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Development and test of an evaluation protocol for heavy gas dispersion models

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Abstract

In order to improve the quality (i.e. fitness-for-purpose) of models used to describe the atmospheric dispersion of heavy gas, an evaluation methodology has been developed and tested through a small evaluation exercise. This activity was carried out by the Heavy Gas Dispersion Expert Group, which was set up by European Commission's Model Evaluation Group. Its objective was to develop a protocol for evaluation of the models and to make an overview of the experimental data available for such an evaluation. The main results of the Expert Group's activities are: (i) a tested heavy gas dispersion model evaluation protocol, (ii) a list and classification of available models and (iii) a list and classification of relevant data-sets. Furthermore, it is concluded that there is a need for a more extensive evaluation exercise and that the scientific evaluation requires more attention. © 1997 Elsevier Science B.V.

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1. Introduction

The European Commission (EC) has been supporting research in industrial safety for 13 years. A major part of the work funded falls into the category of consequence modelling. This involves the modelling (mathematically as well as physically), of the

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chemical and physical phenomena associated with major industrial hazards. The primary use for such models is in risk assessments for safety reports and by safety officers. As a consequence, they may influence very important decisions such as the design of, or granting of permission for, chemical plants. There is a widespread concern over the quality of these models, i.e., whether these models are scientifically and technically correct, compare favourably with experimental data and are fit for purpose.

To answer these quality concerns the EC, Directorate General XII Science, Research and Development (DG XII) initiated a study carried out by Britter [1]. This study provided a framework for the management of the quality and evaluation of technical models. As a consequence a Model Evaluation Group (MEG) was set up by the EC. The current situation is described by Petersen [2]. A generic evaluation protocol for consequence models was produced by MEG [3].

Heavy gas dispersion is an area in which there has been a particularly large amount of EC-funded research related to industrial safety. This started in 1980 with the Thorney Island field trials on dense gas dispersion (see e.g., Britter and McQuaid [4]). Since then the EC has supported two other major series of field tests in parallel with wind-tunnel and modelling work. In addition, there are many heavy gas dispersion (HGD) models of varying quality and applicability, ranging from simple box models through more complex 'shallow layer' type models to fully three-dimensional computational fluid dynamics (CFD) models. Each type of modelling has its merits and disadvantages, and the plethora of models presents a baffling situation for those having to choose and use models. A more structured and unified approach to evaluation and quality enhancement is thus particularly urgent in this field.

Therefore, MEG set up an expert group on heavy gas dispersion in 1993, one of the aims of which was to produce an evaluation protocol specific to HGD models. The group further developed a protocol that had been produced by Bakkum under the EC project REDIPHEM (Review and Dissemination of Physical Effect Models, an overview can be found in Cole and Wicks [5]) taking the MEG protocol as a starting point. The protocol produced by the group was tested in a small exercise, the results of which were presented at an EC workshop in Mol on November 1994, Cole and Wicks [5]. This paper describes the activities of this Heavy Gas Dispersion Expert Group (HGDEG). The problems related to model quality are of course not restricted to research initiated by the CEC, but because the HGDEG operated under the CEC's umbrella, the CEC's considerations are specially relevant.

In this paper, we adopt the terminology as suggested by the MEG protocol [3], i.e., evaluation includes the whole review of any model with respect to proper scientific formulation (called assessment), correct coding (called verification) and comparison with experimental data (called validation). We are aware that sometimes different terms are used and that there is some philosophical criticism on the use of the term 'validation'.

2. Objectives of the group

The members of the group were:

1. Alf Mercer, Health and Safety Executive (HSE), UK (chairman)

2. Claude Bartholome, Solvay, Belgium
3. Bertrand Carissimo, Electricité de France (EDF), France
4. Nijs Jan Duijm, Netherlands Organisation for Applied Scientific Research TNO, Netherlands (presently at Risø National Laboratory, Denmark)
5. Hartmut Giesbrecht, BASF, Germany.

The tasks of the group were:

1. To draw up a classified list of HGD models.
2. To identify experimental data sets for use in validation.
3. To review and adapt the MEG documents 'Guidelines for Model Developers' [6] and 'Model Evaluation Protocol' [3]
4. To arrange an open (i.e., allowing participation of any interested party) exercise to test the protocol.

3. Modus operandi of the group

Membership of the Expert Group was on invitation by the EC. The group performed its tasks between November 1993 and September 1995. The basis for the group's activities were the MEG Guidelines for Model Developers [6] and the MEG Model Evaluation Protocol [3].

Main results of the group were obtained through round table discussions during 3 formal meetings. In between the meetings, the members communicated frequently on draft documents and progress of activities. Informal comments on the documents were also made by Steve Jones (AEA Technology, UK, member of the MEG). Although documents were circulated to members of the group for comment, the round table discussions proved essential to obtain consensus.

