	65	1082	10608.	7.6	74510.	36
87	01	10	930	945	0.490	0.102	129	1029	10088.	4.8	47059.	36
87	01	10	930	945	0.810	0.102	144	1049	10284.	3.7	36275.	36
87	01	10	945	1000	0.140	0.102	54	1161	11382.	8.3	81373.	36
87	01	10	945	1000	0.440	0.102	132	1337	13108.	5.2	50980.	36
87	01	10	945	1000	0.820	0.102	237	1486	14569.	3.4	33333.	36
87	01	12	930	945	0.150	0.102	49	1060	10392.	11.1	108824.	36
87	01	12	930	945	0.300	0.102	68	437	4284.	2.7	26471.	36
87	01	12	930	945	0.460	0.102	115	633	6206.	2.3	22549.	36
87	01	12	945	1000	0.160	0.102	52	988	9686.	8.6	84314.	36
87	01	12	945	1000	0.300	0.102	58	741	7265.	5.8	56863.	36
87	01	12	945	1000	0.440	0.102	113	774	7588.	2.8	27451.	36
87	01	17	1000	1015	0.150	0.102	41	637	6245.	6.9	67647.	36
87	01	17	1000	1015	0.470	0.102	98	484	4745.	3.3	32353.	36
87	01	17	1000	1015	0.900	0.102	134	2732	26784.	7.6	74510.	36
87	01	17	1015	1030	0.150	0.102	69	256	2510.	1.7	16667.	36
87	01	17	1015	1030	0.490	0.102	79	1327	13010.	6.2	60784.	36
87	01	17	1015	1030	0.900	0.102	131	1138	11157.	5.8	56863.	36
87	02	09	1000	1015	0.190	0.102	55	2342	22961.	29.6	290196.	36
87	02	09	1000	1015	0.410	0.102	95	3411	33441.	9.7	95098.	36
87	02	09	1015	1030	0.190	0.102	59	4770	46765.	45.8	449020.	36
87	02	09	1015	1030	0.430	0.102	98	5328	52235.	20.0	196078.	36

DIST_L.DAT

YR	MO	DY	HRE	NUARC	D1	D2	D3
87	01	10	945	3	0.160	0.490	0.810
87	01	10	1000	3	0.140	0.440	0.820
87	01	12	945	3	0.150	0.300	0.460
87	01	12	1000	3	0.160	0.300	0.440
87	01	17	1015	3	0.150	0.470	0.900
87	01	17	1030	3	0.150	0.490	0.900
87	02	09	1015	2	0.190	0.410	
87	02	09	1030	2	0.190	0.430	

5.4 Indianapolis

5.4.1 Experimental set-up

Release from an 84 m stack. 170 one-hour samples

The EPRI Indianapolis field study involved SF_6 tracer releases from the 83.8 m stack (with diameter 4.72 m) at the Perry K power plant in Indianapolis, Indiana, USA. The geographic coordinates of this stack are UTM-N 4401.59 km (39.8° latitude) and UTM-E 571.40 km (86.2° longitude). The elevation of the plant is 214 m. 170 hours of tracer data are available from September and October, 1985, and represent all stability classes and most wind speed ranges. Data were taken in 8 or 9 hour blocks. There are a total of 19 such blocks in the Indianapolis dataset. During a test day, trace gas emission and stack measurements began one to two hours before the field sampling began.

Hoosier Dome and other buildings

The 83.8 m stack at the Perry K plant is located in a typical industrial/commercial/urban complex with many buildings within one or two kilometres of the stack. For example, the Hoosier Dome sports stadium is a few hundred meters to the east. Concerning potential influence by this building, Steve Hanna writes:

"Our analyses of the data (Hanna and Chang; 1991, 1993) and an independent wind tunnel study have suggested that the Hoosier Dome and the other buildings do not influence the plume, which tended to rise a hundred meters or more above the stack top most of the time. As a result, our modeling exercises have ignored the effects of nearby individual buildings. We specify a surface roughness length of 1 m in order to parameterize the overall effect of the buildings on the boundary layer. We also specify a "minimum Monin-Obukhov length, L" of 50 m during stable conditions for the urban area in order to account for the fact that the urban boundary layer does not stabilize significantly due to the mechanical mixing generated by the buildings and due to the anthropogenic heating in the urban area (Hanna and Chang, 1991). If other modelers would like to directly model the influence of the buildings or other aspects of the urban area, they can find the buildings' locations in the TRC (1986) report."

The EPRI report "Urban Power Plant Plume Studies", EPRI EA-5468, contains the following description of the urban meteorological site (D on the map):

"The urban site was located at the northwest corner of Ohio and Senate Streets, adjacent to a State employees' parking lot. This area was surrounded by large buildings and received a heavy volume of traffic. The site was located approximately 1.5 km northeast of the Perry-K plant."

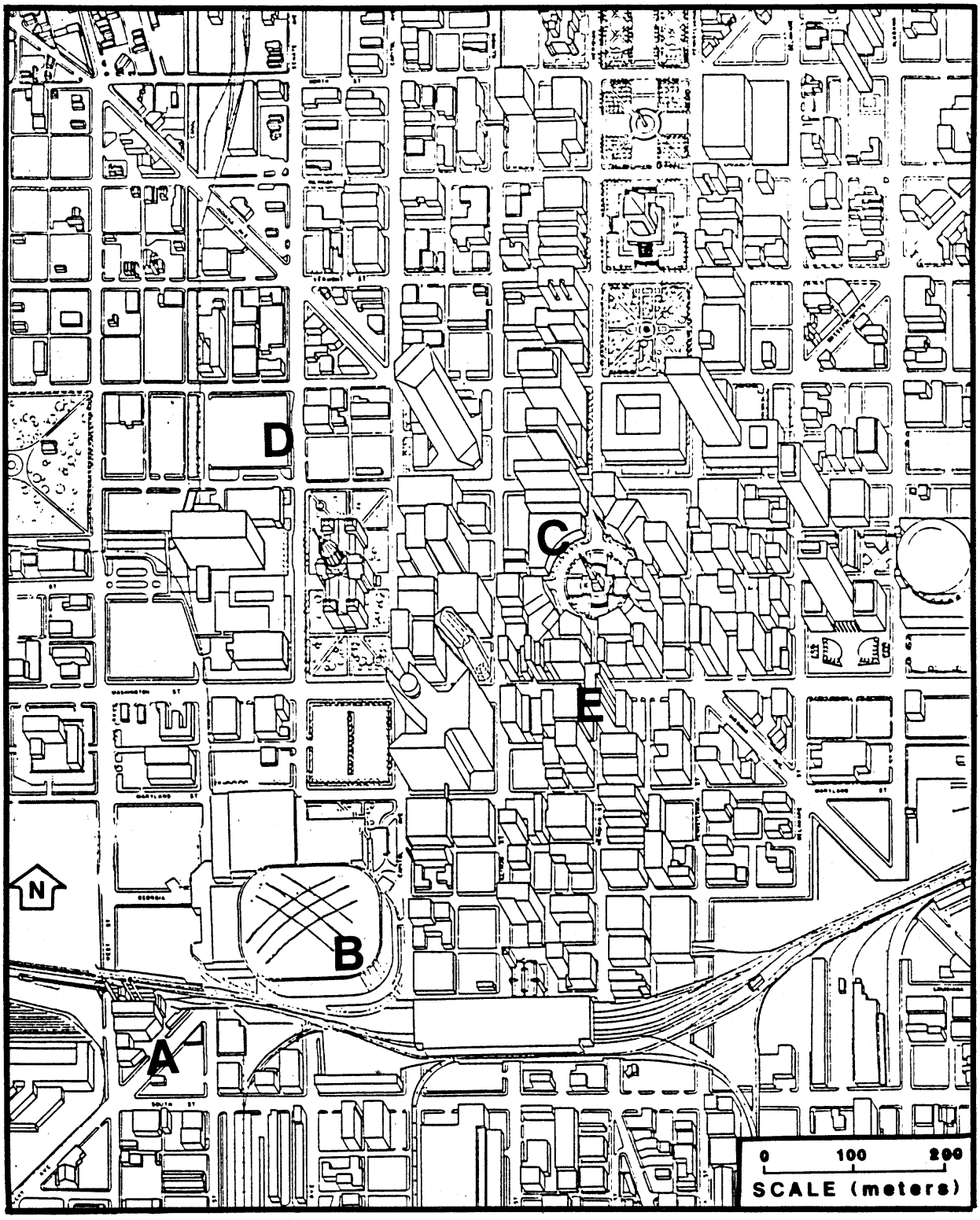


Figure 4 Map showing the relationship of the Perry-K Station (A), the Hoosier Dome Sport Stadium (B) and the central Indianapolis business district (C). The downtown surface meteorological site is located at (D) and the "bank tower" site was on the top of the building at (E). The horizontal and vertical scales are equal (from TRC, 1986).

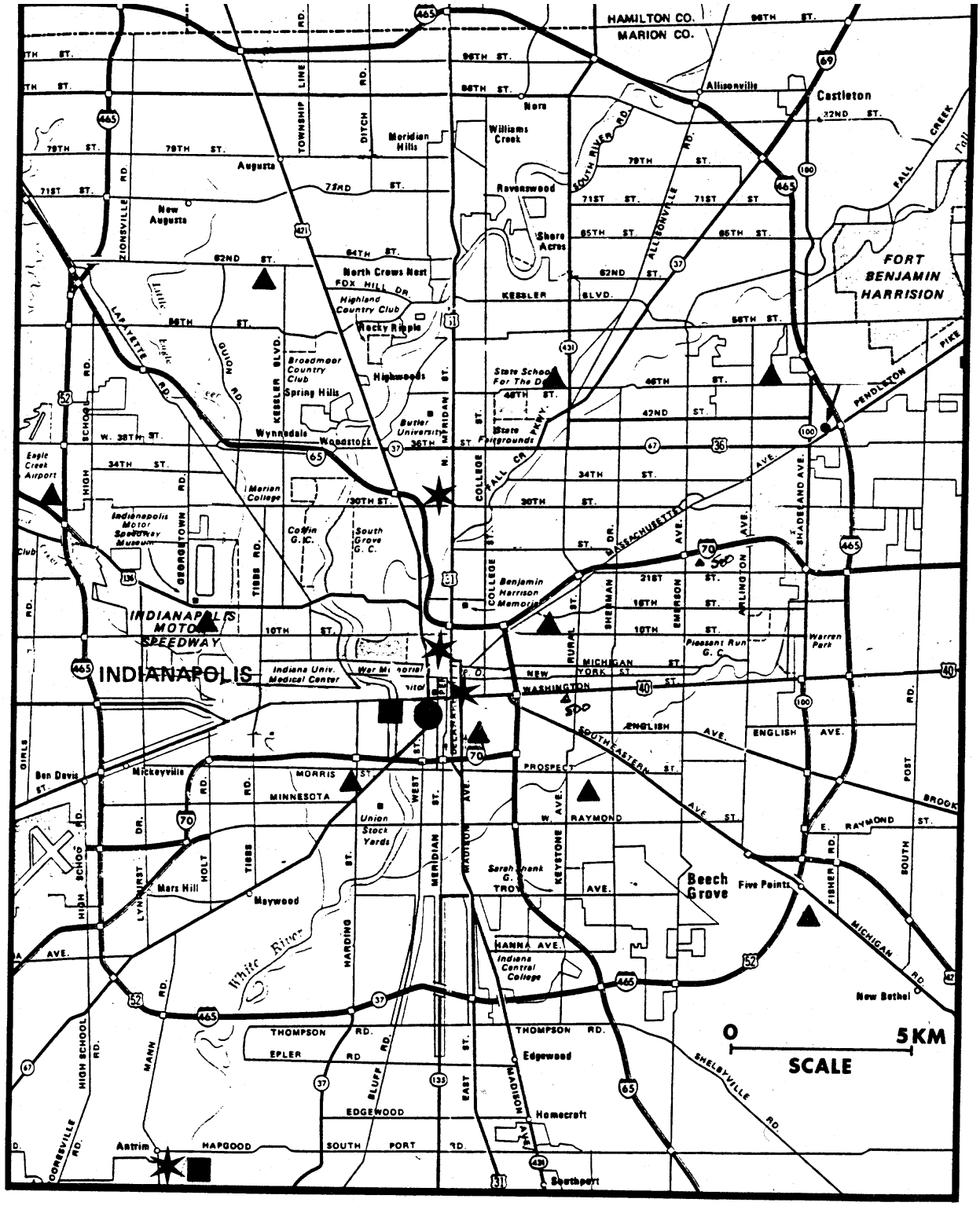


Figure 5 Location of meteorological sensors. The filled circle is the Perry K power station. The filled triangles are measurements of surface temperature. The asterisks are the primary meteorological sites. The filled square is the rawinsonde launch site (from TRC, 1986).

