SMEDIS FINAL REPORT

DRAFT CONTENTS (with responsible partners)

Executive Summary (HSL with contributions from CERC and EdF)

Contents

In addition it is intended to produce CDs containing the data used in and the results of the validation exercise.

1. INTRODUCTION

1.1 Background

Complex industrial processes are increasingly incorporated into computational models in order to predict possible outcomes resulting from changes in the process, accidents and environmental impact. In order to have confidence in these models the usually "non-expert" user requires independent confirmation that the model is "fit-for-purpose". Such confirmation requires an assessment of the validity of the model assumptions and approximations relevant to the process, information about Quality Assurance, and evidence that the model has undergone some validation testing. Without this information the user must rely on the claims of the model supplier. An independent assessment allows informed judgements to be made when using the model results for the basis of financial, managerial or technical decisions.

SMEDIS (Scientific Model Evaluation of dense gas DISperson models) is a project designed to develop and apply an independent assessment procedure to a class of technical models. The class under consideration, dense gas dispersion or DGD models, contains sophisticated mathematically-based computer models. There are over 100 different models which purport to address this problem, ranging in complexity from empirically-based screening tools through integral models to shallow layer and Computational Fluid Dynamics (CFD) models.

DGD models occupy a central role in the study of the consequences of accidental releases of flammable or toxic materials. The formation of a gas cloud denser than ambient air is a common feature of industrial processes involving low storage temperatures, or materials stored above their boiling point under pressure, such as LNG or LPG. Dense gas models also provide the bridge between the source models and the fire/explosion models, say, describing the hazardous consequences of the release of a flammable material, or between the source and population affected by the release of a toxic material.

The motivation for studying such problems derives primarily from the pressure of legislation introduced following major disasters (Flixborough, 1974; Seveso, 1976) which, in the European context, is enshrined in the so-called Seveso Directive (1) and more recently the updated version, Seveso II (2). Such legislation requires the owners of industrial sites to safeguard people against potential injury and property against damage on and near the site by carrying out an assessment of the consequences of various accident scenarios.

Since the ability of a site to operate depends on the acceptance of the resulting "safety report" by the relevant competent authority, the modelling plays a significant role. Important decisions are made based on the results of such models, and, if there were an accident, models used in formulating safety plans, and the calculations which were performed, will come under scrutiny and need to be defensible. The model user therefore needs to be able to demonstrate that they have used the model for problems to which it is applicable and that the model has been tested against observations from relevant situations.

The concerns over model quality and appropriate use of complex technical models have led to the concept of *scientific model evaluation*, i.e. the objective examination of a model according to a well-defined procedure documented in the evaluation *protocol*. Scientific model evaluation comprises three main elements:

(a) *scientific assessment* – objective examination of the scientific and user-oriented aspects of a model

(b) *vertification* – confirmation that the (computer) implementation is an accurate translation of the mathematical model

(c) *validation* –comparison of the predictions of the model against experimental observations

The terminology scientific is used to emphasise the difference between model evaluation and the more restricted process of model validation.

1.2 Previous work

The impetus to study this subject within Europe dates back to previous model intercomparison work carried out in the framework of a cooperation between UK AEA and France CEA (3). More recently further activity arose from the interest of the European commission through DGXII and, in particular, the programme on Major Industrial Accident Hazards. Following a report by Britter (4) discussing issues associated with model evaluation, quality and application, an EC Model Evaluation Group (MEG) was set up. The MEG produced two documents:

(a) A generic protocol suitable for adaptation for the assessment of many classes of models (5); and

(b) a set of guidelines for model development (6).

Additionally specialised 'expert groups' were formed with the task of focusing on issues particular to individual model types. Thus groups were set up to examine problems with assessing models used to predict for example the efforts of gas explosions or jet fires.

A Heavy Gas Dispersion Expert Group (HGDEG) was one such sub-group. This forum adapted the general guidelines of the MEG by drawing up a list of heavy gas dispersion models, identifying data sets, further developing the protocol to be more specific to dense gas dispersion models (7) and conducting a modest evaluation exercise to test the protocol (8). This open exercise comprised the distribution of a very limited number of data sets to interested parties followed by an attempted statistical analysis of returned model predictions. Details and experience of this limited exercise are given by Cole and Wicks (9).

This methodology was further developed by Duijm et al (10). They performed a comprehensive validation exercise for a restricted number of the simpler dense gas dispersion models over flat unobstructed terrain. They made use of data from the REDIPHEM data base and selected a total of 41 experiments from 6 experimental programmes, including field and wind tunnel trials, for processing into a form suitable to perform two types of comparison with model predictions:

(a) using spatially distributed data involving the comparison of observed and predicted concentrations paired in space and time at all locations in the measurement array.

(b) using the maximum observed concentrations at several distances from the release point to compare with the predicted plume centre line concentration at that distance.

Duijm et al investigated the use of a number of statistical performance measures with which to quantitatively assess model performance. They concluded that the evaluation and ranking of dense gas dispersion models on single performance measures and data sets is fraught with difficulty and in general should not be attempted. At least two performance measures should be used to determine both the bias and variance in the data. They suggested that a good combination might be the mean relative bias and mean relative square error used together with the easily-understood factor of two statistics; the fraction of observed/predicted values which agree to within a factor of two. Similarly a procedure based on maximum concentrations might result in a model ranking inconsistent with the general model capability. The geometry of the plume/cloud must always be taken into account and an evaluation procedure based on spatially distributed data is of value, particularly where more advanced models which can account for details of the release or obstacles, for example, are involved. Finally they suggest that statistical evaluation is only one aspect of assessing model quality and that scientific evaluation is at least as important.

In the United States, there has also been considerable activity in this area during the 1980s and 1990s. Hanna et al (11) carried out a seminal validation study on a number of commonly-used dense gas dispersion models : they focused on flat unobstructed terrain and did not include any element of scientific assessment. However, they were the first to introduce the use of quantitative statistical measures of model performance to the dense gas dispersion field and recognised that, for any model ranking exercise to be valid, models must be compared against exactly the same data sets. Thus they developed the Modeller's Data Archive (MDA); a database comprising centre line concentrations at various downwind distances derived from 90 experiments from more experimental field campaigns. The main conclusion derived from this model ranking exercise on flat unobstructed terrain was that the performance of a model was not found to be related to its cost or complexity and simpler models yielded as good agreement with experiment as any of the more complex dense gas dispersion computer codes tested.

More recently, Lazaro et al (12) carried out a study of many dense gas dispersion models, combining elements of both validation and assessment, although the former was restricted to parametric studies of model response to differing input data coering realistic but non-experimental scenarios.

1.3 The need for SMEDIS

In practice, however, industrial sites consist of complex, obstructed terrain often with a high degree of confinement, and failure of pressurised storage or transportation vessels will commonly lead to the formation of a dense cloud or plume containing a liquid droplet fraction in the form of an aerosol. Such complex effects – releases in aerosol form, terrain effects and obstacles – are therefore crucial elements in a real site and accident scenario.

The work described above has also identified the importance of scientific assessment in the evaluation process and particularly the need to understand why a model performs well in one situation while poorly in another, the physical limitations of a model and model user oriented aspects which might affect how it is applied.

There is therefore a need for a study of scientific model evaluation of dense gas dispersion models combining both scientific assessment with validation against observed data, while including the complex effects of aerosol release, complex terrain and obstacles. SMEDIS is the first attempt to apply this procedure to a large number of dense gas dispersion models – the majority in use across Europe. In so doing, SMEDIS seeks to encourage continual model improvement rather than to rank a set of models at one instant in time by leaving in place an evaluation protocol and an archived database of test cases which can be used by all dense gas dispersion model developers and users in the future.

1.4 Overview of SMEDIS

The overall objectives of SMEDIS are:-

- to develop further and test a protocol for scientific model evaluation of dense gas dispersion models;

- to carry out scientific model evaluation of all current dense gas dispersion models in Europe using this protocol with particular emphasis on the complex affects of aerosol formation, complex terrain and obstacles; and

- to leave in place a methodology for scientific model evaluation.

The project therefore involves many organisations involved in the development and application of dense gas dispersion models throughout Europe. The project is coordinated by the Health and Safety Executive (HSE, UK) with two other main partners, Cambridge Environmental Research Consultants (CERC, UK) and Electricit• de France (EdF, Fr). There are also ten other associated partners participating in the project: British Gas (BG, UK), Det Norsk Veritas Research (DNV, No), Finnish Meteorological Institute (FMI, Fin), Giz de France (GdF, Fr), The EC Joint Research Centre (JRC Ispra, It), The National Centre for Scientific Research 'Demokritos' (NCSR, Gr), RISO National Laboratory (RISO, Dk), TNO Institute of Environmental Scientific (TNO, NL), University of Hamburg (UH, De) and W S Atkins (WSA, UK). Additionally a number of external organisations have contributed both financially and technically to the project.

At the outset an initial list of dense gas dispersion models to which the methodology was to be applied was compared from these models regularly used by project participants. This initial list comprised a total of 24 models filling broadly into four main types : empirical screening tools, one-dimensional integral models, models based on the shallow layer equations and those designed computational fluid dynamics (CFD) models derived from solutions of the Na….-Stokes equations. These types increase in complexity and, in general, the resolution of detail required in model input and provided in model results.

In order that as many of the currently used dense gas dispersion models be included in the exercise attempts were made to augment this initial list of models. Thus:-

- an open call for participation in the exercise was placed in CORDIS (13); and

- through project partners contacts were made with other model developers and users outside the project both in Europe and the United States.

As a result a further 4 models were added to the list to give a total of 28. This full list of models is given in Table 1.1, those added from the initial set being marked by an asterisk. This table also gives the name of each model developer together with a model 'proponent' for SMEDIS, this being the organisation responsible for providing information on the model and carrying out the model runs for the validation exercise.

Scientific model evaluation comprises three main components; assessment, verification and validation. In SMEDIS the emphasis has been placed on assessment and validation. Verification has been handled through reference to previous verification activities.

Model	**Version**	**Year**	**Developer**	**Proponent**
Screening tools				
Britter-McQuaid Workbook	1	1988	HSE & CUED, UK	HSL
VDI Guideline 3783 Part 2	4.0	1990	Met. Institute, U. Hamburg, GERMANY	UH
Integral models				
AERCLOUD	1.0	1993	Finnish Met. Institute, FINLAND	FMI
DEGADIS *	2.1	1989	US Coastguard, US EPA and GRI, USA	UA
DRIFT	2.23	1991	AEA Technology	HSL
EOLE	3.0	1996	Gaz de France, FRANCE	GDF
ESCAPE	6.10	1996	Finnish Met. Institute, FINLAND	FMI
GASTAR	3.06	1999	CERC Ltd., UK	CERC
GReAT	2.0	1994	Ris❷ National Laboratory, DENMARK	Ris❷
HAGAR	4	1996	BG Technology, UK	BG
HGSystem	3	1994	Shell Research, UK	HSL
OHRAT/Multi-Stage	1.3.1	1996	Det Norske Veritas, UK/Norway	DNV
PHAST/UDM	6.0	1999	Det Norske Veritas, UK/USA	DNV
SLUMP	2B	1989	WS Atkins Safety & Reliability, UK	WSA
WHAZAN/HVYCLD	2.1	1993	Det Norske Veritas, UK/USA	DNV
Shallow-layer models				
DISPLAY-1	1.0	1996	EC Joint Research Centre, Ispra, ITALY	JRC
DISPLAY-2	1.0	1996	EC Joint Research Centre, Ispra, ITALY	JRC
SLAB	-	1990	Lawrence Livermore Natl. Lab., USA	TNO
SLAM	1.0	1996	Ris❷ National Laboratory, DENAMRK	Ris❷
TWODEE	10	1997	HSE/HSL, UK	HSL
CFD models				
ADREA-HF	2	1996	NCSR "DEMOKRITOS", GREECE	NCSR
CFX	4.1	1996	AEA Technology, UK	HSL
COBRA	4.06	1995	Mantis Numerics Ltd., UK	BG
FLACS *	2.0	1997	Christian Michelsen Research, NORWAY	CMR
FLUENT *	5.0.2	1998	FLUENT, UK	NH
FAMELEON FireEx 98 *	-	1997	SINTEF, NORWAY	SINTEF
MERCURE	3.2	1996	Electricit• de France, FRANCE	EDF
STAR-CD	2.300	1996	Computational Dynamics Ltd., UK	WSA

Table 1.1 Models and participants in SMEDIS.

In this table: HSL = Health & Safety Laboratory, UK; CUED = Cambridge University Engineering Department, UK; UA = University of Arkansas, USA; NH – Norsk Hydro, Norway; US EPA = Environmental Protection Agency, USA; GRI = Gas Research Institute, USA.

In the SMEDIS procedure, therefore, each model has undergone a detailed scientific assessment or review, focusing on its scientific basis and taking into account practical user-oriented aspects. This has been done according to a prescribed draft protocol with input of information from the model developer. This protocol has been devised to highlight the importance of complex affects. The product is a Model Evaluation Report (MER). This report is then finalised only after consultation with and agreement of the model developer. Finally, in the light of experience gained with each model, a revised protocol has been produced for use by future model developers/users.

Additionally each model has been the subject of a validation exercise using specially-selected data sets. Thus a database comprising data sets comprising at least one complex affect of interest has been assembled and the data processed into an agreed set of validation comparison parameters. These data have been circulated to model 'proponents' and the models run against selected cases. The results of this exercise have been collated centrally in terms of agreed statistical comparison parameters. These results together with a brief commentary on how the model 'proponent' undertook the comparison, have been incorporated in the MER.

Table 1.2 shows the principal tasks involved in each part of the evaluation. SMEDIS was largely concerned with assessment and validation and in both cases there are preliminary stages, setting up the procedures followed by implementation/application of these procedures to each mode. Hence the 'methodology' or 'protocol' comprises the documented form of these procedures.

The responsibility of the development of the procedures has been largely that of the main partners (HSL, CERC and EdF) but with discussion and input from all other partners. The implementation of the procedures is primarily the responsibility of one organisation (CERC) for the scientific assessments and the model proponents for the validation exercise (but with coordination by EdF and HSL). The production and circulation of the SMEDIS database has been the responsibility of EdF and HSL.

ASSESSMENT (♏2)	VERIFICATION (♏3)	VALIDATION (♏4)
1. Development of protocol for scientific assessment	1. included as part of assessment through evidence of previous verification undertaken	1. data set group identification
2. information gathering		2. scenario classifiction
		3. identification of specific cases
3. application of protocol to information supplied		4. development of validation procedure (a) physical parameters (b) statistical parameters (c) rest of procedure
4. agreement of Model Evaluation Reports		5. production and circulation of data sets
5. revision of protocol		6. application of procedure to data sets supplied

Table 1.2 Project tasks in SMEDIS for assessment, verification and validation.

1.5 SMEDIS Outputs

A description of each of the tasks listed in Table 1.2 is given in Sections 2 – 4 of this report. These detail the development of the procedures and their application to the models listed in Table 1.1. The final output from this exercise comprises:-

- A fully developed and tested protocol for use by future model developers/users. This is found at Appendix 5.

- A database for use in future validation exercises. This is found at Appendix 2.

- A model evaluation report (MER) for each model involved in the exercise. These are found in Appendix 6. Due to Commercial-in-Confidence concerns all means of identifying the model with its MER have been removed. Elsewhere all references connecting models to results have also been removed for the same reasons. Only project partners retain the means of identifying specific models.