4. Results of the activities of the group

4.1. Task 1—classified list of HGD models

Clearly, this task is never ending as new models are developed or improved versions of existing models are produced. The list of models below presents the status at the end of the HGDEG's activity, i.e., September 1995

The Heavy Gas Dispersion Protocol (see Section 4.3) distinguishes 3 to 4 classes of dispersion models:

1. Phenomenological models, in which the dispersion behaviour is described by a series of nomograms or simple correlations;

2a. Intermediate models. To this group belong the box-type models or 1-dimensional integral models that describe the evolution of the cloud or plume with time or distance, respectively;

2b. Models based on the shallow-layer equations in the 2 horizontal co-ordinates, and
3. Models based on the solution of the full set of 3-dimensional, time-dependent Navier–Stokes [2] equations.

It should be noted that the later models of class 2a and the models of class 2b are often based on the same equations and theory, so the difference seems mainly related to a difference in dimensions. However, most class-2a models are not able to treat effects of (gentle) topography. whereas most class-2b models claim to be able to do so.

The following is based on an existing list from the UIC [7] report and results from the REDIPHEM project, as well as input from the individual Heavy Gas Dispersion Expert Group members:

4.1.1. Models of class 1

- Britter and McQuaid Workbook [4]
- VDI Guideline 3783 Part 2 [8]

4.1.2. Models of class 2a

Most models within this class can be traced back to original developments 2 decades ago. One can set up a kind of hereditary scheme or 'family tree' for these models, showing on what earlier models and algorithms they are built (Kolkman [9]). The following list mentions the most important original work (without claiming to be complete).

- SAFER, TRACE (based on Kaiser and Walker [10])
- CONSEQ, PHAST, WHAZAN, SAFETI (based on Cox and Carpenter [11])
- DENZ, DRIFT, CIGALE 2, SLOPEFMI (based on Fryer and Kaiser [12]; an overview of DRIFT can be found in Webber et al. [13])
- HEGADAS, HEGABOX, HGSYSTEM (Colenbrander [14])
- DEGADIS (Colenbrander [14]; van Ulden [15]; and Havens [16])
- CHARM, EOLE, (Eidsvik [17])
- DENS1, DENS8, DENS20 (Meroney and Lohmeyer [18])
- SLAB (Zeman [19]; Ermak and Chan [20])
- CRUNCH, GALON (Jagger [21])
- GASTAR (Britter [22])
- CAMEO (E.P.A.-U.S.A.)
- PAMPA (Rhone-Poulenc, France)
- HASTE (ERT, USA)
- MIDAS (Woodward, Pickard Lowe and Garrick, USA)
- CLOUD (Hewitt et al. [23]; Martini [24])

4.1.3. Models of class 2b

During the REDIPHEM project it was concluded that within this class no models were yet available for operational use, but that a lot of effort is currently put into

[2] In fact, only models based on the Reynolds equations, i.e., the Navier–Stokes equations after averaging out the turbulent fluctuations, are being used, together with a closure assumption about the turbulent processes.

development of these type of models. Although these models were not used for consequence analysis at the time of the evaluation exercise described below, it is expected that they will be used for such analysis in the near future.

- SHALLOW (Webber et al. [25])
- TWODEE (Hankin and Britter [26])
- DISPLAY1, DISPLAY2 (Würtz [27]; Würtz et al. [28])

4.1.4. Models of class 3

Here only models are listed that have been used specifically for atmospheric dispersion of dense gases. The claim of many 'general purpose' CFD software packages to be able to treat these problems with equal accuracy should be backed up by proper validation.

- SIGMET (England [29])
- TRANSLOC (Schnatz and Flothmann [30])
- FEM3 (Chan et al. [31])
- ZEPHYR (Hertel and Teuscher [32])
- MARIAH (Taft [33])
- HEAVYGAS (Deaves [34])
- MERCURE (Riou [35])
- ADREA-HF (Bartzis [36])
- MERADIS (Vergison et al. [37])

4.2. Task 2—classified list of relevant data

The list of classified experiments on dense gas dispersion is extracted from the REDIPHEM database (Nielsen and Ott [38]). The REDIPHEM database, presented below, contains easily accessible data, with a reference to the original source and an assessment of data quality. It differs substantially from the Modellers' Data Archive (MDA) (Hanna et al. [39]) in that it contains the full time series of meteorological and concentration data at all sensor positions. The MDA contains only time averaged meteorological parameters, and maximum concentration and plume width as a function of distance. The REDIPHEM database is not extensive in that it focuses on data from experiments performed in relation to EC-sponsored research and some data obtained in the USA. The well-known Thorney Island data-set is lacking however, because the original data are not easily accessible in electronic form at the moment. (It is intended that this data, involving mainly the instantaneous release of about 2000 m^3 of a Freon/nitrogen mixture, will be transferred to CD-ROM in the near future.)

The data-sets included in the REDIPHEM database are listed in Table 1.