5.4.2 Meteorological data

Meteorological observations were taken from a 94 m height at the top of a building in the middle of the urban area, and from three 10 m

towers in urban, suburban, and rural locations (at the urban site the measuring height for some variables was 11 m, however). Standard National Weather Source (NWS) observations were available from the local airport. In addition, vertical profiles were taken by minisondes and acoustic sounders.

5.4.3 Tracer data

Concentrations were observed on a network of about 160 ground-level monitors on arcs at distances ranging from 0.25 to 12.0 km from the stack. Vertical cross-sections of the plume were made by a lidar a few hundred meters downwind of the stack. The design of the field experiment was similar to earlier EPRI field experiments at the Kincaid and Bull Run power plants.

As in the case of Kincaid, a quality indicator was assigned to the arc-wise maximum concentrations. A subjective numerical ranking of the quality of the data on that monitoring arc was undertaken (by Steve Hanna). It has been determined by studying the ground level SF_6 observation patterns during each hour and assigning a quality index ranging from 0 to 3 to each monitoring arc. Monitoring arcs are recommended to be used in the model evaluation exercises only if their quality indicator is 2 or 3.

5.4.4 Data files

Concentration data are summarized in the SF6_IND.DAT data file where a separate line of data is given for each monitoring arc for each hour. The hour notation refers to the one hour period *ending* at that time. The file INDI_description.doc provides a description of data which is more detailed than the one presented above..

The following files are supplied in the `Field_data\Ind` folder:

Information-carrying files

README.TXT Gives an overview of the material.
INDI_description.doc A brief description of the available data sets for the Indianapolis study.
PAR_INDI.TXT Can be regarded as an Appendix to the description in INDI_description.doc. Contains details on missing parameters etc.
XY_DOC.TXT Describes format of files with detailed concentrations for each hour. There are 170 such files located in the subfolder XY_conc.
SOND_DOC.TXT Describes the format of upper air data (file INDY30.DAT).

Data files

INDI.DAT and its equivalent, INDI.XLS. INDI.DAT is in ASCII format. It contains mainly meteorological variables, but also includes information on emission. This file contains all information needed to model dispersion. It has very long lines (the record length is 542).
INDI.XLS contains the same information as INDI.DAT, but in EXCEL format.
SF6_IND.DAT Contains SF6 measurements. Modellers need normally not use this file. If they want to compare model results to measurements,

it is easiest to use the program COMBINE_INDI, as described in Chapter 6.

85101123.DAT etc. 170 files in this format are provided with detailed concentration measurements, one for each hour. These data files are located in the subfolder XY_conc. They are not necessary for normal use of the Model Validation Kit..

INDY30.dat Radiosonde data from an urban and a rural radiosonde.

5.4.5 Additional information

A full description of the Indianapolis field study is given by TRC (1986) and some results of analysis are given by Hanna and Chang (1991, 1993). The data included here represents a subset of the full data set, which includes many magnetic tapes full of lidar data and fast-response turbulence data.

The data have been supplied by the EPRI "Atmospheric Science Data Center" operated by Earth Tech, USA. The persons involved were Steve Hanna and Joe Chang. Further preparation of the data was performed by H.R. Olesen, National Environmental Research Institute, Denmark.

5.4.6 Points to be noted

There are missing values for a number of variables. Details are listed in the file PAR_INDI.DAT. To most modellers, the missing values will not be any problem, except possibly for the case of September 29, where winds from the 94 m level are missing.

Further, note that there is a mixing height of 0 m for several night-time hours (September 21, 28 and 29). Rawinsonde showed a ground-based inversion on the hours in question.

Table 10 Sample from SF6_IND.DAT and one of the files with detailed concentrations, 85091611.DAT

The file INDI.DAT (or INDI.XLS) has too long records to display in a table.

SF6_IND.DAT

YR MO DY HR	DIST. (km)	TOTAL SAMPLE	NONZERO SAMPLE	ARC MAX (PPT)	ARC MAX (nG/M**3)	Emission rate (g/s)	ARCMAX / Q	QUALITY INDEX	AZIMUTH TO MAX	CY (uG/M**2)	SIGY (M)
YR MO DY HR	DIST	N_TOT	NONZERO	ARCMAXPP	ARCMAXNG	Q	C_OBS	QUAL	AZMAX	CY	SIGY
85 9 16 11	0.25	1	1	7.0	42.6	4.94	8.6	0	65.3	-999.0	-999.0
85 9 16 11	0.50	8	4	155.0	942.4	4.94	190.8	3	84.9	309.5	101.5
85 9 16 11	0.75	4	3	84.0	510.7	4.94	103.4	1	93.1	-999.0	-999.0
85 9 16 11	1.00	6	3	206.0	1252.5	4.94	253.5	1	105.3	-999.0	-999.0
85 9 16 11	1.50	11	5	444.0	2699.5	4.94	546.5	2	91.8	1595.8	391.9
85 9 16 11	2.00	17	4	55.0	334.4	4.94	67.7	1	79.6	465.6	557.0
85 9 16 11	3.00	21	5	467.0	2839.3	4.94	574.8	2	91.5	2692.3	418.6
85 9 16 11	4.00	13	4	258.0	1568.6	4.94	317.5	1	94.5	1398.2	655.7
85 9 16 11	6.00	20	7	200.0	1216.0	4.94	246.2	3	99.0	3005.9	1121.8
85 9 16 12	0.25	5	3	110.0	666.8	4.94	135.0	1	107.9	-999.0	-999.0
85 9 16 12	0.50	8	4	337.0	2042.8	4.94	413.5	2	84.9	833.6	147.1
85 9 16 12	0.75	13	6	458.0	2776.3	4.94	562.0	2	111.9	1209.1	237.1
85 9 16 12	1.00	12	9	327.0	1982.2	4.94	401.3	2	105.3	1362.3	296.3
85 9 16 12	1.50	15	6	150.0	909.3	4.94	184.1	2	83.9	1068.1	340.6

85091611.DAT

X	Y	Conc	Dist
0.129	0.280	7.	0.310
0.042	0.470	155.	0.470
0.170	0.440	9.	0.470
0.228	0.330	0.	0.400
0.383	0.240	0.	0.450
0.417	0.120	0.	0.430
-0.387	0.320	0.	0.500
-0.310	0.450	18.	0.550
-0.101	0.470	143.	0.480
-0.039	0.720	84.	0.720
0.410	0.520	0.	0.660

6 Step by step instructions

After a few general comments, a step-by-step explanation on the processing of the Kincaid data set follows in Section 6.2 – which is quite long.

Structure of this chapter

Processing of the other three data sets follow the same principles, but with some deviations. Such deviations are explained in the subsequent three sections, one for each of the three remaining data sets. Indianapolis data are treated similarly to Kincaid data, while Copenhagen and Lillestrom data should be processed a bit differently.

Outcome from the tools

Typically, when the results of a model run are processed with the enclosed tools, the outcome is the following products:

(1) A file with statistics (FB, NMSE etc.)

(2) A scatter plot (c_{mod} vs. c_{obs})

(3) A quantile-quantile plot (cumulative distribution)

(4) Plots for diagnosing model behaviour

- *(4a)* Box plots analyzing the ratio c_{mod}/c_{obs} in terms of physical parameters.
- *(4b)* Box plots analyzing the behaviour of c_{obs}
- *(4c)* Box plots analyzing the behaviour of c_{mod}

The file with statistics is generated using the BOOT program, while the plots can be generated using RESIDUAL and SIGPLOT.

All of the required programs and files are assembled in the **`Tools`** folder on the CD. Thus, for convenience, the Tools folder includes a copy of the BOOT program as well as of the SIGPLOT program. These two utilities can also be found in the folders **`BOOT`** and **`SIGPLOT`**, where they are accompanied by user manuals and sample files.

The subsequent sections describe in detail the procedure for processing of Kincaid data.

6.1 File naming conventions; conventions for the example

Avoid spaces in file names

Avoid using file names with spaces in their name, as some of the utilities will not work.

8-character limit for files used by SIGPLOT

Furthermore, the SIGPLOT utility that can optionally be used for graphical analyses, will not recognise names of files or folders that are longer than 8 characters. This is because SIGPLOT is quite old. However, when you work with SIGPLOT, you will need only relative path names, so there is no problem in locating all of your work in a folder with a long, complicated name, as long as you stick to short, relative names in your 'conversation' with SIGPLOT (a detailed example follows).

Format changes since previous version of the Model Validation Kit

If you have used a previous version of the Model Validation Kit, please note there that have been a few changes in the format of the various files. Thus, some files which previously were without header now have one (e.g. 'Modelled.xxx'). Details on changes can be found in Chapter 12.

Assumption about C:\MvK\Tools

In the following, for the example, we will assume that you have copied the **`Tools`** folder of the Model Validation Kit to the folder C:\MvK\Tools on your computer.

Further, we assume that you keep your model results in a subfolder of that folder, namely C:\MvK\Tools\Run1 .

Conventions for file types

In the subsequent explanation the following conventions will be used for file type names:

INP	Input for BOOTW and RESIDUAL.
BOO	Output from BOOTW.
DAT	Data file that can be plotted using SIGPLOT. Some of these DAT files can be generated by RESIDUAL.
QUA	Data file suitable for generating quantile-quantile plots (generated by RESIDUAL).
INQ	Template file for SIGPLOT.
TEK	Picture in Tektronix format (can be shown on the screen using Tekplot).
PIC	Identical to TEK format (picture in Tektronix format).

Some required input files for generating the plots described on the subsequent pages are included in the **`Tools`** folder. Thus, there are 18 *template files* used by SIGPLOT (extension .INQ). They determine the layout of plots (Table 18 on page 52 provides an overview of the files).