In addition, it is also intended to make the assessment protocol and evaluation database available both on CD and via a SMEDIS website.

A SMEDIS Workshop was also one of the planned project outputs. This was held on the morning of Wednesday 13 October 1999 as a special session of the 'Sixth International Conference on Harmonisation of Atmospheric Dispersion Modelling for Regulatory Purposes' at INSA de Rouen, Rouen, France. This event was attended by most of the thirteen project partners, many of their sponsors, invited speakers who included representatives from regulators, industry, consultants and the US scientific dispersion community and participants at the conference.

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Chapter 2 Scientific Assessments

2.1 Introduction

As we have seen in Chapter 1, scientific model evaluation consists of three elements – assessment, verification and validation – and in this chapter we describe the assessment of the models in SMEDIS.

Model validation – the comparison of model predictions with experimental data – is a familiar part of the process that establishes that a model is able to give “good” results. However, important though this is, it has come to be recognised that there are other aspects of a model that should be considered before applying a model to a given problem. These are concerned with appropriate and defensible use of a model in simulating the problem, with the corollary that the user must recognise and respect the model’s limitations. It is these latter aspects that the scientific assessment addresses through a systematic objective review of the model, giving a picture of *both* the strengths *and* the weaknesses of a model allowing a statement of the situations to which it does or does not appear to be applicable. Thus as well as model “quality” we are concerned with “fitness-for-purpose”.

Intimately connected with the evaluation is the evaluation *protocol*, a document describing the procedure to be followed in the evaluation of each model. It is sometimes used to denote the description of the assessment procedure alone; however, it is important to emphasise that all three elements of the evaluation are covered by the protocol, and any association with the scientific assessment is perhaps due to the dominant contribution to the protocol document from the description of the assessment. For this reason we will discuss the protocol in this chapter.

Similarly, the results of the assessment form the major part of the *Model Evaluation Report* or MER. This document also contains a summary of the results from the validation exercise (and if appropriate the verification exercise) to give a complete record of the evaluation.

The MER is intended for use by both the model developer and model users:

- for the model developer it represents an independent examination of their model according to a protocol which has been applied to a wide range of other dense gas dispersion models.
- for the model user the report assists them in deciding whether the model is appropriate to their intended use (including possibly not to use it at all). The inclusion of both scientific and user-oriented aspects of the model in the assessment helps the user to gauge how well the model can simulate the specific scientific problem of interest as well as how well the model performs from a practical point of view.

In all cases, the report can form part of the standard documentation accompanying the model in the specific version.

Together with participation in the validation exercise, the scientific assessment of each model in SMEDIS represents one of the two principal parts of the scientific evaluation. The detail with which every model has been examined in SMEDIS plus the large number of models taking part – 28 in total – has meant that this has been a major undertaking.

Having given an overview, the remainder of this chapter is organised as follows. We begin with a description of the two main ingredients of scientific assessment, namely the protocol and the gathering of information on each model – the “raw data” for the scientific assessments. The next section presents an analysis of the results of the scientific assessments, in which we aim to make statements on the appropriateness of the various models for application to dense gas dispersion problems. We organise this by highlighting the key features of a realistic dense gas dispersion problem and then for each discuss how the four generic classes – and the models we have examined within each class – would fare in terms of being able to handle the features of the problem. The "results" also include findings from the evaluator's perspective. We conclude the chapter with a discussion of lessons learned from carrying out the exercise, a summary of the major findings and how the work might be extended or applied to new areas.

2.2 Preliminary tasks

Before the scientific assessments could begin, two main tasks were required in SMEDIS, namely the development of the evaluation protocol – which deals with the handling of not only the scientific assessment but also the validation and verification elements – and the gathering of the necessary information on models for the scientific assessments.

2.2.1 Development of SMEDIS protocol

One of the early tasks in SMEDIS was to develop an evaluation protocol. This task was undertaken by CERC, with contributions/comments from all partners, in particular Risø, HSE and EDF.

The SMEDIS protocol was developed in a form consistent with the EC Model Evaluation Group (MEG) generic protocol [REF] and the Heavy Gas Dispersion Expert Group (HGDEG) protocol [REF]. However, for a project such as SMEDIS the MEG protocol was much too general and has been used as a guide only. Similarly, the HGDEG protocol, although far more detailed and having been made specific to dense gas dispersion compared with the MEG protocol, was still considered to be not explicit enough in its description of the evaluation procedure. In developing the SMEDIS protocol we have therefore tried to make it as structured and explicit as possible.

However, we have taken the protocol still further. In addition to the evaluation procedure itself we have also included a description of the additional stages before and after the evaluations: these are stages that have been undertaken in SMEDIS, such as the development of the protocol, but which would not necessarily be required every time the protocol is used: this would depend on the aims of any model evaluation project using the protocol. Thus the protocol document becomes further self-contained and allows for future developments beyond simply the same procedure being applied to additional (or possible re-applied to the same) models.

The guiding principles in SMEDIS may be summarised as follows.

1. The models considered by SMEDIS are all models either specifically designed for or capable of being applied to dense gas dispersion problems. Both types of model are referred to as dense gas dispersion or DGD models.
2. Although DGD models are often used in association with other models, in particular with various release models, or may simply represent one type of application for a more complex model, it is beyond the scope of the procedure to consider evaluation of the "extended" model. In particular, jet models, which are often used prior to a DGD model, are not considered.
3. Application of DGD models to problems featuring the effects of aerosols, complex terrain and obstacles is addressed explicitly – the so-called context-of-use. Hence the ability of a model to simulate problems containing such features is of particular interest.
4. Validation is treated actively, while assessment and verification are treated passively. This requires the protocol to deal with validation in much more detail than if all three parts had been treated passively.

5. There is some scope for self-evaluation, i.e. by the model developer, as well as evaluation by an independent third party. During SMEDIS, validation is treated in this way since the model proponent, who in many cases is the model developer, runs the model – they are also permitted to know the experimental data before running the model and may run the model more than once following further changes to the model, i.e. model evolution. This was allowed in order to encourage model improvement.
6. Parts of the procedure involving the active use of the model must be documented to make them auditable and results reproducible. This would apply even if an independent third party were performing the evaluation, since they may need to carry out pre- or post-processing of data for the model. In the case where model evolution is allowed, such documentation is even more important.
7. The performance of the models is quantified using a range of data sets and performance measures, including quantitative statistical comparison techniques. However, ranking of models according to their performance is *not* carried out.
8. Models are treated in a uniform way as far as possible, but the range of DGD models, with their differing capabilities and requirements, is taken into account. Individual circumstances of a model, such as the way it is currently used, are also acknowledged when assessments are made.
9. A policy of comment from participants (evaluator, model developer, information supplier) is adopted to help to improve the procedure/protocol.
10. The aim is that the procedure put in place will continue to be used to evaluate models beyond the end of the project. Application of the procedure should be useful in the development of a given DGD model (through self-evaluation) as well as DGD models in general by highlighting where the strengths and weaknesses lie. Areas are identified where further data would benefit the evaluation process.
11. Ideally, the information produced by the evaluation should be available to the public domain. However, it is recognised that for proprietary models this may not be possible, although some form of openly-available results would be desirable, and it is hoped the Model Evaluation Report would be treated in the same way as other documentation on a model.

We end with a brief outline of the SMEDIS model evaluation protocol – see Table 2.1. A more detailed outline is given in an Annex to this chapter, and the full description is, of course, to be found in the protocol document itself, which is reproduced in Appendix 5 of this report.

2.2.2 Obtaining information on models

Once the protocol has been developed, the other initial main task as far as the scientific assessments are concerned is to gather information on each model. The approach taken in SMEDIS was to use as far as possible pre-existing documentation on the model to cover the topics of interest, e.g. the technical specification, user manual, validation document, etc. for the model, or their equivalent.

In SMEDIS, it is the responsibility of the model proponent in the project to supply this information. In 75% of cases the proponent was also the developer of the model, while in the remaining cases they were a licensee/experienced user of the model.

Stage 1 Pre-evaluation tasks (a) List models and responsible parties (b*) Define the scope of the model evaluation project (c*) Assess whether there is a suitable protocol that is applicable to the models (d*) Develop/modify protocol (e*) Develop/modify validation database *Note that the parts marked with an asterisk* would not be necessary for application of the procedure to additional models (or, say, new versions of the existing models).* **Stage 2 Carry out the scientific assessments** Obtain information on models and apply protocol to this information to produce the MER. **Stage 3 Carry out the verification exercise** (This is simply part of Stage 2 in SMEDIS.) **Stage 4 Carry out the validation exercise** Set up input data, run models and make comparisons according to protocol. *Note that Stages 2, 3 and 4 can take place in parallel.* **Stage 5 Post-evaluation tasks** (a) Seek agreement of evaluation with model developer/proponent (b) Refine the protocol

Table 2.1 The main stages of the SMEDIS evaluation procedure

Clearly, such information should cover all aspects of the model that are to be considered in the assessment in order to give the evaluator the most complete picture possible of the model. To facilitate the task of the information supplier two questionnaires were formulated and circulated to information suppliers for completion.

- The first questionnaire was intended to obtain summary information on the models in the project, so that the general scope of participating models was established at an early stage. The survey concentrated on their broad capabilities and implementation features, e.g. can a model handle two-phase releases, what computer platforms does it run on, etc. The results from the questionnaire returns were collated for each of the four model types. The questionnaire is included within the protocol (see Appendix 5 to this report).
- The second questionnaire was intended to obtain the detailed information on the models required for the scientific assessments. The questionnaire was therefore structured according to the topics of the assessment (see 2.2.1), with spaces for the information supplier either to give a cross-reference to a supplied document that covered that point or to include the information explicitly in the completed questionnaire. The latter situation can arise for even the most well-documented model, since certain topics are unlikely to be included in documentation, e.g. current model users, run times for given problems. The completed questionnaire was returned together with copies of the documents referred to therein. The questionnaire is also included in the protocol (Appendix 5).

2.3 Results from scientific assessments

2.3.1 Evaluation aspects

Before discussing the models themselves, we consider the SMEDIS scientific assessments from the point of view of the evaluator(s).

Documentation

The approach used in SMEDIS for the scientific assessments is to rely on pre-existing information to minimise the imposition on the model proponent/information supplier. This works well provided there is enough documentation of sufficient detail available and/or the model proponent is willing to supplement the existing documentation with new material. If such information is not made available then the comprehensiveness of the assessment may be compromised.

In practice, the documentation supplied fell short of expectations/requirements on several counts.

- The quantity of documentation provided varied greatly between models. Despite the fact that 75% of the information suppliers were also the model developers, none of the models supplied the “ideal” combination of technical description, user manual, validation document and verification document, although one or two came close. However, in general, the documentation was a long way from this ideal situation and in some cases it was virtually non-existent. There was no consistent trend with model type.
- For many models the quality of documentation supplied (which is assumed to be the best available) was not high – incomplete, poorly-written, unnecessarily complicated. It was adequate at best in most cases. On the whole the commercial or widely-available (public domain) models were documented most clearly and completely, as one might expect.

This survey would therefore suggest that there is a need for improvement in the documentation at least to some minimum level of completeness. The SMEDIS MER could provide some basis for improving documentation, at least the scientific description and possibly other parts, through the MER template.

Confidentiality

During the course of the preliminary stages of SMEDIS, there was discussion of how to handle the confidentiality nature of some of the models being considered – after all, a number of the models were proprietary and information on them was therefore of a commercially sensitive nature. There were two main aspects to consider:

- supply of information to the evaluator for the scientific assessment
- the fate of the MER once completed

The first of these was handled through (a) developing a document (Ref. SMEDIS/98/6/Z, “Information management procedures for SMEDIS”) setting out how information should be handled and (b) a formal written request issued by the information supplier to treat the information in accordance with this document and the evaluator sending a formal written acceptance of these terms.

This procedure has been followed where requested (only two information suppliers followed this procedure, although several other organisations supplied information that was marked as confidential without a formal agreement from the evaluators).

As far as the second of these was concerned, it was agreed that the MER would be the property of the information supplier and therefore theirs to control the distribution. However, the hope was expressed that the information suppliers would in fact distribute these documents freely.

In practice, the amount of detail taken from the documentation supplied, including confidential documentation, has not been great, e.g. only limited mathematical formulae have been reproduced in the MERs. Thus no information has been used that would not have been available to a user/customer, and so at the very least the MER for a given model should not present confidentiality problems with the users of that model. Indeed, since the MER is an agreed document with the developer, it is likely that it will prove useful for the developer in promoting the use of the model.

Application of protocol
As noted above, the application of the SMEDIS protocol to information on the models began using a "working" version of the protocol. This contained a provisional set of headings (together with accompanying instructions), to be revised (if required) as a result of carrying out the assessments. It was found that in the vast majority of cases the content of the protocol was satisfactory in terms of the headings used; however, the major addition to the reports was in providing the summary information given in the most important sections (see Section 2.5). It was felt that this was important because it gave a rapid overview of the model, for those who did not wish to read the full details of the assessment and could form the basis of a summary document (formed by extracting these summary boxes).

Faced with documentation to digest with such a variety of completeness as well as style and organisation, experience began to suggest a most efficient way to absorb the information before carrying out the assessment.

- The documents that describe the technical content of the model were surveyed first. Ideally these would comprise a single technical specification, but generally a mixture of papers with short descriptions, reports with longer descriptions was supplied. In many cases these described features that were not implemented in the model in the same way, or in some cases not at all.
- If available, the User Manual was one of the most useful documents to consult at an early stage, since in particular it (normally) describes the input data for the version of the model being evaluated. This helps to confirm the actual capabilities of that model version. The description of input data also reveals the properties of the released substance and the environment that the user is required to specify.
- If necessary, the documents describing technical content may then be reviewed in the light of the limitations of the implementation.

2.3.2 Scientific aspects

We turn now to the scientific aspects of the dense gas dispersion models examined in SMEDIS. As noted earlier, the approach in this section is to focus on the most important aspects of a problem that need to be addressed and to consider how each of the categories of models handles the aspect in question.

Recall that the total numbers of models in each category is: Screening Tools (2), Integral Models (13), Shallow Layer Models (5), CFD Models (8).

(a) Release conditions

We are concerned here with the treatment of the dense gas source and the stages leading to production of the source.

Release conditions – *the stages leading to the dense gas source*	
Screening tools	Both screening tools take into account in a global way the source of the dense gas, but neither is able to model these stages directly – only its effect on the initial conditions, in particular the density.
Integral	It is quite common for integral models to have available directly release models for one or more of the common release scenarios. The commonest example is for a jet release option to be incorporated directly within the DGD model, interfaced transparently to the dense gas calculation. Several models were also interfaced with a vaporising pool model.
Shallow layer	Shallow-layer models have some disadvantages over integral models in this respect, in that they need the release configuration to be consistent with the shallow-water assumptions. It is quite difficult to include general release models within the framework of shallow-layer theory.
CFD	Users should expect to model the initial release either with a separate model or using the model itself – in the latter case, a separate simulation would be advisable given the need to grid the entire domain (possibly not if adaptive refinement is allowed). Some CFD models have been developed explicitly for dispersion problems, and these may simulate jet releases directly, effectively through sub-grid scale modelling. However, flashing jets are outside the scope of even these models.

Release conditions – *time-variation of source*	
Screening tools	The only consideration of time variation of the source is to define equivalent instantaneous or continuous releases. Hence there is no time variation of the solution corresponding to time variation of source conditions.
Integral	Approximately half the integral models consider time variation of the source. In all cases, they use a combination of "equivalent" instantaneous and continuous releases – some just use a single representative release while some segment the source in time and superpose a set of continuous releases with suitably defined starting conditions to give the spatial distribution at a given time. There does not appear to be a clear consensus on how the general time variation and the continuous/instantaneous sources should be related.
Shallow layer	In principle these are better able to solve the time-dependent equations directly. Usually models restrict the form of the time variation to continuous releases.
CFD	By definition, CFD codes are based on the time-dependent equations and solve for the time variation explicitly. This is true of all the CFD models here (with the possible exception of one). CFD models can also usually calculate the time evolution towards a steady state for a *steady* source.

Release conditions *– geometry of source*	
Screening tools	The specific geometry of the source is not taken into account in these models, only some representative length scale (other length scales are derived from the source strength and density). Thus multiple sources could be aggregated into a single source.
Integral	Normally only a right circular cylinder for instantaneous and a rectangular vertical plane at the start of the plume for a continuous release.
Shallow layer	For the 2-D models there is scope for defining a more general (2-D) spatial distribution. In some cases the user may also specify a vertical mass flux, i.e. a more realistic representation of a low momentum area source.
CFD	Normally complete generality is possible for the geometry of the source, including multiple and elevated sources.

(b) Substance released

Substance released *– the range of release materials*	
Screening tools	The primary characteristic of the specific released substance is its density. Hence the models may treat a very general substance including mixtures.
Integral	All the integral models in the study took the released substance to be a single material, i.e. no true mixtures unless it could be described as an effective single component material. Many models have a set of pre-defined materials (flammable and toxic) in a database. Users may normally define new substances.
Shallow layer	Essentially the same remarks apply here as for integral models, although in general the availability of pre-defined substances was less.
CFD	Generality of set-up continues with the substance released, which appears to be a general mixture in most cases. This is often a necessity due to the consideration of chemical reactions. Databases of pre-defined substances are common.

(c) Atmospheric conditions

***Atmospheric conditions** – wind and stability*	
Screening tools	The main property of the atmosphere is the wind speed. One model uses a worst case wind speed (since it aims at conservative “worst-case” conditions), while the other has a general wind speed. Stability is not taken into account except in some qualifying remarks.
Integral	Typically the user may select a wind speed (at a given height) down to some minimum non-zero value together with any stability conditions through a Pasquill stability category and/or Monin-Obukhov length. Most models adopt a logarithmic vertical wind profile but only in some cases are there profiles modified by the stability. Very few models appear to be able to handle zero wind conditions. These representations capture the features of the atmosphere essential for the description of the physical processes in dense gas dispersion.
Shallow layer	These handle atmospheric conditions in essentially the same way as integral models. There is no account taken of the change in wind due to complex terrain or obstacles. They can operate in zero wind conditions.
CFD	CFD models have the potential to calculate the atmospheric flow field, including both mean flow and turbulence, as well as the effects of terrain and obstacles in modifying it. However, apart from those CFD models that were specifically designed for dispersion, little or no guidance is offered for modelling atmospheric flows. It appears likely that in practice it would be necessary to use empirical profiles for upstream boundary conditions.

(d) Thermodynamics

***Thermodynamics** – cold releases, heat transfer*	
Screening tools	Thermodynamic effects are not considered in these models – only qualifying remarks are given relevant to the determination of the source properties.
Integral	Most of the integral models in the study allow a non-ambient-temperature release to be considered (which is very important for scenarios commonly of interest). Usually both forced and free convection are considered, although the formulae used show some variation. In some cases these convective effects are also taken into account in modifying the entrainment through augmenting the entrainment velocity scale.
Shallow layer	More than half of these models do not take into account thermodynamics, which would be a serious omission for a model that is calculating the evolution of the cloud. Thermodynamics if included, appears through an additional equation formulated in the same manner as the shallow-water equations. This provides a consistent mechanism to include heat transfer.
CFD	Releases of arbitrary temperature may be defined. Heat transfer processes must be characterised in terms of appropriate boundary conditions. In many cases it is possible for the calculation of the heat flow in the ground to be performed and coupled with heat flow into the cloud. Heat transfer to/from obstacles may be treated the same way.

(e) Dispersion effects

***Dispersion effects** – near-source behaviour*	
Screening tools	Since these models are based on empirical evidence, near-source behaviour is automatically taken into account.
Integral	Only a few of the integral models in the study are able to take into account the formation of a secondary vapour blanket, and the resulting increase in the effective width of the plume starting conditions (possibly also a reduction in initial concentration). This is especially important for integral models, with their somewhat inflexible representation of the plume, including the starting conditions.
Shallow layer	None of the shallow-layer models automatically take into account the effects of near source behaviour such as a secondary vapour blanket. The initial conditions can, in principle, be set to include these effects but a preliminary calculation is needed.
CFD	Near-source behaviour should be automatically taken into account in the solution of the governing equations.

***Dispersion effects** – concentration fluctuations*	
Screening tools	The conservative screening tool is able to give a quantitative measure of the mean square fluctuation of the concentration. BMW does not treat fluctuations explicitly.
Integral	None of the integral models give quantitative information on concentration fluctuations. However, some effects of the stochastic nature of dispersion are taken into account through consideration of averaging time – a number of models use an empirically-based correction to the cloud dispersion parameters (and thence to the mean concentrations).
Shallow layer	Neither explicit fluctuation information nor averaging time effects are considered in these models.
CFD	From the available documentation, it appeared that some models might be able to give quantitative information on concentration fluctuations, but details were scarce. The important issue of averaging time is not considered by these models.

***Dispersion effects** – shear dispersion*	
Screening tools	Since these models are based on empirical data, it would be expected that shear dispersion effects (if important in the cases considered) would be taken into account.
Integral	Very few of the integral models provide corrections for shear dispersion, which can have a significant effect on finite clouds (puff releases). This is treated through an addition to the longitudinal dispersion parameter.
Shallow layer	Shallow-layer models do not include the effects of shear dispersion. These models explicitly integrate over the depth of the cloud and include the effects of the atmospheric flow in a similar way.
CFD	In general, it would be expected that CFD models would capture the effects of shear dispersion since they are able to model both the vertical turbulent mixing and the velocity shear well.

Dispersion effects *– passive dispersion*	
Screening tools	The screening tools considered are explicitly concerned with the dense gas phase and not the passive phase.
Integral	Many of the integral models allow the passive dispersion phase to be considered. Standard Gaussian concentration profiles are adopted, while a matching condition is employed at the transition point to relate the passive cloud parameters to the cloud at the end of the dense regime. There did not appear to be a consensus on the matching conditions that should be applied.
Shallow layer	The essence of a shallow-layer model is the presence of a well-defined layer over which properties are assumed to be vertically uniform. Thus the passive limit is not a natural extension. However, models can deal with this in some form by increasing entrainment by the ambient flow in this limit.
CFD	CFD models continue to calculate the evolution of the cloud without specific regard to whether it is passive or not. The only likely restriction is whether the computational domain is able to extend far enough to encompass the passive dispersion region.

(f) Complex effects

Complex effects *– aerosol releases*	
Screening tools	Two-phase effects are not taken into account explicitly: they are only treated in the accompanying guidance on source definition (or are neglected altogether).
Integral	Most (10/13) of the integral models in the study had some capability to model releases containing a mixture of vapour and liquid droplets, a situation commonly encountered in real releases. All except one of these used the homogeneous equilibrium assumption rather than an explicit droplet model (although this was not a full dispersion model; one other model had elements of both). This is appropriate for the integral formulation. The important phenomenon of rainout is only addressed by one dispersion model.
Shallow layer	Few (2/5) shallow layer models in the study had an aerosol release capability. One used the homogeneous equilibrium assumption (the other some different treatment). Rainout is not addressed.
CFD	Only some of the CFD models appear to provide a capability for aerosol releases, which is slightly surprising. Only one definitely used an explicit droplet model (although possibly others did also), which also appears to be the only model that can handle rainout (which would require further post-processing).

***Complex effects** – complex terrain/slopes*	
Screening tools	Not taken into account by these models (only considered in the discussion of their importance).
Integral	Only three of the integral models take slopes into account, although for one of these only for instantaneous releases. Both the other models allow cross-wind slopes and multiple slope segments.
Shallow layer	Three of these models allow general 2-D sloping terrain in principle. Complex terrain must be consistent with the shallow-layer approximations, i.e. small slopes. One considers simple 1-D slopes and the other does not consider this complex effect.
CFD	General sloping terrain may be defined through the computational grid surfaces, with the effects on dispersion handled automatically through the governing equations.

***Complex effects** – obstacles*	
Screening tools	The conservative screening tool takes into account a wide variety of generic obstacle arrangements. The other only discusses obstacles in terms of their potential importance.
Integral	Only three of the integral models take obstacles into account. They all consider collections of 2-D fences and finite buildings and calculate the *net* effect on the cloud, in particular the change in width and height of the cloud as a result of the interaction.
Shallow layer	Some shallow-layer models claim to treat obstacles. Where included, obstacles are usually treated as an extension of the complex terrain. This is questionable in the context of shallow-water approximations.
CFD	CFD models treat obstacles in essentially the same way as terrain, through the computational grid and appropriate boundary conditions, and hence with the same generality as for terrain. They can calculate the detailed effect of the obstructions on the flow field and the dispersion.

(g) Output

Output *– concentration distribution*	
Screening tools	Screening tools are not designed to give concentration distributions – they provide an estimate of the maximum concentration or the greatest concentration (under worst case conditions) likely to be encountered at a given distance downstream.
Integral	Integral models calculate a “top-hat” concentration (uniform over the volume for instantaneous and over a cross-section for continuous releases) and then apply concentration profiles to these uniform distributions. Some of the integral models did not use concentration profiles, so that these models would tend to provide an arbitrary measure of the cloud width (and height) and would tend to under-estimate the maximum ground-level concentrations. A variety of profiles were used, although most were based on error functions or Gaussian curves.
Shallow layer	The 2-D shallow layer models give the distribution of depth-averaged concentration in two dimensions, with in one case shape functions to provide the vertical distribution. The 1-D models are much like integral models either using vertically averaged values or imposing profiles.
CFD	CFD models are able to provide the complete 3-D concentration distribution at all points in the flow domain. For time-dependent situations, this information is usually also available at any specified time.

Output *– concentration derived data*	
Screening tools	Other than the maximum concentration (see above), which could be considered as derived data, screening tools do not provide directly any derived data – these must be calculated separately by the user.
Integral	Many integral models provide a subset of the derived concentration data of interest, such as distance to LFL, concentration contours, toxic dose, flammable mass, although there did not appear to be a clear priority for which data to provide.
Shallow layer	Derived concentration data was sparse for this model type. Only one 2-D model gave limited derived data and one 1-D model gave a good selection of derived data (at least for continuous releases).
CFD	Due to their general-purpose nature, CFD models do not normally provide derived concentration data such as dose or flammable inventory directly: they have all the necessary “raw material” available and any of the derived quantities would be available provided suitable post-processing were applied.

Output – *other output*	
Screening tools	Screening tools do not provide any output other than concentration output (although one of the two considered does give a measure of the cloud width).
Integral	Most integral models provide an estimate of the temperature (although only the "top-hat" value and not a distribution), together with a (bulk) advection speed and cloud dimensions.
Shallow layer	Those models with thermodynamics capabilities give the temperature; the 2-D models give two velocity components.
CFD	As for the concentration distribution, CFD models provide complete distributions (including time evolution) of all the dependent variables. These would typically include three components of velocity, pressure, density and temperature as well as properties of the turbulence such as kinetic energy and dissipation rate.

2.3.3 User aspects

Turning now to the consideration of the user-oriented aspects of the models, the approach we take here is to consider the different stages of usage of a model, from initial usage by a new user, through the familiarisation process and then finally to routine usage of the model by a (sufficiently) experienced user.

(a) Initial usage

Availability
Only 5 of the models appear to be freely-available public domain models: both the screening tools, two integral models and one shallow layer model. The remainder are proprietary: integral models typically cost around 1000-1500 GBP to licence; the two shallow layer models stated to be available were around 2000-4000 GBP; while CFD models were typically cost more than 10,000 GBP. Several models were of uncertain status.

Installation
The proprietary models tended to have a more sophisticated, user-friendly installation procedure using a script or application, while non-proprietary models tended to require simply copying the files to a specified directory together with possibly some adjustments to the operating environment.

(b) Familiarisation

Documentation
Although, as already noted in 2.3.1, the general standard of documentation supplied was disappointing, some of the better documentation was to be found in the User Manual and other user-oriented material. This documentation generally gave a reasonable introduction to the use of a given model, although it was not uncommon that

- information was spread over several different documents, meaning that it sometimes was difficult to obtain clear and unambiguous information on a particular topic relating to the model. It would be preferable, if possible, always to have a single user reference for a specific version of a model
- input data parameters were not defined very carefully/comprehensively, and advice and guidance on how to select model options and parameter values was often sparse

- worked examples, at least in the documentation supplied for this project, were almost non-existent except in very few cases.

Experience requirements
As one might have expected, the length of the familiarisation period suggested by model proponents increased with the complexity of the model – from hours to months at the two ends of the spectrum – and decreased with the amount of prior experience. This latter point is especially relevant to the use of CFD models, where due to their general-purpose nature experience with any CFD code will be of some value; however, it should be recognised that problem-specific experience would be particularly valuable here due to the (apparent) limited application of CFD models to dispersion problems in general.

(c) Routine usage

Computer resources
As for experience requirements, the computer resources follow a predictably increasing path from simple to complex models, with corresponding shifts in the type of computer hardware from simple PCs to high-end PCs, workstations and supercomputers. Such resource requirements clearly play an important role in how a given model is used in practice. This was reflected in the active validation phase of SMEDIS where different numbers of runs were carried out by the different model classes with the number decreasing from simple to complex models.

User interface
A number of models provided a graphical user interface (GUI) as opposed to a text-based one. Although GUIs require considerably more effort to develop (and, to some extent, to maintain) they are much better-suited to a number of useful tasks of the interface that make it more user-friendly, such as

- verifying input – this is a very useful function that can help to eliminate accidental mistakes when entering data, checking the input data against pre-defined ranges (or with other more complex checks) before it is saved as a valid input file
- providing on-line help
- providing lists of options to choose from – e.g. through menus and "drop-down list boxes", helping to standardise input
- allowing significant groups of data to be viewed (and checked) simultaneously
- providing comprehensive error and warning messages
- seamlessly integrating graphical/numerical display of results

It is possible for all these tasks to be accomplished with a text-based interface; however, the flexibility and functionality of a GUI is almost certain to be superior to the textual equivalent. In fact note that for a number of the models with textual interfaces it was stated that development of a GUI was planned for future versions.

Post-processing
The presentation of graphical and numerical results from a model run was available in a variety of formats and at varying levels for the models in this study, and it is therefore difficult to generalise. However, the available presentation was generally fairly limited – certainly not comprehensive in most cases. Most models required extra software for graphical representation of the results, and there was no common standard. All models gave information on the concentration field down wind of the release. In integral and shallow water models this information is the main output and was

usually readily available. For the CFD models much more information was available and it seemed necessary for the user to make special effort to obtain the results in a form suitable for dispersion analysis and risk assessment.