6.2 Kincaid

In order to obtain results that are comparable to those of other groups, you should perform an analysis, where you adhere to the following protocol:

- analyze the behaviour of *normalized* concentrations, ARCMAX/Q, using the same units as in SF6_KIN.DAT;
- conduct an analysis for data with the quality indicator QUAL equal to 3 (the most reliable data), since this is what other modellers have done (the fact that c_{obs} is never zero for data of quality 3 should be kept in mind; this leads to a bias). You can also perform an analysis where you include data of quality 2;
- use your own preprocessor if possible;
- however, use the observed mixing height.

The details are explained in the following.

6.2.1 Instructions on modelling

File with results of model calculations (Modelled.kin)

Perform model calculations for the 12 distances represented in the Kincaid data set (0.5, 1, 2, 3, 5, 7, 10, 15, 20, 30, 40, 50 km). Dump your output in a file. Here, we will call the file Modelled.kin (you may use another name).

The format of Modelled.kin should be the following:

- There is a one-line heading;
- There should be six columns (or more), separated by blanks (the values are read using free-format input);
- There *must* be a line for all 2052 arc-hours (171 hours times 12 distances). The distances must be those indicated above.

An example of the first thirteen lines of a Modelled.kin file is shown below. The date and time is indicated, then the distance, and finally the normalised arcwise maximum concentration, ARCMAX/Q.

```
YR MO DY HR DIST  ARCMAX/Q
80  4 20 14   0.5    0.0
80  4 20 14   1.0   50.4
80  4 20 14   2.0  134.0
80  4 20 14   3.0  107.1
80  4 20 14   5.0   57.7
80  4 20 14   7.0   36.9
80  4 20 14  10.0   23.8
80  4 20 14  15.0   15.9
80  4 20 14  20.0   12.5
80  4 20 14  30.0    9.0
80  4 20 14  40.0    7.1
80  4 20 14  50.0    5.9
```

Please note that the units for ARCMAX/Q should be $s/m^3 \bullet 10^{-9}$ (corresponding to the units used in the file with SF_6 data, SF6_KIN.DAT).

Cross-wind integrated concentrations are *not* included in the present version of the Kincaid data set as they are difficult to assess with confidence (it is not impossible to do, but requires considerable work with quality control – the subject is discussed by Olesen (2001).

6.2.2 Matching model results with observed data

The Model Validation Kit contains a utility for combining model results and observed data, resulting in a file that can be directly used as input to the statistical model evaluation program, BOOT.

Utility to combine model results with observations (Combine_Kin)

The utility (*Combine_kin.exe*) allows selection according to quality level, so that either data with a quality indicator of 2 or 3 are considered (586 observations), or exclusively data with a quality indicator of 3 (338 observations).

Before using the tool, you must edit the file *Combine_Kin.ini*. This is a plain text file, which tells the program where it can find the model results, and where it should place the files that it generates. The file is reproduced in *Table 11*.

Table 11 The file *Combine_Kin.ini*. The user should adjust the three names indicated in yellow to suit his needs. In the example here, the user has placed the utilities in C:\MvK\Tools, while his model results are in C:\MvK\Tools\Run1

```
[Comments: General]
This file contains options for the programme Combine_kin.exe

Capitalisation: Keywords always have the first letter capitalised.


[Files]
Results_path=C:\MvK\Tools\Run1
'   Example: C:\xxx
'   This is the path where the program expects to find the file with model results.
'   The same folder is used to store the output files resulting from the program.

Results_file=modelled.kin
'   Example: modelled.dat
'   File with model results. Indicate only the file name, not the path.

Master_path=C:\MvK\Tools
'   Example: C:\Master
' This is the path where the program expects to find the files MASTER.KIN
' and KIN.BTT (supplied with the Model Validation Kit).
```

The utility produces as well a file that can be used as input for BOOT, as a file that can be used for scatter plots with the SIGPLOT.

The steps for running the utility are as follows:

- Prepare a file with modelled data, e.g. MODELLED.KIN
- Edit Combine_Kin.ini to reflect the correct path and file names.
- Double-click the icon for Combine_Kin.exe
- Follow the instructions (you are asked for a title).

The output consists of two files:

- a file of type .INP (e.g. KI3.inp, designed as input to BOOT and RESIDUAL).
- a file of type .DAT (e.g. KISCAT3.DAT, designed for SIGPLOT scatter plot).

The file names depend on the user-prescribed quality level. Thus, KI**2**.inp contains data of quality 2 and 3, while KI**3**.inp contains data exclusively of quality 3.

The procedure for generating statistical analyses and plots is explained in the following sections.

6.2.3 Analysing data with BOOT

Capabilities of BOOT

The BOOT package is capable of computing performance measures such as the Fractional Bias (FB), the Normalised Mean Square Error (NMSE), the Geometric Mean Bias (MG), the Geometric Variance (VG), the fraction within a factor of 2 (FAC2), the Measure of Effectiveness (MOE), as well as several others. (FB and MOE are in fact closely related).

Note that a useful extension to FB and MG has been implemented in the current BOOT package. FB is of limited value because overpredictions and underpredictions compensate each other. However, FB and MG can be separated into overpredicting and underpredicting components. Thus, FB_{fn} (false negative) only considers underpredictions, while FB_{fp} only considers overpredictions.

Bootstrap resampling is used to estimate the confidence limits of a performance measure – hence the name BOOT of the package. Consult the BOOT User's Guide for a detailed discussion of the interpretation of results from BOOT. The User's Guide (Chang and Hanna, 2005) is part of the Model Validation Kit.

(1): File with statistics

Proceed as follows in order to generate a file containing statistics for data of quality 3 with the use of BOOT.

As noted above, we assume that the tools reside in C:\MvK\Tools.

BOOT can be launched in various ways. E.g., you can use Explorer to show C:\MvK\Tools and then double-click on the icon for BOOT.

Alternatively (assuming some familiarity with DOS), BOOT can also be launched by these steps:

- Open a Command Prompt window (explained in Section 6.2.5)

Table 12 Dialogue when using the BOOT programme.

```
Name of input file:
Run1\ki3.inp

Name of output file:
Run1\ki3.boo

Select one from the following options:
(1) straight Co and Cp comparison
(4) consider ln(Co) and ln(Cp)
1

Use ASTM procedure? (y/<N>)
n

Print out original data? (y/<N>)
n

Use E- or F-format for mean, sigma, and bias? (<F>/e)
f

Calculate partial correlation? (y/<N>)
That is, the influence from a certain model is removed.
n

Do the bootstrap resampling? (<Y>/n)
y

Print out detailed information on confidence limits? (y/<N>)
n

Create files containing FB (with its 95% confidence limits) and NMSE that
can later be plotted? (<Y>/n)
n
Reading data
Calculating performance measures...
Start resampling procedure...
Computing c.l. of performance measures for each model...

Make another run? (y/<N>)
N
```

- Change to the folder where BOOT and the associated data files reside, using the CD command.
- Type BOOT to launch the program.

The latter option has the advantage that it is possible to automatize the procedure (see Section 6.5).

Table 12 shows an example of a dialogue with the BOOT programme, which results in a file with statistics, Ki3.boo. A central part of the resulting file is shown in *Table 13*.

Table 13 Table with statistics, which is a central part of the output file produced by BOOT.

```
Nominal (median) results          (No. of regimes =    1)
  MODEL      MEAN      SIGMA       BIAS       NMSE   CORR   FA2     FB      HIGH   2nd HIGH   PCOR
  C_OBS       54.      40.25       0.00       0.00  1.000  1.000  0.000      319.      225.    n/a
                        (FBfn=  0.000, FBfp=  0.000, MOEfn=  1.000, MOEfp=  1.000, FB=FBfn-FBfp)

  C_MOD       47.      45.48       6.88       1.24  0.146  0.547  0.135      256.      248.    n/a
                        (FBfn=  0.428, FBfp=  0.292, MOEfn=  0.600, MOEfp=  0.687, FB=FBfn-FBfp)
```

6.2.4 SIGPLOT: A tool for graphical analyses

Exploratory data analysis is a 'must'

When performing model evaluation, it is not sufficient to consider just statistical evaluation that produces some performance metrics. Rather, it is recommended that exploratory data analysis also be performed using graphical techniques.

SIGPLOT: capabilities and limitations

The Model Validation Kit includes some tools for such graphical analyses in the form of the SIGPLOT graphical package. The SIGPLOT package is offered as an option that is specifically tailored for model performance evaluation. The package can produce residual plots, where model residuals are depicted as a function of independent variables such as the downwind distance and time of day. However, SIGPLOT is an old software package. Thus, in order to use SIGPLOT, you will have to work in a DOS environment (as explained in the following).

Alternatives to SIGPLOT

More modern and interactive tools than the SIGPLOT package can certainly be used to achieve the same goals. For example, a potential alternative is to use Microsoft Excel for data handling and graphical analyses. Excel offers some very powerful tools for interactive data analysis. Nevertheless, Excel does not offer the specialised plots that SIGPLOT produces. The advantages of using SIGPLOT are that you will be able to produce residual and other types of specialised plots in a relatively standardised format, that the required utilities are already prepared, and that the procedures are described in detail here.

Reference information on SIGPLOT

There is reference information on SIGPLOT to be found in the SIGPLOT handbook and its addendum – see Chapter 7 for an introduction. In order to get started with SIGPLOT you do not need that information, but can just follow the instructions given here.

Overview of products from BOOT and SIGPLOT

As noted previously, the following products are a typical outcome when the results of a model run are processed:

(1) A file with statistics (FB, NMSE etc.)

(2) A scatter plot (c_{mod} vs. c_{obs})

(3) A quantile-quantile plot (cumulative distribution)

(4) Plots for diagnosing model behaviour

- *(4a)* Box plots analyzing the ratio c_{mod}/c_{obs} in terms of physical parameters.
- *(4b)* Box plots analyzing the behaviour of c_{obs}
- *(4c)* Box plots analyzing the behaviour of c_{mod}

BOOT was used to create the first product. Here, we will here explain how to create the remaining products.

6.2.5 Preparations to work with SIGPLOT

Preparing to work in a command-line environment

First, make a few preparations, so that SIGPLOT can be used in a convenient manner. You will have to work in a command line environment (DOS environment). You can ensure that the system can find the utilities of the Model Validation Kit, if you once and for all adjust the *Path* variable in your system environment.

In Windows 2000 or XP, follow the subsequent steps.

Redefine the 'Path' environment variable

Select *Start* > *Settings* > *Control Panel* > *System* , choose the *Advanced* tab, select *Environment variables*, in the panel with *System variables* choose *Path*, *Edit*. In the field *Variable value* you should edit the contents, so it ends with, e.g. **`;C:\MvK\Tools`** – namely, a semicolon followed by the location of the tools. After you have finished, the *Path* may look like this:

```
%SystemRoot%\system32;%SystemRoot%;C:\MvK\Tools
```

(the path may be longer, depending on your system).

You need to know a few things in order to work in a command line environment (DOS). First, you enter this environment by selecting

Use 'CMD' to open a command-line environment (DOS)

Start > *Run*, write *cmd*, and then press the Enter key.

You will need to use the command *cd* (Change Directory), and possibly *dir* (show Directory).