Databases

Many of the models in the study provided a database of materials and their properties. In general this is a valuable user-oriented feature of a model, since it helps to standardise input – further databases of other features of a problem, such as the surface roughness length, would also be valuable in standardising this parameter. However, databases must be controlled carefully – in particular in the way they are modified, since unregulated changes to a database can cause more problems than use of a database solves. In some of the models in this study there appears to be little control over who modifies the database together with possible local copies of the database being used. Thus databases are effective when used carefully.

2.3.4 Verification aspects

(a) Direct verification

Explicit evidence for this is very limited, but assuming that this forms part of ISO 9001 compliance approximately a quarter of the models appear to have undergone line-by-line checking. This may apply to further models that have been developed according to internal QA standards (see (c) below), but to rather less than a half of the models in total.

(b) Indirect verification

Those models for which indirect verification was claimed, such as comparisons of predictions against exact solutions of simplified problems, either did not give the specific tests or, in the cases where the tests were given, they did not seem to particularly helpful in establishing the model had been accurately implemented. This may be due in part to the lack of convenient comparisons available. A centralised source of such comparisons could perhaps usefully be made available to developers of DGD models.

(c) Quality assurance

For only 3 models (one integral and 2 CFD) was there evidence that an external QA standard had been gained (ISO 9001). For a further 8 models it was claimed that internal QA standards applied in developing the model (implementation). Not surprisingly perhaps, there was a high correlation between the adoption of QA standards of one sort or another and the proprietary nature of a model.

(d) Evidence of verification by model group

Considering the overall evidence to create confidence that verification had been carried out satisfactorily, the CFD models appear to present the best evidence as a group, although this relies to some extent on implications for QA standards. This would not be a surprising outcome, given the generally commercial nature of these models together with their complexity.

Not far behind are the integral models, approximately half of which give good to excellent overall evidence of verification (but again relying on QA standards being worth something). Some further models did not provide much evidence, but given their large numbers of users it is likely that inaccuracies in coding would be highlighted through extensive practical use.

The implementation of screening tools is essentially simple, and since both examples in this study have been used widely, it is to be expected that their verification is satisfactory.

This leaves the shallow layer models, which trail the other groups in providing convincing evidence of verification. There was no evidence for any of the models in the group that any form of QA standard applied, no evidence of direct verification and only limited indirect verification. With the exception of one model, a large user population could also be ruled out in assisting to increase user confidence in this respect. These observations reflect the largely non-commercial nature and restricted user population for these models.

2.3.5 Validation aspects

This is concerned with validation carried out prior to the SMEDIS project, as reported in the documentation supplied for the scientific assessments.

(a) Field data vs. laboratory data

The vast majority of data sets cited as having been used in validation comparisons are field data sets. Furthermore these are mostly taken from the Modeler's Data Archive (MDA) developed by Hanna and co-workers from the large-scale field tests in the US, with a few examples of more recent EU-research-funded data sets (BA, FLADIS) used by some models (tending to be those that originated in a European research context). This shows that the SMEDIS database, which uses many data sets of European origin, may be considered complementary to the MDA.

(b) Substances range

Given the bias towards the MDA tests, the substances for which the models have been validated are largely those considered there – for models that have attempted the full range of tests, this means a wide variety of hazardous substances, including a range of both toxic (ammonia, hydrogen fluoride) and flammable (LNG, propane) materials. There are also series of passive releases for testing models that include the capability to model this type of release.

(c) Presence of complex effects

Of the three types of complex effect considered by SMEDIS, by far the commonest effect present in the tests is the aerosol release, since many of the experiments used liquefied gases stored under pressure. This was true of both the older data sets (MDA) and the newer European field tests. However, these release conditions also tended to mean that the release was a jet, making it difficult (or impossible) to isolate performance of the dense gas model with respect to aerosol effects.

The next most common complex effect was that of obstacles. However, field tests exhibiting this effect are largely confined to Thorney Island (in the MDA) together with some of the more recent European tests, which used mostly fence-like obstructions.

Finally, slopes/complex terrain were represented very sparsely. There were no field-scale tests cited showing significant slope; and in only three cases did any (laboratory) tests appear to have been used to investigate slope effects.

These observations show that the SMEDIS database is again complementary to the earlier well-established MDA.

(d) Evidence of validation by model group

Looking at each group of models, it may be concluded on the available evidence that the integral models offer the most comprehensive accounts of validation comparisons for dense gas dispersion problems, with some models providing extensive and carefully prepared documentation of validation carried out. This is probably due to the common use of integral models operationally.

The weakest group, again based on the available evidence, are probably the CFD models, many of which showed scant evidence of *any* application to dense gas dispersion problems. There may be several reasons for this: for example, it is relatively uncommon to apply CFD models to this type of problem; the relatively high cost of running CFD models means that simulating many different cases, and even re-running the same case in order to produce better agreement through parameter tuning, could be too expensive. Exceptions to this were the CFD-style models developed specifically for dispersion problems.

The shallow layer models lie somewhere in between, which is consistent with their general status.

Finally, the screening tools are based on experimental data, and so require independent experimental evidence of their predictions. Evidence exists for both models of this type.

(e) Other general remarks

This examination of previous evidence of validation highlighted several problems.

- As already remarked above, many of the experimental set-ups involve either a jet release or a vaporising liquid pool, which provide at least one stage preceding the dense gas dispersion phase. Hence it is difficult to separate out the dense gas dispersion part for consideration in isolation. For those models that have a well-defined methodology/model to calculate the initial stages this is not a problem provided the dense gas dispersion model is always used with the same methodology/model.
- There is no guarantee that the version of the model used in these earlier validation studies is the same as that currently available, or even that the studies refer to the same version. This emphasises the point that model results should always be accompanied by the version number of the model that generated them.

2.4 Conclusions

2.4.1 Revision of protocol

Considerable effort was invested in developing the protocol, including the validation exercise procedure and the explicit and detailed nature of the MER template. The result of this was that relatively little adjustment was required following use of the protocol in the evaluations, and changes to the "working version" of the protocol have largely been restricted to making it as complete as possible (the part dealing with the validation exercise could not be included as this had not yet been fully developed) and to rearrangement of the material for clarity. As far as the details of the assessment part of the protocol are concerned, the headings for the assessment have not been changed significantly, and the summary information, introduced while carrying out the first model assessment, have proven to cover not only all the models of the same type without need for significant change but also the other models in different classes.

2.4.2 Conclusions

The scientific model evaluation procedures developed and used in SMEDIS were aimed at providing a mechanism for the independent evaluation of dense gas dispersion models. This project used model evaluation procedures developed in earlier EC projects and applied them to DGD models, with particular reference to complex effects – aerosols, obstacles and complex terrain. The major part of the model evaluation was the production of a Model Evaluation Report or MER for each model submitted to the project. A total of 28 models were evaluated. These were divided into four classes: screening models (2), integral models (13), shallow-layer models (5), CFD models (8).

A new protocol was developed during SMEDIS for the generation of MERs. This protocol was designed to apply to each model class, and to provide a uniform basis for their evaluation. As far as the scientific assessments are concerned, this protocol bases them on different aspects of the model, such as some general information, its scientific basis, its treatment of source and output, the implementation of the algorithms and user aspects. The aim of the protocol was to provide the evaluator with a template so that all models were treated uniformly in the assessments. This template proved to be very successful, and allowed models to be assessed by different persons within the project.

The approach adopted within SMEDIS was to request information provided by the model proponents and to use only this information in the assessments. This approach has some limitations since in many circumstances the documentation that was supplied was poorly organised and did not provide sufficient details of the model. The model itself was not supplied to the evaluator, so there was no attempt to determine information by inspecting or running the model. This approach was chosen since it was felt that the assessment should be based on information available for a potential user who was deciding which model to use and did not have access to the model. A consequence of this approach was that it was impossible in many cases to determine precisely how the model dealt with some aspects.

From the model assessments it is clear that the integral models form the most mature class of models for dense gas dispersion problems. This is reflected both in the large number of models in that class and also in their widespread use. Integral models provide information relevant to consequence analysis and risk analysis, and have been developed over the last twenty years or so into a mature tool. Because of their relative simplicity they have been extended to deal with the complex effects relevant to SMEDIS. Generally speaking integral models have been tested against data more than the other classes and there is more confidence in their applicability.

The next level of complexity is represented by shallow-layer models. These models include the dynamics of gravity driven flow in a more direct way than integral models. They have been developed more recently than integral models and are, therefore, not as well tested. In fact, most shallow-layer models are still in the process of evolution. For example, they can be used to deal with complex terrain and two-dimensional flows. However, this aspect is not without scientific difficulties – in, for example, the specification of the front condition – and so these models may be regarded as somewhat experimental. Note that three of the five models considered cannot handle thermodynamic effects, which would be a severe limitation for operational use of such models.

Fully three-dimensional computational fluid dynamics models based on solutions of the Navier-Stokes equations with a turbulence model, represent the most sophisticated class of models for dense gas dispersion. Most CFD codes were developed for engineering purposes and their use in dispersion calculations is still in its infancy. So, while in principle, they can be used for the full range of complex effects, their use and testing for dense gas dispersion to date has been minimal, and there are some serious issues concerning how this type of model should be applied to dense gas dispersion in the atmosphere.

Within each class there is considerable variability in the capabilities of the different models. The details are given in the text of this chapter and we simply comment here that an assessment of the strengths and weaknesses of a given model can be found in the relevant MER. SMEDIS was not intended to rank models and it remains up to the user to decide what model is suitable for a particular problem. However, it seems as though for most practical purposes, integral models are the class chosen for most practical problems, despite their limitations in dealing with complex obstacles and terrain.

The protocol and the MER template can be used in future by others to evaluate models and we believe will assist in model improvement.

- We believe it will be useful for developers to evaluate their own models. The assessment, via the MER template, provides a checklist of features that a model might wish to include – the headings chosen refer to properties of a model that would generally be considered desirable (so that a model that was able to "tick all the boxes" would be likely not only to have a very wide range of capabilities but would also take into account all the important physical processes)
- The assessment also provides guidelines for the organisation of the documentation (at least the scientific part) for a model.
- Together with, say, the Modeler's Data Archive, the data sets in the SMEDIS validation exercise database provide targets for a model to attempt to achieve in terms of quantitative performance

2.5 Postscript – Main stages in protocol

Stage 1 Pre-evaluation tasks
This initial stage contains all the setting-up activities that are required before the model evaluations can begin. In SMEDIS these were achieved either at the proposal stage or in early tasks of the project and associated discussion between the partners. Parts (b)-(e) of this stage would not be necessary for application of the procedure to additional models (or, say, new versions of existing models).

(a) List models and responsible parties

- Identify models for inclusion – the general group, e.g. dense gas dispersion.
- Identify specific models of interest
- Identify a proponent for each model, i.e. who is willing to supply the model and carry out some or all of the evaluation tasks
- Identify an independent third party to carry out some or all of the evaluation tasks

(b) Define the scope of the model evaluation project

- Identify a specific context-of-use for these models, e.g. problems exhibiting complex effects such as aerosol releases, complex terrain and obstacles.
- Decide to what extent the evaluation of each model will take an active or a passive approach, where the former employs a "hands-on" approach, while the latter relies on pre-existing information
- Decide to what extent self-evaluation is to be catered for (rather than by an independent evaluator) and whether model evolution will be allowed, i.e. changes to the model during the evaluation process.

(c) Assess whether there is a suitable protocol that is applicable to the models

- Identify a protocol
- Assess its suitability based on the requirements of (a) and (b)

(d) Develop/modify protocol

- Includes all three elements of the evaluation, i.e. development of the validation procedure will be included under this heading
- Takes into account the conclusions of (a)-(c).
- Define a classification system for the models, e.g. screening tool, integral, shallow layer, CFD.
- Formulate a framework to describe the problems to which the models are applied, e.g. source-environment-targets framework
- Develop/modify procedure for scientific assessments – use the above framework to define the categories
- Also includes development of questionnaires to obtain information on models, for use in the scientific assessments

The part of the protocol dealing with the scientific assessments describes a series of categories according to which the model is to be examined. The main section headings have largely been adopted from the MEG protocol, and are shown in Table 2.2, together with the next level of categories.

1. General model description
    1.1 Name, version number and release date
    1.2 Short description of model
    1.3 Model type
    1.4 Route of model into evaluation project
    1.5 History of model
    1.6 Quality assurance standards adopted
    1.7 Relationship with other models
    1.8 Current model usage
    1.9 Hardware and software requirements
    1.10 Availability and costs
2. Scientific basis of model
    2.1 Specification of the source
    2.2 Specification of the environment
    2.3 Model physics and formulation
    2.4 Solution technique
    2.5 Results or output available from model
    2.6 Sources of model uncertainty
    2.7 Limits of applicability
    2.8 Special features
    2.9 Planned scientific developments
3. User-oriented aspects of model
    3.1 User-oriented documentation and help
    3.2 Installation procedures
    3.3 Description of the user interface
    3.4 Internal databases
    3.5 Guidance in selecting model options
    3.6 Assistance in the inputting of data
    3.7 Error messages and checks on use of model beyond its scope
    3.8 Computational costs
    3.9 Clarity and flexibility of output results
    3.10 Suitability to users and usage
    3.11 Possible improvements
    3.12 Planned user-oriented developments
4. Verification performed
    4.1 Summary of verification
    4.2 Comments
5. Validation performed
    5.1 Validation already performed
6. Conclusions
7. References

Appendix 1: Actively-generated information

Appendix 2: Comments from model developer

Table 2.2 Summary of main headings in scientific assessment.

The main headings would be suitable for virtually any model. To make it more specific to SMEDIS, we use the framework developed earlier (in Stage 1) to divide these into a number of sub-categories relevant to the particular group of models being analysed, and indicated (to the first sub-level) in the above list.

To accompany the protocol a template for the MER is also developed. This ensures that there is a common format for the report for every model in the project, further standardising the assessment process across models. The organisation of this report template is to use a combination of summary information and qualifying text. Thus for some headings summary information is given using a “check box” format for rapid overview of the capabilities and formulation of the model together with qualifying text that expands on and complements the summary information; while for other headings summary information is not appropriate and text alone is used. A considerable effort was made to make the layout as clear as possible, while at the same time ensuring the summary options were covered all the model types and most likely responses. An example is given below.

2.2.2.1 Mean wind field

☑ Mean wind parameterised

☑ Vertical profile ☒ Horizontal field ☒ Time-varying

[M] Dependence on stratification [] *Other*

☑ Vertical velocity profiles used

☑ Logarithmic ☐ *Other*

[U] Velocity at reference height ☒ Friction velocity specified

☐ *Mean wind modelled*

[] *Vertical profile* [] *Horizontal field* [] *Time variation* ☐ *Other*

☒ Zero wind allowed

<Qualifying remarks here>

Sections 1-3 form the principal part of the assessment, and each uses the summary information format where appropriate. Section 4 represents the treatment of verification in SMEDIS, i.e. through consideration of previous verification undertaken. Section 5 is a summary of previous validation carried out on the model, which acts as a useful complement to the validation taking place within SMEDIS. Finally, Section 6 summarises the contents of Sections 1-5, including a set of advantages and disadvantages for using the model. There is also a section listing the references used for the assessment and appendices containing a summary of the actively-generated information (SMEDIS validation results) and the comments from the model proponent on the draft report.

Turning now to the part of the protocol dealing with the validation exercise, the main points to develop here are the choices of comparison parameters and the procedure itself (the data sets are considered in a separate part, (e), below).

- Define physical comparison parameters for use in validation comparisons.
  - ∗ A mixture of pointwise and arcwise comparison parameters were chosen, i.e. comparing values at specified points and comparing values for specified arcs of points, respectively.
  - ∗ Distinction was made between continuous and instantaneous releases, with the time-averaged concentration and the dose (time-integrated concentration) being used as the basis for the two types of release, respectively.
  - ∗ Continuous releases were characterised with pointwise and arcwise-maximum concentrations together with cloud width; instantaneous releases were characterised with

pointwise and arcwise-maximum dose, time-of-arrival and time-of-departure and cloud width. (See Appendix 3 to this report for a precise list of parameters together with their definitions.)

- Define statistical comparison parameters for use in validation comparisons.
  * The principal statistical comparison parameters were chosen to be the Mean Relative Bias and the Mean Relative Square Error, together with the Factor of n; the Geometric Mean Bias and Geometric Mean Variance were also considered as secondary parameters for the purposes of possible comparison with earlier exercises. (See Appendix 3 to this report for definitions of these parameters.)

- Define procedure for validation comparisons
  * Carry out pre-processing for the dense gas dispersion model, e.g. to provide single-phase dense gas source conditions from a flashing two-phase jet release.
  * Set up the input data for each scenario.
  * Run the model.
  * Make the validation comparisons, possibly involving post-processing, e.g. calculation of dose from the concentration time history, before comparisons can be made.

(e) Develop/modify validation database

- Only required for active validation.
- Aim is to produce a collection of data sets for specific experiments in a suitable format against which to make comparisons in the validation exercise.
- Data set groups are identified, e.g. Thorney Island
- A framework for the experimental scenarios is developed
- Individual data sets within selected groups are chosen to span the range of possible scenarios as far as possible
- The chosen data sets are put in a common format appropriate to the validation task

These activities are described in further detail in Chapter 4.

Stage 2 Carry out the scientific assessments

SMEDIS treats the scientific assessments passively by using pre-existing information about each model[1]. The principal stages are therefore

- obtain the information on each model through circulation of questionnaires
- carry out scientific assessment of each model according to the protocol and record results in the Model Evaluation Report for the model. See Appendix 5 for the model evaluation protocol and Appendix 6 for examples of complete MERs that have been produced using this protocol.

Note that Stage 2 can take place in parallel with Stages 3 and 4.

Stage 3 Carry out the verification exercise

In SMEDIS, this is treated passively and forms part of Stage 2: evidence for verification of the model (supplied as part of the model information) is examined within the scientific assessment of

[1] Other than direct interrogation of the model developers, it does not appear to be possible to take an active approach to assessment.

the model. This treatment of verification was selected for SMEDIS because of the large number of models in the project and the potentially labour-intensive nature of verification. A section was included in the MER summarising this evidence.

In the general case, this would be a separate activity for all the models in the project. The most comprehensive form of verification in a model evaluation project would be to examine the (computer) implementation itself for each model and check that the mathematical algorithms had been translated accurately into code.

Stage 4 Carry out the validation exercise

SMEDIS treats this actively by requiring that the models be run to simulate a number of experimental tests. The experiments to be used were chosen and their data sets put into a suitable format in a database in the earlier setting-up stage (see Stage 1), which also defined the procedure for carrying out the exercise for a given model.

SMEDIS allowed the model proponent to carry out the model validation rather than an independent third party. Those running the models were also allowed to see the experimental data prior to carrying out the validation runs of their models, and they were also allowed to modify their model and re-run the cases (provided the same version is used for *all* cases). These aspects of the validation exercise were included so as to encourage model improvement – realistically, they are also the conditions that would apply to use of the protocol outside SMEDIS.

Ideally all cases would be attempted, but in reality resource constraints would be likely to mean that for the more complex models only a subset would be attempted and/or minimal re-runs would be performed to improve agreement. This was acknowledged in SMEDIS by defining specific subsets of the entire database that should be simulated by each class of model.

Stage 5 Post-evaluation tasks

(a) Seek agreement of evaluation with model developer/proponent

In SMEDIS this process applies principally to the scientific assessment of the model, in that a draft MER is sent to the information supplier (the model developer in the majority of cases) for their comments, and the MER is then revised to incorporate these comments where possible – an appendix records the comments received and if agreement is not possible then the appendix also contains the reaction of the evaluator to the comment, so that the reader may judge for themselves.

There is also an element of agreement in the validation exercise, in that the model proponent (who, in the case of SMEDIS, has also carried out the model runs) is allowed to check that the results of the model runs have been correctly compared against the experimental data.

If there were an active verification exercise then the results would also be provided to the model proponent for checking/comment.

(b) Refine the protocol

Following use of the protocol in evaluating a significant number of models in SMEDIS, the protocol is refined to take into account any improvements that have been suggested in the course of the earlier stages.

The protocol has now been tested as a result of carrying out the evaluations, and so the opportunity should be taken to improve the protocol where it appeared to be weak or unsuitable. As for the previous stage this could be applied to all three elements of evaluation, but in the case of SMEDIS it applies principally to the scientific assessment aspect of the protocol.

3 MODEL VERIFICATION

Although verification is to be regarded as an essential element of evaluation, detailed verification of each model is outside the scope of the present project for pragmatic reasons: in a project of this size resources are considered more usefully concentrated on the other two elements.

Thus we rely on pre-existing evidence of verification of the model, and this can take two main forms.

(a) direct verification

Complete verification of the model would comprise checking of the code line by line against a detailed technical specification of the model algorithms to ensure that there has been an accurate translation of the technical specification into computer code. In practice this is unlikely to have been carried out in many cases since the specification is often not available in sufficient detail for many models. Such direct verification is linked to quality assurance (QA) procedures, which would tend to include this type of checking as part of the code development process itself.

(b) indirect verification

This is intended to mean comparisons of model predictions with known results. If the model algorithms may be solved in certain cases for which the solution is known analytically (exactly), then by running the model to simulate these situations agreement of the two provides evidence that those parts of the model involved have been implemented correctly.

A variation on this theme is when a model algorithm represents, say, a conservation relation such as conservation of mass: in this situation, the total calculated mass may be summed and its expected variation assuming conservation may be checked.

Note that evidence of either of the above types of verification is requested as part of the information supplied for a model and has been included as part of each model is evaluation report (MER).

h:/Novreports/modelverification

Chapter 4 : The Database and Validation Exercise

This chapter describes the validation procedure developed and applied in SMEDIS.

It starts by describing how the datasets were selected and processed to form what we refer to as the SMEDIS database. The chapter then describes the parameters that have been selected for the statistical comparison between model and experimental results. Finally, after a description of the procedure to distribute the database and collect the model results from participants, the chapter ends on a complete analysis of the first set of model results returned.

4.1. Database description

4.1.1 Data selection

Identification of suitable data sets for the model validation was carried out with input from all participants. First a preliminary list of over 40 data sets and corresponding references was prepared by collecting information from partners (cf. Appendix 1). Based on this preliminary list, a detailed questionnaire was sent to all partners to obtain information about the data sets, including previous use of the data for model validation, availability of data and an opinion of the user on the data set quality in several areas, e.g. source specification and concentration measurements.

The replies were then analysed to produce a priority list of data sets which had been previously used for the validation of a range of models, including integral and CFD models, and were judged of sufficient quality by the participants. There turned out to be relatively few high quality data sets available for validation in these complex situations. These are presented in Table 4.1 A provision was made to include more recent data sets, which had not already been used for validation, as the project progressed, including data sets for which near-field effects are important (BMT and ETH-Z datasets). These datasets, processed within the project, were added to the REDIPHEM database.

Identifier	**Scale**	**Material**	**Source type**	**No. tests**	**Complex effects**
Burro	field	LNG	pool	8	fast aerosol evaporation
Desert Tortoise	field	Ammonia	jet	4	aerosol
FLADIS-Risø	field	Ammonia	jet	16	aerosol
BA-Hamburg	wind tunnel	Sulphur hexafluoride	continuous instantaneous	146	obstacles, slopes
BA-Propane	field	Propane	jet/cyclone	51	aerosol, fences
BA-TNO	wind tunnel	Sulphur Hexafluoride	continuous instantaneous	13	fence
Thorney Island	field	Freon	instantaneous	30	fence, building
EMU-Enflo	wind tunnel	Krypton	continuous	2	buildings, real site

Table 4.1 Data set groups selected based on questionnaires returned by all participants.

There is a mixture of the well-established experimental programmes used by Hanna *et al.* (1993) and more recent EC-funded programmes. Most of the data sets from both categories can be found in the REDIPHEM database (Nielsen and Ott, 1996); see also Britter (1998) for a review of the European experimental programmes.

Both field trials and wind tunnel experiments were allowed, although preference was given to field trials where these were available. However, it became clear that the exclusion of wind tunnel tests would be unduly restrictive to the range of scenarios considered and so a mixture of field trials and wind tunnel experiments was used in the final selection.

4.1.2 Scenario classification

It is clearly preferable to test any model over as wide a range of conditions as possible, i.e. for a broad range of scenarios. In order to delimit the possible range of scenarios, a scheme was devised to classify them. This scheme is based on four main characteristics of a scenario, as shown in Table 4.2.

Main code	Main characteristic	Values	Value code
S	source type	continuous	c
		instantaneous	i
C	complex effect	aerosol	a
		complex terrain	t
		obstacle	o
		congestion/confinement	c
		none	n
D	gas density	weak	w
		strong	s
A	atmospheric conditions	neutral/unstable	n
		stable	s
		low/no wind	l

Table 4.2 Classification scheme for dense gas release scenarios. The code letters can be used to denote a particular scenario, e.g. ScCnDwAn refers to a scenario with a continuous source, no complex effects, weak dense gas effects and neutral atmospheric conditions.

The complex effect “congestion/confinement” and atmospheric conditions “no/low wind” were added later to the basic formulation in order to highlight situations where near-field effects are particularly important, e.g. because of very low wind or where there is interaction with obstacles near the source. After a search for suitable data sets, two groups of wind tunnel tests were identified, namely continuous dense releases inside an offshore module and instantaneous dense releases on a slope in calm conditions (Daish *et al.* 1999).

This gives a total of 45 combinations, or cells in a four-dimensional matrix, and so ideally there would be at least one high quality data set per combination. In fact, based on the short list given in Table 4.1 there were data sets to fill most but not all of the cells in the four-dimensional array, as described in Daish *et al.* (1999). There are few instantaneous releases showing aerosol effects and no releases with terrain (slopes) for stable atmospheric conditions. There is heavy reliance on the wind tunnel experiments designated “BA Hamburg” which were necessarily carried out under neutral conditions. Nevertheless, there is a sufficient spread of conditions for which data sets of adequate quality can be found to carry out effective validation

4.1.3 Specific cases

The final stage in the selection of cases to simulate is to choose one or more cases from as many of the complete cells as possible. Taking into account resource constraints, it was decided to limit the exercise to a total of 30 cases, divided into three main batches: some details are given in Table 4.3. The number of cases a particular model is required to simulate depends on the type of model: thus screening tools and integral models are required to simulate all 30 cases, shallow layer models approximately 50% of these and CFD models approximately 20% of the total. For all model types the cases are specified, so that all models of a given type simulate the same (or a subset of the same) cases.

Data set group	Test name	Code	Rationale	C/I	F/W	A	T	O	ST	I	SL	3d
Prairie Grass	PG8	ScCnDwAn	Simple, well-used data set	C	F				o	o	o	
	PG17	ScCnDwAn	As Test 17, but with unstable atmosphere	C	F				o	o		
Desert Tortoise	DT1	ScCaDsAn	Aerosol and stronger dense gas effects	C	F	x			o	o	o	
	DT2	ScCaDsAn	Repeat of DT1 with different flow rate	C	F	x			o	o		
BA Propane	EEC360	ScCnDsAn	Strong density effects	C	F	x			o	o		
	EEC361	ScCoDsAn	As EEC360, but with one obstacle (fence)	C	F	x		x	o	o		
	EEC362	ScCoDsAn	As EEC360, but with two obstacles (fences)	C	F	x		x	o	o		
	EEC550	ScCnDsAn	Strong density effects	C	F	x			o	o	o	o
	EEC551	ScCoDsAn	As EEC550 but with one obstacle (fence)	C	F	x		x	o	o	o	
	EEC560	ScCnDsAn	Strong density effects	C	F	x			o	o		
	EEC561	ScCoDsAn	As EEC560, but with obstacle (porous fence)	C	F	x		x	o	o	o	
	EEC170	ScCnDsAn	Strong density effects	C	F	x			o	o		
	EEC171	ScCoDsAn	As EEC170, but with obstacle (circular fence)	C	F	x		x	o	o	o	o
	LAT49	SiCaDsAn	Instantaneous release with aerosol effects	I	F	x			o	o		
BA Hamburg	DAT638	SiCtDsAn	Instantaneous source with steep slope	I	W		x		o	o	o	o
	DAT648	SiCtDsAn	As DAT638 but slope less steep	I	W		x		o	o		
	DAT231	SiCoDsAn	Instantaneous release with wall parallel to wind	I	W			x	o	o		
	DAT647	ScCtDsAn	Continuous release on slope	C	W		x		o	o	o	
	DAT458	SiCoDsAn	Instantaneous release with canyon	I	W			x	o	o	o	
	049101	SiCoDsAn	Instantaneous release and near-field array of obstacles	I	W			x	o	o		
	129034	ScCoDsAn	Continuous release with near-field obstacles	C	W			x	o	o	o	
BA TNO	TUV11	ScCnDsAn	Reference continuous release without obstacle	C	W				o	o		
	TUV13	ScCoDsAn	As TUV11 but with obstacle (oblique fence)	C	W			x	o	o		
EMU ENFLO	EMUDJ	ScCt/oDsAn	Dense release in complex terrain with obstacles (buildings)	C	W		x	x	o	o	o	o
	EMUNJ	ScCt/oDwAn	As EMUDJ but with weak density effects	C	W		x	x	o	o		
FLADIS Risø	FLADIS16	ScCaDwAs	Aerosol effects and stable atmosphere	C	F	x			o	o	o	
	FLADIS24	ScCaDwAn	Aerosol effects and neutral atmosphere	C	F	x			o	o		
	FLADIS9	ScCaDsAn	Dense release with aerosol effects	C	F	x			o	o		o
Thorney Island	TI08	SiCnDsAn	Instantaneous release with strong density effects	I	F				o	o	o	
	TI21	SiCoDsAn	Instantaneous release with strong density effects and fence	I	F			x	o	o	o	o

Table 4.3 Specific cases used in SMEDIS validation exercise. Additional cases will also be selected for the near field cases (BMT and ETH-Z).

KEY: C = continuous release; I = instantaneous release. F = field trial; W = wind tunnel experiment. An “x” indicates aerosol effects (A), terrain effects (T) and obstacles (O) important. Fences are linear unless otherwise stated. An “o” indicates the case should be attempted by screening tools (ST), integral models (I), shallow-layer models (SL) and CFD models (3d).

4.1.4 Validation procedure

Finally, we consider how the validation comparisons between observations and predictions are made. This comprises two aspects, namely defining the parameters used in the comparisons - physical parameters and statistical parameters - and setting up and running the models.