The Change Directory command

Write *cd..* (CD followed by two dots) to move up in the tree of folders. The command *cd* can also be used to move down to a branch. Thus, if your current folder is the root of C:, the command

cd mvk

will change the current folder to *C:\MvK*

6.2.6 Using SIGPLOT

(2): Scatter plot

We assume that you have used the utility Combine_kin.exe to produce KISCAT3.DAT as explained in section 6.2.2.

Next, create a scatter plot showing c_{mod} versus c_{obs}, by following the following steps.

Use *Start* > *Run*, write *cmd* to open a command-line environment.

Change directory with *cd* so your current folder is C:\MvK\Tools\Run1

Write *SIGPLOT* in order to run SIGPLOT.

You are asked for the name of a template file. Such a file is part of the Model Validation Kit. It is called Kiscat.inq, and it is located together with the other tools in C:\MvK\Tools. In response to the question you can write

..\kiscat.inq

where `..\` serves to indicate that in the tree of folders, the file is one level closer to the root.

The input data file is Kiscat3.dat (this file was created by Combine_kin.exe)

You are asked for the name of 'tektronix picture file' which is the resulting output file. Enter

kiscat3.tek

You can view the plot on the screen using the command Tekplot. Write

Tekplot kiscat3.tek

(You may have to enter the command twice – sometimes there is no reaction the first time). The Tektronix file format is typically not supported by modern Windows applications. Therefore, if you wish to produce a file that can be included in a report, you should convert the file to another format.

We recommend using the EPS format (Encapsulated PostScript); HPGL is a possible alternative, which is not recommended[1].

A file in EPS format can be produced by writing

ps kiscat3.tek

(PS is a utility in the `Tools` folder.) The result is kiscat3.eps. This file can be included in, e.g., a Word document.

The scatter plot produced has linear axes and there is an offset so that zero values are clearly displayed. The layout can be changed by changing the template file (Kiscat.inq); see the SIGPLOT User's guide and its addendum for details.

Table 14 displays the conversation described above.

[1] An alternative - not recommended - is HPGL format (HP Graphics Language). An eps file can be converted to HPGL by the command EPS2HP Kiscat3 (don't indicate the extension .eps).
You may receive an error message even if the conversion is successful. However, HPGL is a format which is typically *not* recognised by modern applications. A standard installation of MS Word does not recognise it; anyhow, it is possible to download an unsupported import filter for Word at the Microsoft web site (look for hpgl32.exe).

Table 14 Commands required to produce a scatter plot as described.

```
C:\MvK\Tools\Run1>sigplot

Type "sigplot nolabels" instead if you want to disable labelling.

Name of template file :
..\kiscat.inq

Name of input data file :
kiscat3.dat

Name of tektronix picture file :
kiscat3.tek

Plotted frame     1

C:\MvK\Tools\Run1>tekplot kiscat3.tek

C:\MvK\Tools\Run1>ps kiscat3

TekPS, version 2.0, (c) 1988 Arlindo da Silva.
       version 3.0, revised by J. Chang, SRC, June, 1993,
       to make the output comply with the encapsulated PostScript file format

kiscat3.tek ---> kiscat3.eps

working...done!
```

6.2.7 Creating Q-Q plots and box plots

(3): Q-Q plot

In order to create items (3) and (4) (Q-Q plots and various box plots), you will have to run the RESIDUAL utility several times to generate the necessary data files, and then create the plots with SIGPLOT.

Running Residual

As before, we assume that you are in a command line environment with C:\MvK\Tools\Run1 as your current folder. Write RESIDUAL on the command line in order to run the utility.

Table 15 shows a set of commands, pertinent to running Residual with Kincaid data.

Certain thresholds are indicated in order to assure that the ratio c_{mod}/c_{obs} lies in the interval [0.01, 100]. Furthermore, to make the values of the ratio less noisy, a filter value has been set to 15. This is suitable for Kincaid data, and many other modellers have used this value.

The procedures can be automatized

If you have to repeat such runs several times with slight variations, the task of running Residual becomes tedious, and you will probably feel a desire for some degree of automatition. You will find various hints on this in Section 6.5.

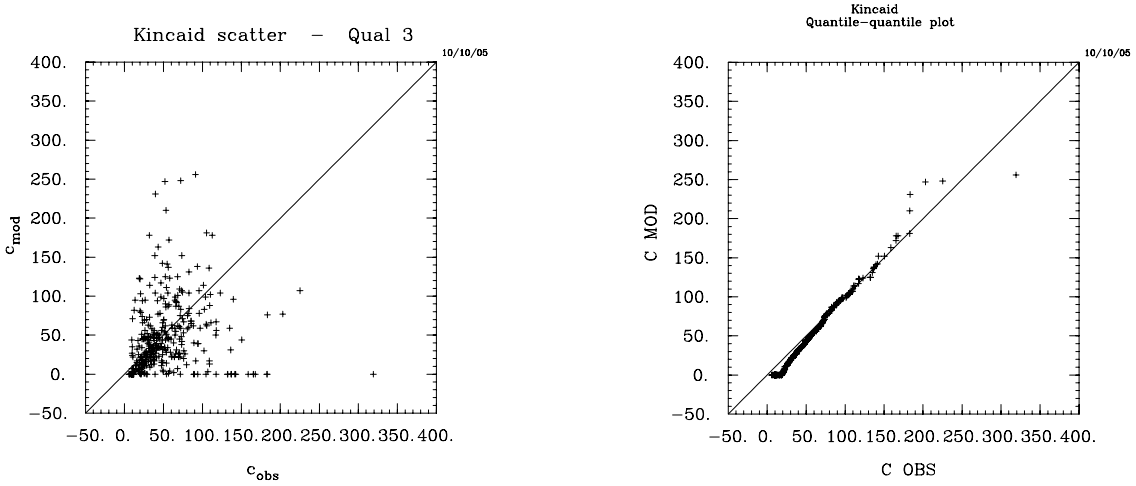


Figure 6 Sample plots produced with SIGPLOT using the template files KISCAT.INQ (a simple scatter plot) and KIQUA.INQ (a quantile-quantile plot.

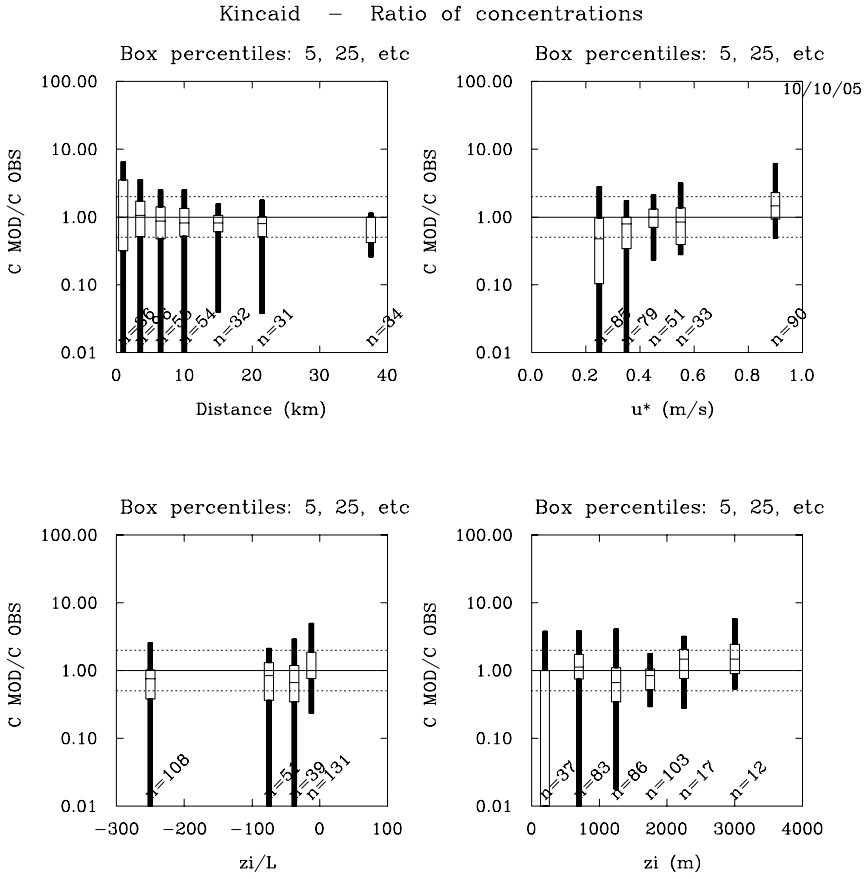


Figure 7 Sample plot produced with SIGPLOT using the template file KIRATIO.INQ.

Table 15 Commands entered in a dialogue with the RESIDUAL utility in order to prepare data files for both a quantile-quantile plot and a box plot of ratios.

```
C:\MvK\Tools\Run1>residual

Name of input file:     ki3.inp

Name of output file:    ki3ratio.dat

Following models are available, choose two models, i and j,
where the ratio of Model(i)/Model(j) will be analyzed against
the independent variables:
1 )  C_OBS
2 )  C_MOD
0 )  All 1's
Enter the two numbers, in order, between 0 and  2

2 1
Implement a lower threshold on the ratio (<Y>/n) ?
y
Enter the lower threshold on the ratio (e.g. 0.01)
0.01
Implement a upper threshold on the ratio (<Y>/n) ?
y
Enter the upper threshold on the ratio (e.g. 100.)
100
Do you wish to use extended capabilities of RESIDUW (<Y>/n) ?
y

Do you wish to impose a filter, so that the ratio C_MOD/C_OBS is
considered unity when both C_MOD and C_OBS are small ?

(This will remove noise, thus making it easier to
diagnose tendencies in data)
                                        (<Y>/n)  y

What is the threshold for this filter (e.g. 15.) ?   15


Normally, on box plots produced by RESIDUAL, the following
percentiles are indicated:
(1)      2.4    16       50       84   and   97.6

For plots of ratios, this is not always pertinent. Often, the
boxes stretch over many decades, so that no tendencies can be
seen in such plots.

Therefore, you can choose to use an alternative set of
percentiles:
(2)      5      25      50       75          95

Enter 1 or 2, according to your desire >>>>   2


Do you want to create a file suitable for a
quantile-quantile-plot (<Y>/n) ?   y

Name of additional output file (suggested type: .QUA):  ki3.qua

Reading data

Summary of choices made:
A lower threshold of  9.99999978E-03  has been imposed on the ratio,
An upper threshold of  100.000000  has been imposed on the ratio.
A filter has been imposed on small values of variables.
The filter value is    15.00
The ratio has been changed to unity in   23 of  338 cases.
The alternative set of percentiles (5, 25, 50, 75, 95) is used.
The file ki3ratio.dat has been created.
The file ki3.qua has been created as basis for q-q plots.

C:\MvK\Tools\Run1>
```

Table 16 Creating four box plots with SIGPLOT

```
C:\MvK\Tools\Run1>Sigplot

Type "sigplot nolabels" instead if you want to disable labelling

Name of template file :
..\kiratio.inq

Name of input data file :
ki3ratio.dat

Name of tektronix picture file :
ki3ratio.tek

Plotted frame     1
Plotted frame     2
Plotted frame     3
Plotted frame     4

C:\MvK\Tools\Run1>
```

Next, you should run *SIGPLOT* with an appropriate template file for a quantile-quantile plot. In our example, all templates reside in a folder one level closer to the root than the current. Therefore, in order to create the quantile-quantile plot, indicate that ..\KIQUA.INQ is the template file, while KI3.QUA is the input file.

(4a) Box plot of ratios

In order to create a box plot of ratios, you have already established the required data set (KI3RATIO.DAT) through your previous dialogue with RESIDUAL. Now, run SIGPLOT once more with ..\KIRATIO.INQ as template file and KI3RATIO.DAT as input

(4b): Box plot analysing c_{obs}

In order to generate item (4b), you will have to run RESIDUAL once more. This time again use KI3.INP as input, but KI3OBS.DAT as output file.

Indicate the numbers 1 0 in order to analyze c_{obs}. You need not impose thresholds, as this is a plain analysis of concentration data. You will not be asked whether to use extended capabilities when the ratio – as here – has 1 in the denominator. In this case the boxes will automatically represent percentiles 2.4, 16, 50 , 84 and 97.6.

Run SIGPLOT to plot the KI3OBS.DAT file. A template file, ..\KIOBS.INQ has been prepared for this purpose.

(4c): Box plot analysing c_{mod}

The last item, (4c), can be produced exactly corresponding to (4b). Run RESIDUAL, where you indicate the numbers 2 0 in order to analyze c_{mod}. Then run SIGPLOT with template file ..\KIMOD.INQ.

6.2.8 Recapitulation

- Run your model.
- Run Combine_kin.exe (after having prepared Combine_kin.ini).
- Run BOOT
- Run RESIDUAL and SIGPLOT a number of times. It is not necessary to use Residual to generate a simple scatter plot, but it must be used if you wish to generate a quantile-quantile plot, or plots with boxes.
- Run TEKPLOT to see plots, and PS to produce EPS versions of the files.

Figure 6 and *Figure 7* show samples of plots produced by the procedures outlined here.

Table 17 gives an overview of utilities in the `Tools` folder. Table 18 lists all of the predefined template files for SIGPLOT.

Note that the procedure can be automatized – see Section 6.6.

Table 17 Overview of utilities

Tool	What it does
COMBINE_xxx (xxx is kin, indi or CphLil)	Produces a file of type .INP that can be directly used as input for BOOT, and a file suitable for scatter plots.
BOOT	Produces files with statistics.
RESIDUAL	Used repeatedly to prepare input files to SIGPLOT (not needed for scatter plots, but for all other plots)
SIGPLOT	Produces plot files in Tektronix format: • Scatter plot • Quantile-quantile plot • Box plots analysing ratios stratified by physical parameters • Box plots analysing observations • Box plots analysing model results
Tekplot	Displays plot file on screen
PS	Converts plot file to EPS format

Table 18 **Overview of template files for SIGPLOT**

		Template file (supplied on diskette)	**Input file** (created by one of the 'Combine' utilities or by the RESIDUAL program)	**Resulting plot**
Kincaid	Max. concentration	KISCAT.INQ	KISCAT3.DAT	Scatter plot
		KIQUA.INQ	KI3.QUA	Quantile-quantile plot
		KIRATIO.INQ	KI3RATIO.DAT	Ratio. 4 plots on a page, log. ratio axis
		KIOBS.INQ	KI3OBS.DAT	Observations. 4 plots on a page, lin. conc. axis.
		KIMOD.INQ	KI3MOD.DAT	Model results. 4 plots on a page, lin. conc. axis.
Copenhagen	Max. concentration	CPSCAT.INQ	CPSCAT.DAT	Two pages of plots, presenting a scatter plot and a quantile-quantile plot.
		CPQUA.INQ		
	Crosswind concentration	CPYSCAT.INQ	CPYSCAT.DAT	Two pages of plots as above – but for crosswind integrated concentration.
		CPYQUA.INQ		
Lillestrøm	Max. concentration	LISCAT.INQ	LISCAT.DAT	Two pages of plots (centerline concentrations) as for Copenhagen.
		LIQUA.INQ		
	Crosswind integrated	LIYSCAT.INQ	LIYSCAT.DAT	Two pages of plots – crosswind integrated concentrations – layout as above.
		LIYQUA.INQ		
Indianapolis	Max. concentration	INSCAT.INQ		Five pages of plots for Indianapolis: Scatter plot, quantile-quantile plot, and box plots as for Kincaid.
		INQUA.INQ		
		INRATIO.INQ		
		INOBS.INQ		
		INMOD.INQ		

6.3 Copenhagen

In order to process Copenhagen data you must go through a procedure somewhat similar to the one outlined above. However, some changes are appropriate.

1) There are only 23 data points, and therefore it does not make sense to produce box plots like those for Kincaid. Scatter plots of various kinds are more informative. You can use SIGPLOT to produce some of these, but in this case SIGPLOT has no particular advantages over other plotting packages. Some template files for SIGPLOT are included – see below.
2) Besides arc-wise maxima, it is pertinent also to consider crosswind integrated concentration values. These are included among the observed data, and can be considered relatively reliable.
3) Note that the format for time is different from that for Kincaid. E.g., 1417 means 14:17 – whereas Kincaid and Indianapolis data are given for integer values of hour.

Procedure for modelling

Perform model calculations for the 13 distances represented in the Copenhagen data set (1.9, 2.0, 2.1, 3.6, 3.7, 4.0, 4.1, 4.2, 5.3, 5.4, 5.9, 6.0, 6.1 km). Dump your output in a file. Here, we will call the file Modelled.cph (you may use another name). The format of Modelled.cph should be the following:

- There is a one-line heading;
- There should be seven columns (or more), separated by blanks (the values are read using free-format input);
- There *must* be a line for all arc-hours (9 hours times 13 distances, altogether 117 lines)
- The distances must be those indicated above.

An example of the first fourteen lines of a Modelled.cph file is shown below. The date and time is indicated, then the distance, then the normalised arcwise maximum concentration, ARCMAX/Q, and finally the normalised crosswind integrated concentration CY/Q.

YR	MO	DY	HRE	DIST	ARCMAX/Q	CY/Q
78	9	20	1417	1.900	332.	374.
78	9	20	1417	2.000	301.	355.
78	9	20	1417	2.100	275.	338.
78	9	20	1417	3.600	101.	196.
78	9	20	1417	3.700	97.	191.
78	9	20	1417	4.000	84.	178.
78	9	20	1417	4.100	81.	174.
78	9	20	1417	4.200	78.	170.
78	9	20	1417	5.300	55.	146.
78	9	20	1417	5.400	54.	145.
78	9	20	1417	5.900	49.	141.
78	9	20	1417	6.000	48.	140.
78	9	20	1417	6.100	47.	140.

Please note that the units for ARCMAX/Q should be $s/m^3 \bullet 10^{-9}$ and for CY/Q $s/m^2 \bullet 10^{-6}$ (corresponding to the units used in the file with SF_6 data, SF6_CPH.DAT).

Merging modelled values and observations

You can use the utility Combine_CphLil.exe to prepare an input file for BOOT, as well as a file appropriate for a scatter plot.

First, you must edit the file *Combine_CphLil.ini*. This is a plain text file, which tells the program where it can find the model results, and where it should place the files that it generates.

Run Combine_CphLil.exe by double-clicking its icon. The program creates 4 files: CP.INP, CPY.INP, CPSCAT.DAT, CPYSCAT.DAT. The letter 'Y' refers to crosswind integrated concentrations.

The two .INP-files are input files for BOOT (for arcwise maximum and cross-wind integrated concentration, respectively), and the two .DAT files can be used to create scatter plot.

You can then run BOOT in a similar way as for Kincaid.

There are so few data that there is not much sense in creating box plots. Therefore, the RESIDUAL programme will not be of very much use in the analysis of the Copenhagen data – except that RESIDUAL can be used to sort data so that quantile-quantile plots can be produced. Template files for SIGPLOT (INQ files) have been prepared so you can use SIGPLOT to produce

- Simple scatter plots (c_{mod} vs. c_{obs} and cy_{mod} vs. cy_{obs})
- Quantile-quantile plots (cumulative distribution) for arc-wise maxima and cross-wind integrated concentrations.

In order to carry out an analysis of the variation of model results with parameters, it is recommended to use a utility like Microsoft Excel.

The starting point can be the INP files, which can be edited slightly.

How does a model behave close to the source?

It is characteristic for the Copenhagen data set that the monitoring arcs never "catch" the maximum ground-level concentration. The concentrations decrease with distance, indicating that the maximum is closer to the source than the nearest arc. Therefore, it is of interest also to investigate how a model behave closer to the source than the monitoring arcs.

In a modelling exercise for a workshop in 1994, it was prescribed that modellers should compute maximum ground-level concentrations and cross-wind integrated concentrations at the following distances (km):

0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.9, 1.0, 1.3, 1.6, 1.9, 2.2, 3.0, 4.0

You may encounter some results based on such data, and you may wish to perform similar calculations with your model.

6.4 Lillestrøm

One experiment has a zero value of u_*

Note concerning selection of data: The experimental period on 87/02/09, 1015-1030 is interesting because it has the highest concentrations. However, it cannot be reproduced by all models requiring L and u_* as input because L is undetermined and u_* indicated as zero. Therefore, for a baseline comparison, you should omit the data from the last experiment.

The procedure for processing Lillestrøm data is similar to that of Copenhagen. Thus:

.

1) There are only 21 data points, and therefore it does not make sense to produce box plots like those for Kincaid. Scatter plots of various kinds are more informative. You can use SIGPLOT to produce some of these, but in this case SIGPLOT has no particular advantages over other plotting packages.

2) It is pertinent to consider crosswind integrated concentration values. On the other hand, one should exert care if model results for arc-wise maxima are compared with observations, because the observations refer to 15-minute averages.

3) Note that the format for time is different from that for Kincaid, but is similar to that of Copenhagen. E.g., 1015 means 10:15 – whereas Kincaid and Indianapolis data are given for integer values of hour.

Procedure for modelling

Perform model calculations for the 14 distances represented in the Lillestrøm data set (0.14, 0.15, 0.16, 0.19, 0.30, 0.41, 0.43, 0.44, 0.46, 0.47, 0.49, 0.81, 0.82, 0.90 km). Dump your output in a file. Here, we will call the file Modelled.lil (you may use another name). The format of Modelled.lil should be the following:

- There is a one-line heading;
- There should be seven columns (or more), separated by blanks (the values are read using free-format input);
- There *must* be a line for all arc-periods (8 periods times 14 distances, altogether 112 lines)
- The distances must be those indicated above.

An example of the first fifteen lines of a Modelled.lil file is shown below. The date and time is indicated, then the distance, then the normalised arcwise maximum concentration, ARCMAX/Q, and finally the normalised crosswind integrated concentration CY/Q.

YR	MO	DY	HRE	DIST	ARCMAX/Q	CY/Q
87	1	10	945	0.140	6930.	313.
87	1	10	945	0.150	9439.	457.
87	1	10	945	0.160	12020.	620.
87	1	10	945	0.190	19044.	1167.
87	1	10	945	0.300	27819.	2691.
87	1	10	945	0.410	25066.	3314.
87	1	10	945	0.430	24351.	3376.
87	1	10	945	0.440	23968.	3400.
87	1	10	945	0.460	23167.	3436.
87	1	10	945	0.470	22755.	3449.
87	1	10	945	0.490	21924.	3464.
87	1	10	945	0.810	11659.	3045.
87	1	10	945	0.820	11448.	3027.
87	1	10	945	0.900	9941.	2885.