(a) Physical comparison parameters

These are the physical quantities, either directly measured or derived from direct measurements. Table 4.4 summarises the physical parameters being considered. There are two main divisions:

- first, distinction is made between continuous and instantaneous releases, where the parameters are broadly based on concentration and dose, respectively
- secondly, there are both pointwise and arcwise comparisons. In the former case, observations and predictions are compared over a given set of points, e.g. the dose at a given set of points; while in the latter case the comparisons are made between sets of arcs, e.g. the maximum concentration across an arc for each of a set of arcs. For a given case (trial) some or all of the arcwise comparisons may not be possible, e.g. when the arcs contain insufficient numbers of points, are not well-defined or when the presence of an obstacle makes the definition of an arc difficult.

Although the arcwise comparisons are often of most practical use, the above difficulty in complex situations has led us to include the pointwise comparisons as well, so as to give credit to models which provide spatial information on the concentration field (e.g. in situations where the cloud is distorted by the presence of obstacles and/or terrain). The cloud width is calculated using moments of the concentration distribution across the arc, while the arrival and departure times of the cloud are defined as the times at which 10% and 90% of the dose, respectively, has been recorded.

(b) Statistical comparison parameters

For a given physical parameter ψ, we need procedures and parameters for comparing the observed values $\{(\psi_o)_i\}_{i=1}^{N}$ and the predicted values $\{(\psi_p)_i\}_{i=1}^{N}$ (where the index i runs over the set of N points or N arcs) to give a measure of the overall agreement between the two sets of numbers. Many so-called statistical comparison parameters have been devised for this purpose (see, for example, Duijm *et al.*, 1996), each with their own merits and limitations, but in general the parameters most commonly adopted (including here) come in pairs, one member of the pair giving a measure of bias in the predictions - do they represent consistent over/under-prediction of the observed values ? - while the other member gives a measure of the spread in the predictions - is there wide scatter in the predicted values compared with the observed values ?

Table 4.5 shows the statistical comparison parameters chosen in SMEDIS. In the table the angle brackets <…> denote an average over N observed/predicted pairs, while the notation $N_{a<\zeta<b}$ denotes the number of members of the set of N values of ζ which lie between a and b. The main parameters are the Mean Relative Bias, MRB, and the Mean Relative Square Error, MRSE, together with the Factor of n with n = 2 and 5. The Geometric Mean and Geometric Variance, MG and VG, respectively, have also been included for comparison with previous studies, although they are not the primary comparison parameters in SMEDIS. All the parameters used are based on concentration ratios, and the MRB/MRSE pair has preferred status on the basis of previous work (Duijm *et al.*, 1996).

APPROACH	RELEASE TYPE	
	Continuous	**Instantaneous**
pointwise comparisons	a) Time-averaged concentration at sensor position ***x***	a) Dose *D* at sensor position ***x*** b) Cloud arrival time at ***x*** c) Cloud departure time at ***x***
arcwise comparisons	b) Maximum concentration across arc at a given radius *x* c) Width of cloud across arc at (*x*, *z*)	d) Maximum dose across arc at a given radius *x* and height *z* e) Maximum concentration across arc at (*x*, *z*) f) Time for maximum concentration across arc at (*x*, *z*) g) Cloud width across arc at (*x*, *z*) based on dose h) Cloud arrival time across arc at (*x*, *z*) i) Cloud departure time across arc at (*x*, *z*

Table 4.4 Physical comparison parameters. A precise definition of each parameter is given in the protocol.

Name	Definition	Advantages	Disadvantages
Mean Relative Bias	$\mathrm{MRB} = \left\langle \dfrac{\psi_o - \psi_p}{\frac{1}{2}\left(\psi_p + \psi_o\right)} \right\rangle$	• Accepts zero values. • Less sensitive than other measures to minimum thresholds. • Symmetric for under/over- prediction.	• Allows differences between models with ψ_o/ψ_p up to ~10 to become apparent, but not so outside this range.
Mean Relative Square Error	$MRSE = \left\langle \dfrac{\left(\psi_p - \psi_o\right)^2}{\frac{1}{4}\left(\psi_p + \psi_o\right)^2} \right\rangle$	• More transparent than VG (see below) in allowing standard deviation of predictions to be obtained.	
Factor of n	$\mathrm{FACn} = \dfrac{\mathrm{N}_{1/n<\psi_o/\psi_p<n}}{\mathrm{N}}$	• Robust, consistent, easy to understand	
Geometric mean bias	$MG = \exp\left\langle \log_e\left(\dfrac{\psi_o}{\psi_p}\right)\right\rangle$	• Log_e(MG) symmetric about zero in under/over-prediction.	• Cannot accept zero values.
Geometric mean variance	$VG = \exp\left\langle \left[\log_e\left(\dfrac{\psi_o}{\psi_p}\right)\right]^2\right\rangle$	• Variance measure related to MG	• Cannot accept zero values.

Table 4.5 Statistical comparison parameters used in SMEDIS. The MRB and MRSE are the principal parameters used together with FA2 and FA5. MG and VG are included for comparison with previous validation exercises which have used these.

Thresholds have been applied to the parameters being compared to allow for cases where either the predicted or observed concentration is zero. In practice, this only applies to the pointwise concentration or dose comparisons, since all other values are non-zero, and is only required by MG and VG unless both observed and predicted values are zero. The effect of thresholds is still being actively assessed, although a working value of 10^{-3} units for concentration (and for dose $10^{-3} t_d$, where t_d is the duration of the test) is being used initially. (It would be preferable to base thresholds on sensor sensitivity, but such information is not available in all cases.)

(c) Other aspects of validation procedure

In general the model proponent is expected to carry out as many of the allocated runs as possible (see Table 4.3). They are expected to document the setting up of their model, especially if there is a deviation from the “normal” method, such as a change to the recommended values of parameters.

In many cases models will not have the capability to handle specific features, in particular aerosol clouds, sloping ground or obstacles. In these circumstances it was agreed that users on a voluntary basis could attempt to simulate all cases assigned to their model type even if their model was missing the necessary capability. Conclusions would be drawn from the results on the effect of using a model beyond its limits of applicability (when validation results are shown, any such mismatch will be clearly indicated).

SMEDIS also allows an element of model development/improvement during the project, since in many cases the model proponent is the same as the model developer. For this reason the validation exercise provides users with the observations (i.e. the “answers”) to assist the improvement process. However, the users are required to document any changes made to the model and provide this as additional input to the scientific assessment of their model. They should also carry out all runs with the same version of the model.

4.1.5 Distribution of data sets

The data for each case (Appendix 2) are circulated in the form of Excel workbooks : there is one workbook per case, containing the data describing the test set-up (to be used in setting up models) together with the concentration measurements (and others, for example temperature if available) against which the model predictions are to be compared. A common format is adopted for each case. The data have been derived from the REDIPHEM database (Nielsen and Ott, 1996) wherever possible. A second workbook (an empty template to allow for automatic processing) is provided for users to return their results.

In the case of wind tunnel experiments, the data workbook contains equivalent “full-scale” data as well, representing (where relevant) the specific full-scale analogue associated with the test. It was agreed that models would be run to simulate this scaled-up version, on the basis that models (other than the general purpose CFD models) were developed to simulate such problems.

The full SMEDIS database is found in Appendix 2 and in the accompanying CD-ROM.

4.1.6 Implementation of validation procedure

Once a given model has been run for its allotted cases, the results workbooks are sent electronically to the two partners responsible for processing the results (EDF and HSL) where the statistical parameters are calculated for all cases and models. The results of the validation exercise are also added to complete the “model evaluation report” resulting from the scientific assessment.

4.2. Analysis of results

The entire exercise involves the collection of over 300 model results returned (each containing up to 130 data points).

In order to allow for time to create the database and to process all the data without delaying all the validation toward the end of the project, the database has been broken into four different sets that were released progressively during the project (table 4.6).

Set 1	Set 2	Set 3	Set 4
PG17 (1)	DAT231	EEC 560	
PG8 (1)	DAT647	EEC 561	
EEC360 (3)	EMUDJ	EEC 170	
EEC 361 (2)	EMUNJ	EEC 171	
EEC 362 (2)	FLADIS16	129034	
DT1 (3)	FLADIS24	LAT49	
DT2 (3)	TI08	DAT 458	
EEC 550 (3)	TI21	049101	
EEC 551 (2)	TUV11	FLADIS9	
DAT638 (4)	TUV13		
DAT 648 (4)			

Table 4.6 : Definition of the database subsets that were progressively released during the SMEDIS project. All datasets are available in the SMEDIS database at the end of the project. For the first set, the value in parenthesis indicates the group type as defined in Table 4.7

A complete analysis has been performed only for the first set of these results (roughly one-third of all datasets in the database). For set 2, all model results have been returned and basic processing made. Further analysis has not been performed due to lack of resources within the project. For set 3 the model results have been returned but no processing has been made and for set 4 no model result has been returned by the participants. The following discussion is based only on the analysis of the first set of data.

Statistical parameters have been computed for all models and all datasets (see Appendix 4), but here we have formed groups to summarize the results. First we have formed groups of models for the four model categories (see Table XXX) and then groups of datasets comprising similar complex effects (including none!). These groups are presented in Table 4.7 (the corresponding datasets are found Table 4.6), which indicates the number of results processed in each group[2].

	Type_effect			
Model_Types	1-no effect	2-obstacle	3-aerosols	4-terrain
1-WorkBook	2	2	4	0
2- Integral	18	17	42	9
3- Shallow-Layer	4	5	8	4
4- CFD-3D	0	7	7	6

Table 4.7 : Number of model results processed in each group.

		Type_effect			
Statistical Parameter	Model_Types	1-no effect	2-obstacle	3-aerosols	4-terrain
ln(MG)	1-WorkBook	-0,88	-0,73	1,06	

[2] Note that the term “Workbook” is used here since there is only one model - the Britter-McQuaid Workbook - included in the analysis of results (see also caption to Table 1).

	2- Integral	-0,01	0,01	0,18	1,07
	3- Shallow-Layer	-0,49	0,75	0,35	1,79
	4- CFD-3D		-0,01	-0,27	0,50
ln(VG)	1-WorkBook	1,46	0,82	10,20	
	2- Integral	0,39	0,52	2,34	1,74
	3- Shallow-Layer	1,04	1,04	1,51	7,32
	4- CFD-3D		0,14	0,35	0,40
MRB	1-WorkBook	-0,72	-0,66	0,14	
	2- Integral	-0,00	0,01	0,03	0,88
	3- Shallow-Layer	-0,39	0,65	0,31	0,94
	4- CFD-3D		-0,01	-0,25	0,47
MRSE	1-WorkBook	0,98	0,65	1,39	
	2- Integral	0,33	0,37	0,61	1,08
	3- Shallow-Layer	0,66	0,74	1,01	1,31
	4- CFD-3D		0,13	0,30	0,35

Table 4.8 : Results of statistical analysis of **arcwise** comparison between model results and experimental values. Model and datasets have been grouped into four categories.

Table 4.8 and Fig. 4.1 present the results of the arcwise comparison. This part can be compared to previous studies that have similarly used the maximum arcwise comparison. For the "FAC2" statistics (Fig. 4.1), we can first notice the weakness of integral models with complex terrain and shallow layer model with aerosols. All other results are above the 40% that have been reported elsewhere (for example in Duijm *et al.* 1996). We can also note a general improvement of the FAC2 with increasing complexity of the models (more than 70% within a factor of two for CFD).

For the two measures of bias (ln(MG) and MRB, Table 4.8) there is no clear over- or under- prediction if obstacles or aerosols are present. However with no complex effects, the models over-predict whereas with complex terrain they under-predict. Based on these numbers alone, the best model type is the integral model excepted for terrain effects.

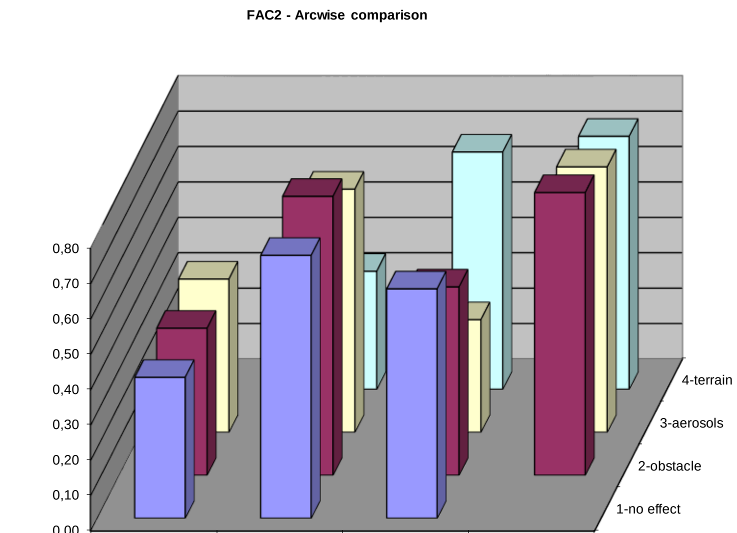
Finally for the two measures of spread (ln(VG) and MRSE) we again see the improvements with model complexity excepted for the shallow layer models.

		Type_effect			
Stat. Parameter	Model_Types	1-no effect	2-obstacle	3-aerosols	4-terrain
ln(MG) =	1-WorkBook	-1,49	0,39	0,54	
	2- Integral	0,45	0,42	0,15	0,87
	3- Shallow-Layer	1,10	1,19	0,77	1,81
	4- CFD-3D		0,90	0,96	0,44
ln(VG)=	1-WorkBook	3,94	8,20	13,85	
	2- Integral	6,43	7,55	9,42	1,56
	3- Shallow-Layer	13,24	6,42	5,48	7,73
	4- CFD-3D		5,53	7,57	0,43
MRB =	1-WorkBook	-0,99	-0,09	0,16	
	2- Integral	0,08	0,11	0,02	0,71
	3- Shallow-Layer	0,16	0,64	0,43	0,92
	4- CFD-3D		0,47	0,37	0,41
MRSE =	1-WorkBook	1,58	1,60	1,91	
	2- Integral	1,40	1,64	1,68	0,97
	3- Shallow-Layer	1,47	1,60	1,45	1,35
	4- CFD-3D		1,08	1,25	0,36

Table 4.9 : Results of statistical analysis of **pointwise** comparison between model results and experimental values. Model and datasets have been grouped into four categories.

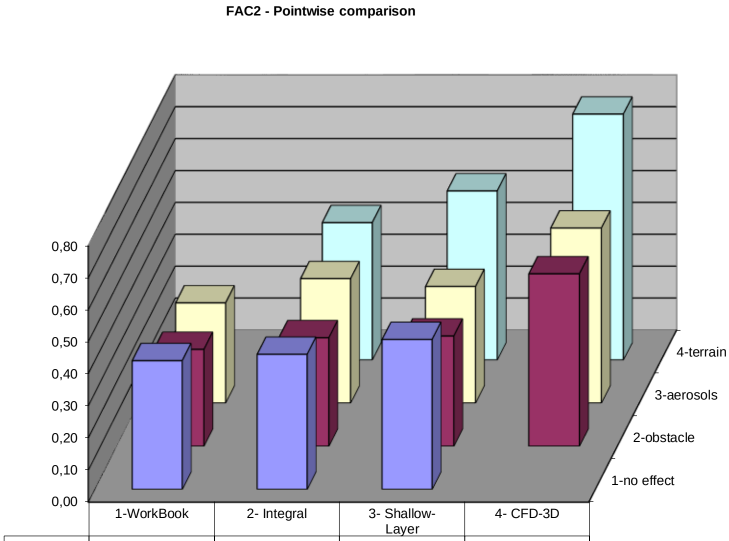
Table 4.9 and Fig. 4.2 present the statistical results obtained for the pointwise comparison. It is important to note that this comparison involves a much larger number of points as all the measurements on each arc are included and there are some additional measurement point that are sometimes not included in any arc.