Please note that the units for ARCMAX/Q should be $s/m^3 \bullet 10^{-9}$ and for CY/Q $s/m^2 \bullet 10^{-6}$ (corresponding to the units used in the file with SF_6 data, SF6_LIL.DAT).

Merging modelled values and observations

You can use the utility Combine_CphLil.exe to prepare an input file for BOOT, as well as a file appropriate for a scatter plot.

First, you must edit the file *Combine_CphLil.ini*. This is a plain text file, which tells the program where it can find the model results, and where it should place the files that it generates.

Run Combine_CphLil.exe by double-clicking its icon. The program creates 4 files: LI.INP, LIY.INP, LISCAT.DAT, and LIYSCAT.DAT. The letter 'Y' refers to crosswind integrated concentrations.

The two .INP-files are input files for BOOT (for arcwise maximum and cross-wind integrated concentration, respectively), and the two .DAT files can be used to create scatter plot.

You can then run BOOT in a similar way as for Kincaid.

There are so few data that there is not much sense in creating box plots. Therefore, the RESIDUAL programme will not be of very much use in the analysis of the Lillestrøm data – except that RESIDUAL can be used to sort data so that quantile-quantile plots can be produced. Template files for SIGPLOT (INQ files) have been prepared so you can use SIGPLOT to produce

- Simple scatter plots (c_{mod} vs. c_{obs} and cy_{mod} vs. cy_{obs})
- Quantile-quantile plots (cumulative distribution) for arc-wise maxima and cross-wind integrated concentrations.

In order to carry out an analysis of the variation of model results with parameters, it is recommended to use a utility like Microsoft Excel.

The starting point can be the INP files, which can be edited slightly.

6.5 Indianapolis

The procedure is completely parallel to that for Kincaid

Procedure for modelling

Perform model calculations for the 12 distances represented in the Indianapolis data set (0.25, 0.5, 0.7, 1.0, 1.5, , 3, 4, 6, 8, 10, 12 km). Dump your output in a file. Here, we will call the file Modelled.ind (you may use another name). The format of Modelled.ind should be the following:

- There is a one-line heading;
- There should be six columns (or more), separated by blanks (the values are read using free-format input);
- Typically, there is a line for all 2040 arc-hours (170 hours times 12 distances). However, it is acceptable that only *some* of these 2040 arc-hours are represented in the file. The distances must be those indicated above.

An example of the first thirteen lines of a Modelled.ind file is shown below. The date and time is indicated, then the distance, and finally the normalised arcwise maximum concentration, ARCMAX/Q.

```
YR  MO DY   HR   DIST  ARCMAX/Q
85  9  16   11   0.250     33.
85  9  16   11   0.500    479.
85  9  16   11   0.750    643.
85  9  16   11   1.000    587.
85  9  16   11   1.500    403.
85  9  16   11   2.000    337.
85  9  16   11   3.000    254.
85  9  16   11   4.000    200.
85  9  16   11   6.000    141.
85  9  16   11   8.000    109.
85  9  16   11  10.000     90.
85  9  16   11  12.000     76.
```

Please note that the units for ARCMAX/Q should be $s/m^3 \bullet 10^{-9}$ (corresponding to the units used in the file with SF_6 data, SF6_IND.DAT).

Cross-wind integrated concentrations are *not* included in the present version of the Indianapolis data set as they are difficult to assess with confidence.

Merging modelled values and observations

You can use the utility Combine_indi.exe to prepare an input file for BOOT, as well as a file appropriate for a scatter plot.

First, you must edit the file *Combine_Indi.ini*. This is a plain text file, which tells the program where it can find the model results, and where it should place the files that it generates.

Run Combine_indi.exe by double-clicking its icon. The program allows selection according to quality level. There are 479 observations of quality 3.

You can then run utilities – BOOT, RESIDUAL, SIGPLOT etc. – in a similar way as for Kincaid. When running RESIDUAL, you may use the same filter value (15) as for Kincaid. The required files are included in the `Tools` folder (Master.ind, .INQ files for SIGPLOT, etc.). Table 18 shows the names of the INQ files (SIGPLOT templates).

6.6 Hints on automatizing the process

It is possible to achieve a high degree of automatition for the programs if you work in a command line environment. This is not the place for a full description of DOS tricks, but a few hints can be given:

If you run, e.g. BOOT from a command line environment, you can enter the command

```
BOOT < boot_commands.txt
```

and then avoid manually entering the responses to the dialogue with BOOT. You just have to prepare the file boot_commands.txt, so it contains all of the responses to the questions asked by BOOT.

A similar approach can be taken with Residual and Sigplot.

There are samples in the files

- Boot_commands.txt (input for BOOT)
- Residual_ratio_commands.txt (input for Residual, when preparing files for box plots of ratio)
- Sigplot_commands.txt (input for Sigplot when producing box plots of ratios)

These samples can be found in the `Tools` folder. However, they should be copied to a different folder. The sample files will work directly if the current folder is the one with model results for Kincaid (such as C:\MvK\Tools\Run1 of the example). For other use, the sample files should be adjusted.

Furthermore, if you are familiar with DOS, you can prepare BAT files and execute several programmes in a sequence.

6.7 Hints on software problems

- Sometimes, when you use TEKPLOT to display a file, nothing is displayed. Just try once more.

- If a file cannot be found even though it exists, then check the length of the filename. Some of the old utilities (e.g. Tekplot) don't recognise filenames of more than 8 characters (+3 characters for file type).

- The BOOT utility and the Combine_xxx utilities are intended to be executed in a Windows environment. If you use them from a command line they will also work, but they behave awkwardly in case of an error: Seemingly, the program just freezes.
  Actually, a separate window has appeared, which may be hidden behind other windows. The window tells you that there is an error, and you have to click an OK button in order to continue working in the command line environment.
  If you work from a command line and want to avoid such behaviour, you can find an alternative version of BOOT called BOOT_NO_PAUSE.EXE (in the `BOOT` folder).

- The required files for input and template files for SIGPLOT has changed in certain respects since the version distributed before 2005. In case of problems, consult the Addendum to the SIGPLOT User's Guide, found in folder `SIGPLOT`.

7 SIGPLOT software

The SIGPLOT software is offered as an option, but it must be recognized that the software is old and the documentation not complete.

The easiest way to get started with Sigplot is to follow the step-by-step explanation in Chapter 6.

SIGPLOT requires that you work in a command line environment (DOS environment). The details are given in Section 6.2.5.

The SIGPLOT software is described in the User's Guide from 1991, which is available as a (scanned) pdf file: SIGPLOT User's Guide 1991.pdf in folder `SIGPLOT`. The software has been enhanced over the years, so you must also consider the *Addendum to the User's Guide*, found in the same folder.

Note that the format of certain template files (INQ files) has changed, so the current version of SIGPLOT will not always work with old template files.

The SIGPLOT software was developed by Joe Chang of George Mason University, VA, USA.

8 Dispersion Visualisation Tool

The Dispersion Visualisation Tool (DVT) was created by Alexandar Markoski, Bitola University, the Former Yugoslav Republic of Macedonia. The present version is preliminary. For updates, see the web site of the Model Validation Kit, www.harmo.org/kit.

Data from the Kincaid experiment are divided into two parts: The "Development data" and the "Evaluation data". Only the Development data are presently included here, but the software has been prepared to use either of the data sets.

When using the DVT, you must first choose the appropriate data set from the menu *Experiment* – i.e., you must select "Kincaid Development".

After this choice, choose date and time. Note that you can step through hours by clicking in the hour field, and subsequently use the arrow keys. With a mouse you can change the viewing angle.

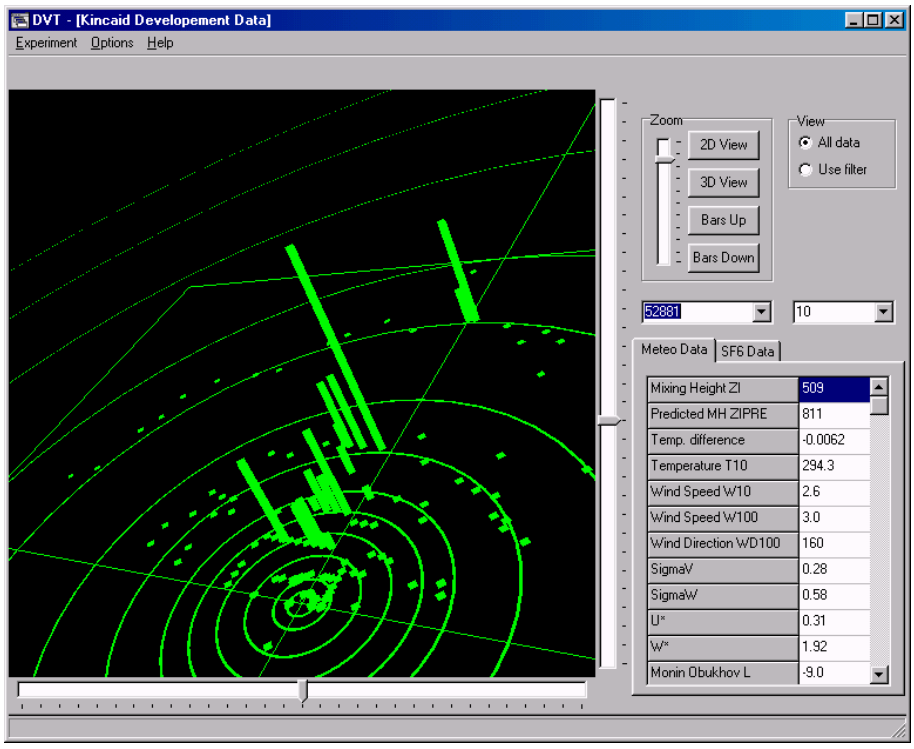


Figure 8 Example of observed SF_6 concentrations at Kincaid, displayed with the Dispersion Visualisation Tool.

9 Tools for Grapher plots

The Dispersion Visualisation Tool provides a very intuitive way of displaying concentration data.

For some purposes, however, it is to be preferred to display data on 2D maps with colour-coding like the one shown in *Figure 9*.

There are utilities for this in the folder **`Grapher_tools`**, and the procedure is explained in the document *XY_Explanation.txt*

You must have installed the commercial software Grapher for Windows if you wish to apply the utilities.