We can first notice that the pointwise comparisons show a global decrease in the statistical performance measure compared with the arcwise values, indicating that all models are better at predicting centerline maximum concentration than the general cloud shape. Putting aside this global decrease in performance, all comments made from the arcwise analysis can be carried over to the pointwise statistics.



	1-WorkBook	2- Integral	3- Shallow-Layer	4- CFD-3D
1-no effect	0,40	0,74	0,65	
2-obstacle	0,42	0,79	0,53	0,89
3-aerosols	0,43	0,69	0,32	0,75
4-terrain		0,33	0,67	0,71

Figure 4.1 : Fraction of model results within a factor of 2 of experimental results ("FAC2") for the arcwise comparison



	1-WorkBook	2- Integral	3- Shallow-Layer	4- CFD-3D
1-no effect	0,40	0,42	0,47	
2-obstacle	0,30	0,34	0,34	0,54
3-aerosols	0,31	0,39	0,36	0,55
4-terrain		0,43	0,53	0,77

Figure 4.2 : Fraction of model results within a factor of 2 of experimental results ("FAC2")
for the pointwise comparison

4. Conclusion

In this chapter we have described the database of experimental results and its use for the model validation performed in the SMEDIS project. This validation was carried out according to the general protocol designed to specify all aspects of model evaluation, including validation but also scientific model assessment.

In the course of constructing the database, we found that there are significant gaps in the experimental data available for dense gas release problems with complex effects, in particular if wind tunnel experiments are excluded. Instantaneous releases featuring complex effects are particularly sparsely studied, with very few examples available for aerosol releases. In addition, stable atmospheric conditions are not well-represented (wind tunnels are not able easily to simulate such cases). Situations where near-field effects dominate (congested/confined releases, low/no wind conditions) are an area in need of further experiments, in particular for flammable clouds.

Information on sensor accuracy and data uncertainty is not always available: this information can have an important role in defining “acceptable” agreement with model predictions, and is necessary to define a threshold to be used for certain statistical measures.

In total, over 300 sets of model results have been returned by the participants (with some having over 100 data points). From these we have carried out a preliminary analysis of approximately one third of the total for the results presented here.

The pointwise statistical measures of model performance are globally lower than for the arcwise comparison, indicating that all models are better at predicting centerline maximum concentration than the general cloud shape. Based on the Fraction within a factor of 2 (FAC2), the Geometric Variance (ln(VG)) and the Mean Relative Square Error (MRSE) we clearly see a general improvement of model performance with increasing complexity, that has been quantified by these statistical measures. However it should be remembered that some results are based on smaller samples size as given by Table 4.7.

References

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APPENDIX 1

List of data sets considered and selection of data sets used

1. INTRODUCTION

As part of preparations for the model validation exercise, a list of all possible validation data sets was assembled. This task was carried out with input from all project participants.

A preliminary list of data sets and corresponding references was first prepared incorporating all data considered of possible relevance by project partners. This initial list is given in Table 1 with summaries of the main characteristics of each data set (where available) and, also, where supplied, at the end of this Appendix, references to each experiment as Table 2. A total of 41 experimental programmes was so identified.

The list of data produced was naturally constrained by the context of the SMEDIS project. Thus Table 1 is biased towards experiments in which the special effects of aerosols, complex terrain and obstacles play a significant role in determining release behaviour.

No restriction was placed on the type of data included in the initial list of data sets. Thus it includes wind tunnel as well as field data and also releases over water.

2. DATA SELECTION

Of the data sets listed there the first twelve are, in some form, already contained in the REDIPHEN database (Nieben and Ott, 1996). These data have therefore previously undergone a quality check and are readily available. The utility of the remaining data was subsequently examined by means of a questionnaire to partners to seek news on their validation experience and particularly to address such issues as data quality and availability.

All partners had used data for validation at some time and in all there were some 60 applications of the data for this purpose. Table 3 shows the way in which this experience breaks down. This shows that many (15) data sets had never been used for validation, conversely some 26 had and 13 had only been used on a single occasion, indication a general lack of availability or perceived poor quality. The maximum number of applications amounted to 7.

Table 4 details the type of model validated against each data set. This shows that several datasets have been used for the validation of different types of models but only three have been used with the full range of model types. In all 8 data sets have been used with empirical models, 20 with box/integral models, 6 for shallow layer and 8 for CFD. It is notable that the data in Table 2 split almost equally between field and wind tunnel/laboratory tests, perhaps indicating that currently both types of data are necessary for a reasonably comprehensive validation exercise.

Table 5 presents partner news on data ‘quality’. The quality of a data set is very difficult to judge in absolute terms. In particular, workers will use different standards and have differing requirements depending on the model type being assessed. Here the approach taken is to rely on the opinions of those who have actually used the data for comparison with models. The data have therefore been rated on a scale from 1 (poor) to 4 (very good) in four different areas:-

- Source specification
- Atmospheric specification

- Site information (including obstacles and terrain).

- Concentration measurement.

In addition information was also sought on the viability of data in terms of format and data file size.

The result is a subjective and approximate composite assessment of dataset quality which although in some respects flowed provides a useful assessment of data utility.

Considering only data examined by two or more of the partners, only one (25 – Lyme Bay) is considered poor, particularly for atmospheric conditions. Failings in several other data sets were identified, indicated by a rating below 3. Thus the source specification was considered weak in 1 Burro, 2 Loyote and 7 BA – Propane. Otherwise the data were considered good to very good in all remaining aspects.

On this basis Table 6 summarises data sets considered of sufficient quality by at least three of the project partners. This list formed the basis from which data will be selected for use in the validation exercise.

All data sets in this list, except the last (12), have been already used for the validation of at least two different types of models

3. SELECTION OF DATA SETS

Further selection of data sets was based on the following criteria:-

- Quality. Only good quality data sets were accepted on the basis of the questionnaire returns.

- Distribution over range of complex effect. On the basis of three complex effects; aerosol, complex terrain and obstacles, an attempt was made to select equal numbers of such cases together with an equal core of ‘simple’ cases with no such influence.

- Laboratory v field data. Where possible field data were to be preferred but due to data gaps the use of significant numbers of laboratory tests would probably be unavoidable.

- Use of passive releases. To provide a base reference case it was decided that two data sets dealing only with passive releases over flat terrain should be included. The commonly – used Prairie Grass and Harford experiments were considered appropriate.

Additional consideration was given to the use of the Modeller’s Data Archieve (MDA) of Hanna et al (1993). However, the constraints of the choice of validation strategy (Appendix 3) using data paired in space and time in addition to maximum arcwise concentrations precluded the use of data from this source.

Resource constraints were also a consideration in data set and selection in that it was agreed only possible for CFD and shallow layer models to simulate of the order of 6 and 12 respectively cases while it might be possible for integral and empirical screening tools to …..about 30 cases. Therefore it was proposed to select of the order of 10 data sets on the basis that shallow models will simulate one experiment for each data set, CFD a subset of these cases and simpler models several experiments from each set.

Satisfying the quality constraint therefore by drawing primarily from data in Table 6 and considering the need to cover all complex effects the following breakdown of data sets were dervied:-

- Aerosols 4 Desert Tortoise, 5 FLADIS Riso, 7 BA Propane
- Slope/complex terrain 6 BA Hamburg, 12 EMU-Enflo
- Obstalces 6 BA Hamburg, 7 BA Propane, 8 BA-TNO, 11 Thorney Island, 12 EMU-Enflo
- 'Simple' case – no complex effect 6 BA Hamburg, 7 BA Propane, 8 BA TNO, 11 Thorney Island.

In addition, as proposed above, a small number of passive releases were included. This selection was made from the Prairie Grass and Hanford experiments.

4. FURTHER DATA CONSIDERED

At a later stage several other data sets were identified as potentially useful and their utility to SMEDIS examined. These included two experimental programmes running concurrent with the SMEDIS project. Thus the Chemical Biological Defence Establishment (CBD) have recently carried out a series of multiple distributed instantaneous propane source releases (Jones, 1998) in Nevada, USA in which aerosol effects are likely to have been significant. Also in the United States, the Petroleum Environmental Research Forum PERF) commissioned a series of large-scale instantaneous two phase releases on slopes (Hanna, 1998). Unfortunately though potentially useful data from both these test programmes were not available within the time-scale of the SMEDIS project. Consideration might be given to their incorporation in the SMEDIS database at a later date.

The identified data sets were also reconsidered by Selmer-Olsen and Fannelop (1998) when it was decided to extend the range of special effects to include releases into low or no wind situations and constrained near field releases into congested enclosures with realistic obstacles and confinements. This latter situation is intended to simulate process equipment and plant elements.

Thus Solmer-Olsen and Fannelop identified the further unpublished and potentially useful data sets summarised in Table 7. None of these data had previously been used for validation by project partners though in several instances the data had been compared with CFD models. Of these data sets Selmer-Olsen and Fannelop concluded that the 4 LINERIS data were not available to SMEDIS and the 43 FALIX Norsk-Hydro 45 (NH) and Christian-Micaelson 44 (CMR) data sets were not of sufficient relevance to the project by British Maritime Technology 46 (BMT) was worthy of further consideration. These tests comprised 1:33 and 1:100 scale simulations of dense gas disperion within the C module of the Pipe Alpha offshore platform and it was decided they might be used as test cases which cover the special effect of release into a constrained near-field environment. These data were deemed of good quality and was therefore added to the list of datasets from which cases might be selected and in particular, to allow the behaviour of models for a release into a constrained congested near-field to be examined.
For data in low/no wind speed conditions Selmer-Olsen and Fannelop re-examined the data already identified by the group. In particular they looked in detail at the large scale laboratory experiments (Datasets 36, 37 and 38), wind tunnel data (6, 10, 20 and 32) and

some field trials (7 and 14). They concluded that near-field and low wind speed effects were better studied in a wind tunnel. They argued that the use of a theoretically derived pseudo-source, as is required by several models not incorporating source calculations, often not well specified in field experiments, is avoided in wind tunnels. Also to test the way models handle the effects of gravity is best examined at low wind speeds in the laboratory since wind effects can often dominate in field and wind tunnel trials, particularly in the far-field. Lw wind speed laboratory experiments therefore can be used to isolate gravity effects and allow entrainment models to be tested.

Thus they sought laboratory data in low/no wind speed conditions and concluded that suitable cases could be identified in the experiments of Grobelbouer (36), Billeter (37) and Muller (38). Due to the use of a cold source the first set of experiments was complicated by heat transfer but the last two, comprising instantaneous releases on slopes, were well-instrumented with concentration sensors and provided high quality data.

As a result it was decided to add these two data sets to the list from which cases might be selected, particularly for the special effect of low/no wind speed conditions.

5. CONCLUSIONS

As a result of the foregoing considerations a short list of datasets was drawn up from which cases could be selected against which the models could be assessed. Particular emphasis was placed on the need for data availability quality and the requirement to cover all complex effects in the data, including the two added during the course of project discussions; releases into a congested/constrained near-field and releases into low/no wind speed conditions.

The final short list, therefore, comprised:

- Aerosols – 4 Desert Tortoise, 5 FLADIS Riso, 7 BA Propane
- Slope/complex terrain – 6 BA Hamburg, 12 EMU-Enflo
- Obstacles – 6 BA Hamburg, 7 BA Propane, 8 BA TNO, 11 Thorney Island, 12 EMU-Enflow
- Congested/constrained near field – 46 BMT
- Low/no wind speeds – 37 Billeter ETH, 38 Muller ETH
- 'Simple' cases – no complex effect – 6 BA Hamburg, 7 BA Propane, 8 BA TNO, 11 Thorney Island
- Passive 'base' case – Prairie Grass

Of these datasets all except 46 BMT, 37 Billeter ETH and the Prairie Grass data had already been transferred into the RADIPHEM data-base (Nielsen and Ott 1996). As a consequence it was decided to similarly transfer the remaining data sets into this format in order to ensure all data were readily accessible in a common format and had all undergone common quality checks.

6. REFERENCES

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TABLE 1 : SMEDIS DATA SETS

#	Identifier	Scale	Material	Source type	Release Size	Nb of tests	Complex effects	Atmospheric stability	Ground type	Concentration [1] Measurements
1	Burro	field	LNG	pool	100 kg/s	8	fast aerosol evaporation	B-F	water pond	C : 29 + 45 T : 96
2	Coyote	field	LNG	pool	100 kg/s	3	fast aerosol evaporation	A-D	water pond	C: 35 + 36 + 12
3	Eagle	field	N204	pool	16-42 kg/s	4	chemical reaction to NO2	C-F	sand	C: 31 + 20 + 24 A : 31 T : 96
4	Desert Tortoise	field	Ammonia	jet	100 kg/s	4	aerosol	D-E	sand	C: 20+31+24+8 T : 36 A : 31
5	FLADIS-RISO	field	Ammonia	jet	0.2-0.6 kg/s	16	aerosol	B-E	grass	C : 34+22+10 T : 95
6	BA-Hamburg	wind tunnel	SF6	continuous instantaneous	adim	146	obstacles, slopes	neutral	-	C : 15-220
7	BA-Propane	field	Propane	jet/cyclone	0.1 – 20 kg/s	51	aerosol fences	A-G	grass	C : 40 + 10 + 6 T : 29
8	BA-TNO	wind tunnel	SF	continuous instantaneous	adim	13	fence	neutral	-	C : 4-16
9	FLADIS-TNO	wind tunnel	SF6	continuous	adim	1	fence	neutral	-	C : 330 DIP (not included)
10	WSL repeat variability	wind tunnel	BCF	instantaneous 50-100 repetitions	adim	40	fence	neutral	-	C : 100-400
11	Thorney Island	field	Freon	instantaneous	2000 m^3	30	fence building	B-E	grass	C : 80 +
12	EMU-Enflo	wind tunnel	krypton	continuous	adim	2	buildings real site	neutral	-	C : 150 – 200
13	FLADIS-ECL	wind tunnel	Freon	continuous	adim	4	fence	neutral	-	C : DIP + fluctuations
14	Maplin Sands	field	LNG Propane	continuous	1-5 m^3/min	34	evaporation		sand,sea	
15	Goldfish	field	Hydrogen Fluoride	continuous	10-20 kg/s	3			sand	
16	USEPA	wind						neutral		

#	Identifier	Scale	Material	Source type	Release Size	Nb of tests	Complex effects	Atmospheric stability	Ground type	Concentration [1] Measurements
		tunnel								
17	Falcon	field	LNG	continuous			evaporation			
18	BG-Shell	field	Propane							
19	U. Arkansas GRI	wind tunnel						neutral		
20	Jet in X flow U. Hamburg	wind tunnel						neutral		
21	HSE Porton	field	Freon	instantaneous	40 m^3	35	slopes	B-E/F	grass	
22	Frenchman Flat	field	LNG		< 350 m^3					
23	Marviken	field	H2O	continuous	9.6 E+3 kg/s	10				
24	Landskrona	field	Ammonia							
25	Lyme Bay	field	Chlorine	continuous		4	none	neutral	sea	c : 10
26	Boliden	field	SO2	continuous	0.2 – 14 kg/s	8	aerosol		-	
27	DOE	field	Propane	continuous	small	21			concrete	
28	EnergyAnalyst	field	Propane	continuous	1.9 kg/s	3			grass	
29	BP-Shell	field	Propane	instantaneous continuous	900 kg 1-12 kg/s	84				
30	TUV-Meppen	field	Propane	continuous	2-60 kg/s	60			farmland	
31	Battelle Europe	field	Propane	continuous	1-10 kg/s		aerosol linear obstruction		flat concrete	
32	Hall (1982)	wind tunnel	Freon Argon		Adim			neutral		
33	Meroney & Neff (1984)	laboratory	Freon		Adim					
34	Briter & Synder (1988)	laboratory	CO2	continuous	Adim			neutral		
35	Moodie & Ewan (1990)	laboratory	Freon	continuous	Adim		none	still air	-	C : 25
36	Gr◇belbauer & Fannel⬢p	laboratory	Nitrogen	instantaneous	Adim		cold slopes obstacles	still air		C : 4 T : 50
37	Billeter & Fannel⬢p	laboratory	Argon	instantaneous	2 m^3			still air		C : 60

#	Identifier	Scale	Material	Source type	Release Size	Nb of tests	Complex effects	Atmospheric stability	Ground type	Concentration [1] Measurements
38	M♦ller & Fannel⬢p	laboratory	Argon, CO2	instantaneous	2 m		slopes	still air		C : 60
39	Havens et al. (1994)	laboratory	LNG	instantaneous	Adim		fast aerosol evaporation			
40	Law et al. (1987)	unknown	water	-	-	-	aerosol			-
41	Dow Chlorine	field	chlorine	continuous	< 75 kg/min	6	water spray			

[1] C : concentration, T : temperature, A : aerosols.

Table 2

SMEDIS Data sets-List of References

1 – Burro

Ermak D. L. et al. 'A comparison of dense gas dispersion model simulations with Burro series LNG spill tests results' UCRL-86713 Lawrence Livermore National Laboratory, Livermore, California, 1981.

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McRae T.G., 'Preliminary analysis of RPT explosions observed in the LLNL/NWC LNG spill tests' UCRL-87564 Lawrence Livermore National Laboratory, Livermore, California, 1982.

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no reference provided

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TABLE 3 : Questionnaire replies for each dataset

#	Identification	total	RISO	GDF	NCSR	FMI	JRC	TNO	UH	EDF	DNV	BG	WSA	HSE	ETH
1	Burro	3	0	1							1	1			
2	Coyote	3	1								1	1			
3	Eagle	1	0					0			1				
4	Desert Tortoise	4	1		1			0		1	1				
5	FLADIS-RISO	5	1	1	1		1	0		1	0				
6	BA-Hamburg	3	1				1		1						
7	BA-Propane	6	1	1	1		1			1	0	1			
8	BA-TNO	3	1					1		1	0				
9	FLADIS-TNO	2	1					1			0				
10	WSL repeat variability	1						0			0	1			
11	Thorney Island	7		1	1	1	1			1	1	1			
12	EMU-Enflo	3			1					1			1		
13	FLADIS-ECL	1								1					
14	Maplin Sands	4		1						1	1	1			
15	Goldfish	1									1				
16	USEPA	0													
17	Falcon	1										1			
18	BG-Shell	0										0			
19	U. Arkansas GRI	0										0			
20	Jet in X flow U. Hamburg	0													
21	HSE Porton	2									1			1	
22	Frenchman Flat	0													
23	Marviken	0													
24	Landskrona	0													
25	Lyme Bay	3								1	1	0		1	
26	Boliden	0													
27	DOE	0													
28	EnergyAnalyst	0													
29	BP-Shell	0													
30	TUV-Meppen	1									1				
31	Barttelle Europe	0													
32	Hall (1982)	0													
33	Meroney & Neff (1984)	0													
34	Britter & Snyder (1988)	1													
35	Moodie & Ewan (1990)	1												1	
36	Grobelbauer and Fannelop	1													1
37	Brilleter and Fannelop	1													1
38	Muller and Fannelop	1													1
39	Havens et al. (1994)	0													
40	Law et al. (1987)	1				1									
41	Dow Chlorine	1													

(0/1 : no used/used for model validation)

TABLE 4 : Suitability for validation: Types of model previously used by the participants

#	Identification	summary	RISO	GDF	NCSR	FMI	JRC	TNO	UH	EDF	DNV	BG	WSA	HSE	ETH
1	Burro	2:4	0	2:4							2	2			
2	Coyote	1:2	1								2	2			
3	Eagle	2	0(chem.)					0			2				
4	Desert Tortoise	1:2:4	1		4			0		2	2				
5	FLADIS-RISO	1:3:4	1	4	4		3	0		4	0				
6	BA - Hamburg	1:3	1				3		1						
7	BA - Propane	1:2:3:4	1	4	4		3			4	0	2			
8	BA - TNO	1:4	1					4			0				
9	FLADIS-TNO	1:2	1					1:2			0				
10	WSL repeat variability	2						0			9	2			
11	Thorney Island	2:3:4		2	4	2	3			2:4	2	2			
12	EMU-Enflo	4			4					4			4		
13	FLADIS-ECL	4								4					
14	Maplin Sands	2	2							2	2	2			
15	Goldfish	2									2				
17	Falcon	2										2			
21	HSE Porton	2									2			2	
25	Lyme Bay	2								2	2	0		2	
30	TUV-Meppen	2									2				
34	Britter & Snyder	2										2			
35	Moodie & Ewan (1990)	2												2	
36	Grobelbauer & Fannelop	2:3													2:3
37	Billeter & Fannelop	2:3													2:3
38	Muller & Fannelop	1:2													1:2
40	Law et al. (1987)	aerosol				aerosol									
41	Dow Chlorine	2									2				

1: empirical, 2: box, 3: shallow-layer, 4: CFD

TABLE 5 : Data accessibility (R:REDIPHEM database, A/N : available/not available freely within the group

						Data Quality			
#	Identification	accessibility	data form	data volume	additional check	source	atmospheric	site	concentration
1	Burro	R	computer files	> 1 Mb	RISO, BG	2;3;3	3;4;4	3;4;4	1;4;4
2	Coyote	R	computer files	> 1 Mb	RISO, BG	2;3	3;4	3;4	4;4
3	Eagle	R	computer files	> 1 Mb		3	3	3	3
4	Desert Tortoise	R	computer files	> 1 Mb	RISO,	4;4;3;4	4;3;3;4	3;3;3;4	4;4;3;4
5	FLADIS-RISO	R	computer files	> 1 Mb	RISO, GDF, EDF	4;4;3;4	3;4;3;3	2;4;4;4	4;4;4;4
6	BA - Hamburg	R	computer files	> 1 Mb	RISO, TNO	4;3;4	4;4;4	4;3;4	4;2;4
7	BA - Propane	R	computer files	> 1 Mb	RISO, GDF, EDF	2;2;4;2;3	3;3;3;3;3	4;2;3;3;4	4;3;4;4;4
8	BA - TNO	R	computer files	> 1 Mb	RISO,	4;3;3	4;3;3	4;3;4	4;3;4
9	FLADIS-TNO	R	computer files	> 1 Mb	RISO,	4;4	4;4	4;4	4;3
10	WSL repeat variability	R							
11	Thorney Island	R * + HSE			EDF, BG	4;2;4;3;4;4	4;3;3;3;3;4	4;3;3;3;4;4	4;3;3;3;4;4
12	EMU-Enflo	A (WSA)	computer files	< 1 Mb	NCSR, WSA	4;3;4	4;2;4	4;4;4	4;3;4
13	FLADIS-ECL	A (EDF)	computer files	< 1 Mb	EDF	2	3	4	3
14	Maplin Sands	A (DNV)	reports		BG	3;3	2;4	2;4	2;4
15	Goldfish	A (DNV)	reports			4	4	4	3
17	Falcon	N							
21	HSE Porton	A (HSE)	reports			3;2	3;2	4;3	3;3
25	Lyme Bay	A (DNV,HSE)	reports		HSE	3;1	1;1	3;1	3;2
30	TUV-Meppen	A (DNV)	reports		DNV	2	2	3	3
34	Britter & Snyder	A (CERC)	computer files	< 1 Mb					
35	Moodie & Ewan (1990)	A (HSE)	computer files	< 1 Mb		4	1	1	3
36	Grobelbauer & Fannelop	A (ETH)	reports			3	3	4	2
37	Billeter & Fannelop	A (ETH)	reports			3	3	4	4
38	Muller & Fannelop	A (ETH)	computer files	> 1 Mb		3	2	4	3
40	Law et al. (1987)	N							
41	Dow Chlorine	A (DNV)	report			3	2	3	4

Data quality estimated by the participants (1= poor, 4=very good)

TABLE 6 - list of SMEDIS datasets

#	Identifier	Scale	Material	Source type	Nb tests	Complex effects
1	Burro	field	LNG	pool	8	fast aerosol evaporation
4	Desert Tortoise	field	Ammonia	jet	4	aerosol
5	FLADIS-RISO	field	Ammonia	jet	16	aerosol
6	BA - Hamburg	wind tunnel	SF6	continuous instantaneous	146	obstacles, slopes
7	BA - Propane	field	Propane	jet/cyclone	51	aerosol fences
8	BA - TNO	wind tunnel	SF6	continuous instantaneous	13	fence
11	Thorney Island	field	Freon	instantaneous	30	fence building
12	EMU-Enflo	wind tunnel	krypton	continuous	2	building real site

TABLE 7 : Further datasets considered

#	Identifier	Scale	Material	Source type	Release size	No. of tests
42	INERIS	Field	NH_z	Continuous	> 1 kg/s	large
43	KALIX	Field	Chlorine	Instantaneous	large	
44	CMR	Wind tunnel	Methane Propane	Continuous	adim	
45	NH	Wind tunnel	Methane Hydrogen	Continuous	adim	
46	BMT	Wind tunnel	Hydrocarbons	Continuous	adim	

APPENDIX 2

Data used in the validation exercise

1. INTRODUCTION

Following the identification of useful datasets detailed in Appendix 1, a procedure to select individual cases was devised to ensure that the widest possible spectrum of special effects was covered in the validation exercise. This procedure is described in Section 4 of the main report.

The resulting selection is summarised in Table 1. This table lists the source of the data, the particular experiment selected from that dataset and a code indicating the trial in terms of instantaneous/source duration; the complex effect present, the important of density effects and the stability of the atmosphere. Thus the code SiCoDsAn denotes an instantaneous release (Si) into an obstacles array (Co) with strong density affects (DS) and a neutral atmosphere (An). This is amplified in the columns at the right side of the Table, where is also found the type of model required to run against each particular case. Hence CFD models were required to carry out six runs only EEC 550, EEC 171, DAT 638, EMUDJ, FLADIS 9 and TI 21 as indicated by the O.

2. DATA LISTINGS

The sheets following Table 1 contain listings of the data in the order found in the Table. All data not already in the REDIPHEM database were initially transformed into the REDIPHEM format and the relevant entries abstracted on to Excel spreadsheets. These are the listings contained here.

The entries generally follow the same format throughout. So that release data, including material properties and release conditions, are followed by details of atmospheric conditions, then information on the site such as the specification of obstacles or ground slope. More detailed information on wind speed and direction is then given, if that was available from the experiment.

Finally, values of the comparison parameters are listed. These are the quantities for comparison with model output and are defined explicitly in Appendix 3. These are quantities derived from experimental measurements of cloud temperature and concentration and include mean and standard deviation of temperature, concentration, …..and, where appropriate, a measure of the cloud width and cloud arrival and departure times.

These data have also been made available in electronic form on the CD accompanying this report.

3. FURTHER DATA

Following discussions among the project partners it was agreed that it would be beneficial to increase the range of special effects covered by the project. In particular it was important to be able to assess the ability of models to predict the behaviour of dense gas releases in a near-field confined/congested by a complex and dense obstacles array and also in low/no wind situations. However, due to lack of resources this could not be achieved within the scope of the SMEDIS project.

As a result it was decided to handle resourcing situations those outside the project but within the SMEDIS group. Work is therefore underway to process two additional run cases from the additional datasets identified in Appendix 1. These data have already been transformed into the REDIPHEM format. Two cases, including the two additional special effects identified, will therefore be selected and added to the following. They will comprise one case from dataset 46 BMT (Appendix 1) for a release into the confined environment of an offshore process module and a further case from either 37-Billeter or 38-Muller for an instantaneous release on a slope in still air conditions to cover the low/no wind speed conditions special effect.

TABLE 2.3 SPECIFIC CASES USED IN SMEDIS VALIDATION EXERCISE

Data set group	**Test name**	**Code**	**Rationale**	**C/I**	**F/W**
Prairie Grass		ScCnDwAn	Simple, well-used data set	C	F
		ScCnDwAn	As Test 17, but with unstable atmosphere	C	F
Desert Tortoise		ScCaDsAn	Aerosol and stronger dense gas effects	C	F
		ScCaDsAn	Repeat of DT1 with different flow rate	C	F
BA Propane		ScCnDsAn	Strong density effects	C	F
		ScCoDsAn	As EEC360, but with one obstacle (fence)	C	F
		ScCoDsAn	As EEC360, but with two obstacles (fences)	C	F
		ScCnDsAn	Strong density effects	C	F
		ScCoDsAn	As EEC550 but with one obstacles (fence)	C	F
	EEC560	ScCnDsAn	Strong density effects	C	F
	EEC561	ScCoDsAn	As EEC560, but with obstacle (porous fence)	C	F
	EEC170	ScCnDsAn	Strong density effects	C	F
	EEC171	ScCoDsAn	As EEC170, but with obstacle (circular fence)	C	F
		SiCaDsAn	Instantaneous release with aerosol effects	I	F
BA Hamburg		SiCtDsAn	Instantaneous source with steep slope	I	W
		SiCtDsAn	As DAT638 but slope less steep	I	W
		SiCoDsAn	Instantaneous release with wall parallel to wind	I	W
		ScCtDsAn	Continuous release on slope	C	W
		SiCoDsAn	Instantaneous release with canyon	I	W
		SiCoDsAn	Instantaneous release and near-field array of obstacles	I	W
		ScCoDsAn	Continuous release with near-field obstacles	C	W
BA TNO		ScCnDsAn	Reference continuous release without obstacles	C	W
		ScCoDsAn	As TUV11 but with obstacle (oblique fence)	C	W
EMU ENFLO		ScCt/oDsAn	Dense release in complex terrain with obstacles (buildings)	C	W
		ScCt/oDwAn	As EMUDJ but with weak density effects	C	W
FLADIS Riso		ScCaDwAs	Aerosol effects and stable atmosphere	C	F
		ScCaDwAn	Aerosol effects and neutral atmosphere	C	F
		ScCaDsAn	Dense release with aerosol effects	C	F
Thorney Island		SiCnDsAn	Instantaneous release with strong density effects	I	F
		SiCoDsAn	Instantaneous release with strong density effects and fence	I	F

KEY: C = continuous release; 1 = instantaneous release. F = field trial; W = wind tunnel experiment. An "x" indicates aerosol effects (A), terrain effects (T) and obstacles (O) important. Fences are linear unless otherwise stated. An "o" indicates the case should be attempted by screening tools (ST), integral models (I), shallow layer (SL) or CFD(3e) models.