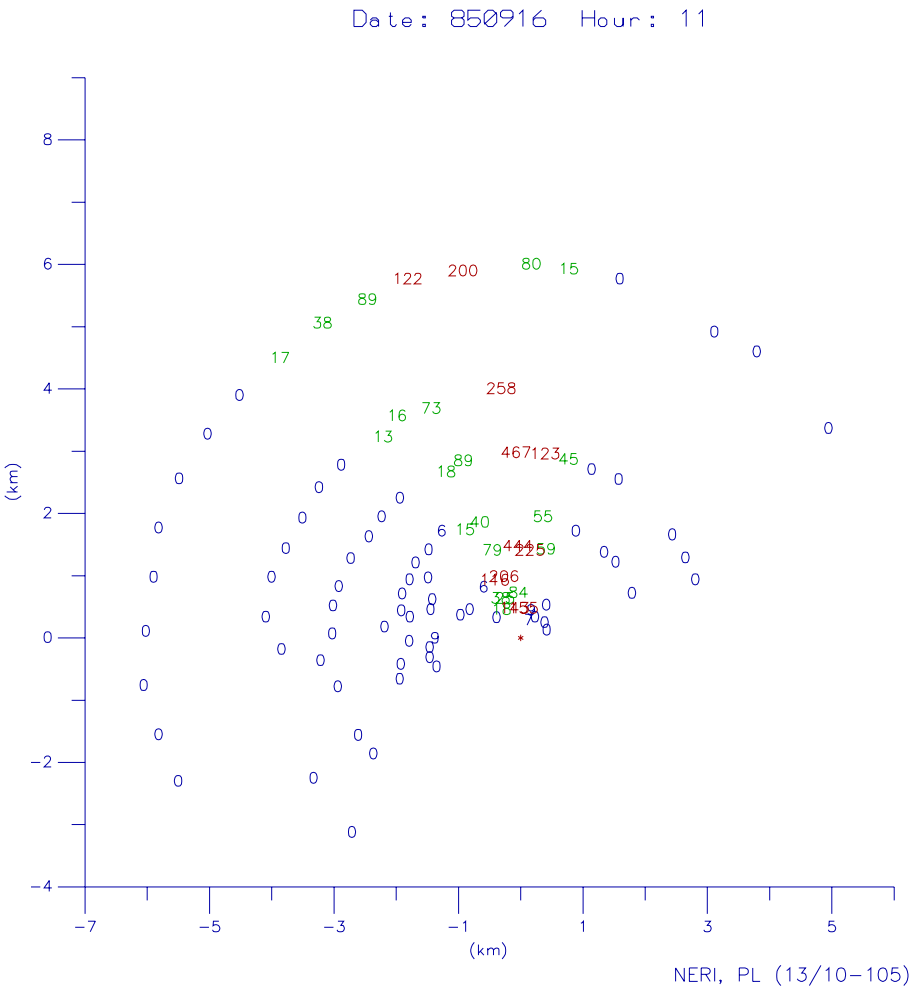


Figure 9 Geographical distribution of concentrations for a specific hour during the Indianapolis experiment.
A plot file has been prepared with the utilities and subsequently displayed with Grapher.

10 Video clips from Kincaid

Introduction

The Kincaid experiment in 1980 was sponsored by the Electric Power Research Institute (EPRI) in the USA. EPRI (through Dr. Charles Hakkarinen) has kindly given permission, so a set of video clips here can be freely distributed.

The video clips were originally on a movie, put together by TRC Environmental Consultants who were contracted to conduct field experiments. The clips have been edited and put in digital format by H.R. Olesen of the National Environmental Research Institute, Denmark.

Most of the video is from time lapse sequences, where a picture was taken every 30 seconds, while the movie was played back at a rate of 9 pictures per second. This corresponds to a rate of 1 "real" hour being played in 13.3 seconds.

The video clips are in MPEG format.

A field observer from TRC wrote a set of notes on the content of the movie, which is reproduced below:

July 12, 1980 (1930 CDT)

Kincaid12JulyPlant
Close-up of plant. Shows stack and "dirty" plume
0:18

Close-up of Kincaid power plant, stack, & "dirty" plume. This is *not* a time-lapse sequence.
Some data about the power plant:

- 600 ft. stack; 2 650 MW boilers; No scrubber
- 4-5% sulphur coal; 2.4 mil. tons burned per year.
- Baseload plant; Generates 4.3 mil MWH per year.
- SO_2 emissions: 200,000 T/yr, 23 T/hr, 5,700 g/s.
- NO_x emissions: 1/3 SO_2 emissions.
- Particulate emissions: 800 T/yr.

July 14, 1980 (0910-1600 CST)

Kincaid14JulyLooping
Study of plume looping periodicity

Study of plume looping periodicity.

The period of the large eddies affecting the plume appears to be several times the time-lapse interval of 30 seconds.

Meteorology: Class B, wind speed = 5 m/s.

July 15, 1980 (1045-1720 CST)

Kincaid15JulyLooping
Study of plume looping periodicity

Study of plume looping periodicity.

Plume appears to stop or back up. Strobe effect implies that large eddies have a period equal to or multiple of the time-lapse interval of 30 seconds.

Meteorology: Class B, wind speed =5 /s.

July 17, 1980 (1130-1820 CDT)

Kincaid17JulyShear
Strong wind shear
1:43

Plume behaviour influenced by strong wind shear.

- North wind aloft initially carries entire plume southward (meanwhile, the surface wind is from the south) .
- During the afternoon, the south winds take over through an increasingly deeper layer.
- By mid-afternoon, wind-shear effect is very apparent. Most of plume continues southward, but chunks are occasionally broken off early in the plume rise by the south wind and are carried northward.
- At 1530 CDT, the bulk of plume is affected alternately by north and south winds. A T-shaped plume results, i.e., two plumes visible at one time going in opposite directions!
- After 1600 CDT, shear is no longer present through plume height. South wind has taken over and entire plume now is carried northward. (Note: clouds aloft still move southward.)

July 23, 1980 1500 CDT

Kincaid23JulyBifurcated
Bifurcated plume

Bifurcated plume often observed at the plant.

July 24, 1980 (0810-1415 CDT)

Kincaid24JulyClassical
Classical morning transition

Classical morning transition from night: stable plume aloft, through inversion break-up fumigation, to the convectively unstable looping plume.

- Initially, a stable, compact plume aloft. No touchdown within 50 km.
- At 1000 CDT, sudden fumigation apparent between plume height and ground.
- By late morning (1150 CDT), strong convective eddies have formed and are propagating through the area in parade fashion.
- As a convective cell passes over the plant area, the plume is rapidly entrained upward into the call. A cumulus cloud then forms in the cell.
- The cloud formation is likely enhanced by added moisture and particulate matter from the plume.

July 25, 1980 (0825-1700 CST)

Kincaid25JulyEntrainment
Plume entrained into convective cells

Plume being entrained into propagating convective cells, with subsequent cumulus development.

- At 1400, bifurcated plume.
- Note: Clock time is wrong.

July 28, 1980 (0820-1530)

Kincaid28JulyCumulus
Plume entrained into convective cells; cumulus formed

Plume producing large, cumulus clouds.

The plume is being entrained into propagating convective cells.

- Note: Clock time is wrong.

11 Notes on the "ASTM package"

ASTM Standard Guide D6589

As noted in chapter 2 ***Key to the Model Validation*** Kit, there is a concern that direct comparison of model predictions against observations could cause misleading results. Therefore, an alternative approach has been proposed by John Irwin, and has resulted in ASTM Standard Guide D6589. This procedure has also been incorporated in the latest version of the BOOT software as an option. However, there exists also a separate package (software and data sets), specifically devised as an implementation of the ASTM procedure – here referred to as the *ASTM package*. It was prepared by John Irwin and is available on the Internet (www.harmo.org/astm). This is not part of the Model Validation Kit, but it can be used as a supplement or an alternative to the Model Validation Kit.

In order to place the Model Validation Kit in a perspective, we will here outline the main principles of the ASTM methodology, and further explain some features that distinguish the two packages.

The ASTM guide is a guide on "statistical evaluation of dispersion model performance", and is general in the sense that it is not confined to the problem of dispersion from an isolated point source – which is the focus of the Model Validation Kit. However, as an example of application of the principles in the Guide, the particular problem of point source dispersion is addressed in an Appendix to the Guide, as well as in the ASTM package.

Premise of ASTM methodology: Average observations within regimes

The fundamental premise of the ASTM procedure is that observations and model predictions should *not* be compared directly, and that observations should be properly averaged before comparison. The comparison takes place within *regimes*, which for example can be defined according to atmospheric stability and distance to the source. The ASTM procedure then calculates performance measures based on *regime averages* (i.e., averaging over all experiments within a regime), rather than the values for individual experiments.

Near-centreline concentrations

In the specific implementation of the ASTM methodology found in the ASTM package, the observations of interest are near-centreline concentrations (NCCs). NCCs bear some relation to arc-wise maxima, but for a given experiment and arc, there may be several NCCs as opposed to only one arc-wise maximum. NCCs are selected among those observations that lie within a distance of 0.67 σ_y from the cloud centre, where σ_y is the cloud width. The software of the ASTM package is capable of retrieving NCCs from observations and process them in accordance with the prescribed methodology. Note, however, that selecting NCCs is not straightforward, as it depends on regime definitions, and there are questions as to which arcs can be considered having enough data for NCCs to be defined.

Datasets: Kincaid, Indianapolis, Prairie Grass

The ASTM package includes software, documentation and three datasets (Kincaid, Indianapolis and Prairie Grass). The data in the package have not been quality flagged, but the software performs certain checks when retrieving NCCs.

The ASTM procedure implemented in the BOOT software in the Model Validation Kit assumes that NCCs have been retrieved separately.

The ASTM procedure represents a framework and is not a fixed protocol. For example, regimes can be defined in many different ways, and this may lead to differing results of a performance evaluation, depending on regime definitions.
Altogether, the ASTM procedure represents a promising approach, but still with some issues that are not fully resolved. Some issues deserving attention are:

- There is a need to study the sensitivity of the evaluation results to the definition of regimes (i.e., how data are stratified).
- There is always only a limited number of regimes (e.g., ~20 to 40) that can be defined. The performance measures are always determined by this limited number of regime averages. It is necessary to carefully examine the implication of accounting for only the variance in regime averages, rather than the full variance in the complete dataset.
- In the current implementation of the procedure with near-centreline concentrations (NCCs), it is problematic that observed NCCs are compared to model predictions in the *exact* centerline, which by definition are higher than near-centerline values.
- The basic assumption that (averaged) model results should fit (averaged) observations may be unwarranted if the quality of observed data is not properly assured. This is especially a concern when experimental data are fed into a statistical "blackbox" where these data are processed and averaged before a result is inspected. Problems with the observed data or the way they are interpreted may easily pass unnoticed. Use of a quality indicator could alleviate such problems.

12 Changes since previous version

The previous version of the Model Validation Kit was distributed between 1993 and October 2005.

There have been *no changes in values in data values* compared to that version. However, the following changes are notable.

Some extra material has been added to the Model Validation Kit, notably the Dispersion Visualisation Tool and the video films.

The BOOT software is version 2.0, which has many additional features compared to the earlier version.

There have been many changes in the utilities in order to allow for unproblematic use of the kit in a Windows environment. The entire documentation is considerably updated.

Some information-carrying files have been renamed, so they now have extension .TXT instead of DAT.

The format for input to BOOT has changed, so there is an additional column of data values compared to previously. See Table 19.

Table 19 Format of an INP file in the previous version (left) and the current version (right)

```
 338   2   1   4                                                    
 338                                                                
'C_OBS'   'C_MOD'   DIST     u*    h/L  zmix  YR MO DY HR QUAL      
'Block of all data'                                                 
  73.3      93.0     3.0  0.300 -241.4  2076. 80  4 20 14  3       
  53.9      85.0     3.0  0.310 -186.8  2092. 80  4 20 15  3       
  30.4      58.0     5.0  0.310 -186.8  2092. 80  4 20 15  3       
  17.2      42.0     7.0  0.310 -186.8  2092. 80  4 20 15  3       
```

```
  338   2   1   4                                                    
  338                                                                
 'C_OBS' 'C_MOD' DIST     u*    h/L  zmix  YR MO DY HR QUAL         
 'Block of all data'                                                
1   73.3  107.0   3.00  0.300 -241.4  2076. 80  4 20 14  3          
1   53.9  111.0   3.00  0.310 -186.8  2092. 80  4 20 15  3          
1   30.4   63.0   5.00  0.310 -186.8  2092. 80  4 20 15  3          
1   17.2   43.0   7.00  0.310 -186.8  2092. 80  4 20 15  3          
```

The format for input to SIGPLOT and for SIGPLOT template files has also changed slightly – see the Addendum to the SIGPLOT User's Guide.

13 Acknowledgements

The material has been compiled through the joint efforts of many persons. Steve Hanna has provided the data sets from Kincaid and Indianapolis, Joe Chang has created much software, Alexandar Markovski has created the Dispersion Visualisation Tool, and Sven-Erik Gryning, Per Løfstrøm, Chuck Hakkarinen, Russ Lee and Dag Tønnesen have contributed in various ways.

The EPRI Air Quality Data Center was operated by Earth Tech in the early nineties, when the data were provided. The Kincaid and Indianapolis data were put at disposal on behalf of EPRI by Earth Tech (Steve Hanna and Joe Chang).

Joe Chang has developed the major part of the software including BOOT, SIGPLOT, while Helge Rørdam Olesen has provided supplementary utilities.

EPRI (through Dr. Charles Hakkarinen) has kindly given permission, so a set of video clips from Kincaid can be freely distributed.

John Irwin has assembled the ASTM package, which is described in Chapter 11 (but is not part of the Model Validation Kit).

14 References

Bowne, N.E. and Londergan, R.J., 1983: Overview, Overview, Results, and Conclusions for the EPRI Plume Model Validation and development Project: Plains Site, EPRI report EA-3074.

Chang, J.C. and Hanna, S.R., 2004: Air quality model performance evaluation. *Meteorol. Atmos Phys.*, **87**, 167-196.

Chang, J.C. and Hanna, S.R., 2005: Technical Descriptions and User's Guide for the BOOT Statistical Model Evaluation Software

Cuvelier, C. (editor), 1994: Proceedings of the workshop "Intercomparison of Advanced Practical Short-Range Atmospheric Dispersion Models". August 30-September 3, 1993, (Manno – Switzerland), CSCS (Centro Svizzero di Calcolo Scientifico). Joint Research Centre, European Commission, EUR 15603 EN. Available from C. Cuvelier, JRC Ispra, TP 690, 21020 Ispra, Italy.

Hanna, S.R. and R.J. Paine, 1989: Hybrid Plume Dispersion Model (HPDM) development and evaluation. J.Appl. Meteorol., 28, 206-224.

Hanna, S.R. and J.C. Chang, 1992: Boundary-Layer parameterizations for applied dispersion modelling over urban areas. Boundary-Layer Meteorology, 58, 229-259.

Hanna, S.R. and R.J. Paine, 1989: Hybrid Plume Dispersion Model (HPDM) development and evaluation. J.Appl. Meteorol., 28, 206-224.

Hanna, S.R., Strimaitis, D.G. and J.C. Chang, 1991: Hazard response modeling uncertainty (a quantitative method). Vol. I: User's guide for software for evaluating hazardous gas dispersion models. Sigma Research Corporation, Westford, Ma.

Hanna, S.R. and J.C. Chang, 1991: Modification of HPDM for Urban Conditions and Its Evaluation using the Indianapolis Data Set. Final Report Prepared for EPRI by EARTH TECH, 196 Baker Ave., Concord, MA 10742.

Hanna, S.R. and J.C. Chang, 1993: Hybrid Plume Dispersion Model (HPDM) improvements and testing at three field sites. Atmos. Environ., 27A, 1491-1508.

Haugsbakk, I. and Tønnesen, D.A. (1989): Atmospheric Dispersion Experiments at Lillestrøm. 1986-1987 Data Report. Lillestrøm, Norwegian Institute for Air Research (NILU OR 41/89).

Gryning, S-E and Lyck, E., 2002: The Copenhagen Tracer Experiments: Reporting of Measurements. Risø-R-1054 rev. 1(EN), Risø National Laboratory, Roskilde, Denmark. ISBN 87-550-3101-3. 75 pp. Available at http://www.risoe.dk/rispubl/VEA/ris-r-1054_rev1.htm

Gryning, S.-E. and E. Lyck, 1984: Atmospheric dispersion from elevated sources in an urban area: Comparison between tracer experiments and model calculations. J. Cl. Appl. Meteor., 23, 651-660.

Gryning, S.E and Thomson, 1979: A tall-tower instrument system for mean and fluctuating velocity, fluctuating temperature and sensible heat flux measurements. J. Appl. Meteor. 18, 1674-1678.

Gryning, S.E, 1981: Elevated source SF6 tracer dispersion experiments in the Copenhagen area. Risø-R-446, Risø National Laboratory, 187 pp. Available from the author (see list of addresses).

Gryning, S-E. and Tassone, C., 1994: The Copenhagen tracer experiment – short description and some model results. In: Cuvelier, 1994.

Grønskei, K.E., 1990: Variation in dispersion conditions with height over urban areas – results of dual tracer experiments. 9th AMS Symposium on Turbulence and Diffusion, 1990.

Olesen, H.R., 1994: Summary of model evaluation discussions in Manno. In: Cuvelier, 1994.

Olesen, H.R., 1995a, The model validation exercise at Mol. Overview of results. Workshop on Operational Short-range Atmospheric Dispersion Models for Environmental Impact Assessment in Europe, Mol, Belgium, Nov. 1994, Int. J. Environment and Pollution, Vol. 5, Nos. 4-6, pp. 761-784.

Olesen, H.R., 1995b, Toward the establishment of a common framework for model evaluation. Paper presented at the 21 International Meeting on Air Pollution Modeling and its Applications in Baltimore, Nov. 6-10, 1995.

Olesen, H.R., 1997, Tools for model evaluation. In: Air Pollution Modeling and Its Application XII, pp. 519-528. Edited by S-E. Gryning and N. Chaumerliac, Plenum Press, New York.

Olesen, H.R., 1997, Pilot study: Extension of the Model Validation Kit. Paper presented at the 4th workshop on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, Oostende, Belgium, 6-9 May, 1996. *Int. J. Environment and Pollution*, Vol. 8, Nos. 3-6, pp. 378-387.
Gives an introduction to data sets from Indianapolis and Bull Run; the Indianapolis data set was later added to the Model Validation Kit. Also conveys general experiences on the preparation and use of data sets for model evaluation.

Olesen, H.R., 1997, Tools for model evaluation. In: Air Pollution Modeling and Its Application XII, pp. 519-528. Edited by S-E. Gryning and N. Chaumerliac, Plenum Press, New York.
Contains additions to previous overviews of model evaluation activities. Also contains a detailed discussion of one particular problem with the methodology of the Model Validation Kit: observed arcwise maxima are compared directly to modelled concentrations. This type of comparison, however, does not have a straightforward interpretation.

Olesen, H.R., 1998, Local-scale regulatory dispersion models. Initiatives to improve "modelling culture". Proceedings of the 10th Joint Conference on the Applications of Air Pollution Meteorology with the A&WMA. American Meteorological Society, Boston, pp. 49-53.
Contains a brief, overview of model evaluation activities.

Olesen, H.R., 2000, The Model Validation Kit – Status and Outlook. *Int. J. Environment and Pollution*, Vol. 14, Nos. 1-6, pp. 65-76.
Reviews status for the Model Validation Kit. A change of the methodology of the kit is considered, based on the concept of near-centreline concentrations. The paper examines some consequences of such a potential change in methodology.

Olesen, H.R., 2001, 'Model Validation Kit – Recent Developments'. *Int. J. Environment and Pollution*, Vol. 16, Nos. 1-6, pp. 129-136. (Paper presented at the 6th International Conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes in Rouen, October 1999)
Supplements the paper on status and outlook mentioned above. Certain problems with the determination and use of so-called near-centreline concentrations (NCC's) are identified and discussed.

Olesen, H.R. (2001), 'A platform for model evaluation'. 7th international conference on Harmonisation within Atmospheric Dispersion Modelling for Regulatory Purposes, Belgirate, Italy, May 28-31, 2001. Available on the web, http://www.dmu.dk/atmosphericenvironment/Harmoni/Conferences/Belgirate/BelgiratePapers.asp

Sozzi, R. and Fraternali, D., 1994: PBL-MET: Library for advanced meteorological and air quality data processing. In: Cuvelier, 1994.

TRC, 1986: Urban power plant plume studies, EPRI Report EA-5468, EPRI, 3412 Hillview Ave, Palo Alto, Ca 94304.

Turner, D.B., 1964: A diffusion model for an urban area. J. Appl. Met., 3, 83-91.

A large number of reports concerning the Kincaid experimental campaign were published by the Electric Power Research Institute, 3412 Hillview Ave, Palo Alto, Ca 94304, USA, www.epri.com.

14.1 Addresses

The main contact for additional information is Helge Rørdam Olesen. However, in the text, some other persons with an intimate knowledge of various parts of the kit have been mentioned. This list of addresses can be used if there is a need to contact them directly.

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Information related to this document can be found on the World Wide Web. Look at

http://www.harmo.org/kit

Danish Summary – Dansk resumé

Det såkaldte *Model Validation Kit* er en 'værktøjskasse' bestående af data fra spredningseksperimenter i atmosfæren samt programmel og dokumentation, der tilsammen udgør en referenceramme for evaluering af atmosfæriske spredningsmodeller. Det er møntet på modeller, der beskriver spredning fra punktkilder lokalt omkring kilden.

Model Validation Kit har vundet vid international udbredelse, siden den første version forelå i 1993. Adskillige hundrede forskningsgrupper har rekvireret materialet. I tiden siden 1992 har det såkaldte *Initiative on Harmonisation within Atmospheric Dispersion Modelling for Regulatory purposes,* (www.harmo.org) afholdt en serie workshops og konferencer om spredningsmodellering til administrative formål. Et fokusområde har været evaluering af modeller, og *Model Validation Kit* er blevet hyppigt benyttet i forbindelse med disse konferencer.

Den foreliggende rapport udgør en brugervejledning til materialet. Den give et overblik over hele 'værktøjskassen', og indeholder ydermere detaljerede anvisninger på brugen af materialet.

Ud over datasæt og programmel til modelevaluering omfatter pakken også supplerende materiale, såsom værktøj til data-visualisering, og videoklip fra spredningseksperimenter.

Model Validation Kit har gennemgået en omfattende revision i efteråret 2005. Den ny version (version 2.0) muliggør de samme analyser som den tidligere, men er blevet opdateret på forskellige områder, især hvad angår software. Endvidere er dokumentationen blevet betragteligt forbedret og opdateret.

Pakken med *Model Validation Kit* kan downloades fra Internettet på adressen www.harmo.org/kit