4.3. Task 3—heavy gas dispersion model evaluation protocol

This task was to produce an Evaluation Protocol specifically for heavy gas dispersion models. The protocol is based on the general evaluation protocol developed by the MEG

Table 1
Data-sets included in the REDIPHEM database

Name	Location/source	Phenomena involved	Release/max. downwind distance
Burro experiments	China Lake, California, 1980 US Lawrence Livermore National Lab.	Atmospheric releases of LNG (liquid); Spill on water pond; Fast evaporation	100 kg/s 1000 m
Coyote experiments	China Lake, California, 1981 US Lawrence Livermore National Lab.	Atmospheric releases of LNG (liq.); Spill on water pond; Fast evaporation; Cloud ignition	100 kg/s 2000 m
Desert Tortoise experiments	Nevada 1983 US Lawrence Livermore National Lab.	Atmospheric releases; Flashing ammonia jet; Dense to neutral clouds; Non-obstructed; Flat terrain	100 kg/s 1000 m
Eagle experiments	Nevada 1983 US Lawrence Livermore National Lab.	Atmospheric releases; Evaporation of N_2O_4; Chemical reaction to NO_2; Flat terrain	35 kg/s 800 m
FLADIS	Landskrona 1993–1994 Risø, HydroCare, FOA, CBDE	Ammonia; Atmospheric releases; Flashing jet; Dense to neutral clouds; Non-obstructed	0.5 kg/s 200 m
EC-Major Technological Hazards-project 'BA' and 'FLADIS' wind-tunnel experiments	Hamburg Univ.	SF_6; SF_6 + air; Continuous and instantaneous; Flat; Various obstacles; Slopes	1 g/s 1 m
EC-Major Technological Hazards-project 'BA' field experiments	Lathen 1988–1989 TÜV, Risø, FOA	Propane; Flashing jet/cyclone; Atmospheric releases; Dense cloud; Flat terrain; Obstructions (fences)	3 kg/s 100 m
MT-TNO 'project BA' wind tunnel experiments	Apeldoorn, Netherlands, 1988–1990 TNO	Continuous plume; Instantaneous release (Thorney Isl. No. 17); Plume hitting fence; SF_6 gas	0.001 kg/s 5 m
'FLADIS' wind tunnel experiments	Apeldoorn, Netherlands, 1992 TNO	Continuous plume; Many sensor locations; SF_6 gas	0.001 kg/s 5 m
Warren Spring repeat variability	Stevenage, UK, 1988–1991 Warren Springs Laboratory	Instantaneous isothermal release of Thorney Island type in 1:100 model scale. Variable bulk release stability. Solid fence/crenellated fence/no fence. Variable fence height. 50–100 repetitions of each case.	0.01 kg 2 m

[3], but enhanced and made more specific for the application to heavy gas dispersion models. The Heavy Gas Dispersion Expert Group was particularly fortunate in that Emil Bakkum at TNO, had already produced such an Evaluation Protocol for the CEC project, REDIPHEM. The protocol produced by the group is basically that produced by Bakkum, with some relatively minor changes.

The protocol has been finalised, taking into account the comments that were made in the context of the evaluation exercise, which was concluded by a one-day meeting in Mol, on November 25, 1994 (see Section 4.4). At this meeting the draft protocol was widely accepted with some minor remarks only. The final protocol is included in the final report from the Heavy Gas Dispersion Expert Group to the EC Model Evaluation Group (Mercer et al. [40]).

4.4. Task 4—arrange an open exercise to test the protocol

An informal open evaluation exercise was organised, following the guidelines contained in the protocol. The main purpose of the exercise was to test the protocol and to bring problems out into the open, not to evaluate the models themselves. It was agreed that results should be presented at a workshop, but that there would be no attempt to rank the models and that results would be presented anonymously. Since preparation for the exercise took place over rather a tight time-scale some mistakes were made (involving the definition of the source dimension in the wind tunnel data and the correct name of one of the performance measures).

About 40 invitations to participate were sent out. 6 responders provided quantitative data. The evaluation exercise package, containing the protocol, the data sets and an explanatory note specifying the test parameters to be calculated, was sent out about a month before the meeting. Participants were therefore given a rather a short time to carry out the calculations.

Two data sets—the EC 55 propane field test results (Heinrich and Scherwinski [41]), and some TNO wind-tunnel data (Oort and Builtjes [42])—were sent to a large number of model developers, including both the input and output data. The modellers were invited to run their models, compare their predictions with the experimental data, and to make general comments on the procedure. Thus, the exercise was not a blind test, since the experimental data were available to the modellers throughout.

The two data-sets were selected because they were considered to be fit for this particular evaluation exercise and they were readily available to the members of the Heavy Gas Dispersion Expert Group. The statistical performance measures referred to in the Protocol, namely those adopted by Hanna et al. [39,43], are intended only as an example of what can be done. These measures are not to be regarded as the recommendations from the HGDEG. In fact, the evaluation exercise package required that the statistical evaluation should be performed by using spatially distributed data and a performance measure that Duijm et al. [44] call the 'Mean Relative Bias', MRB (In the explanatory note this was erroneously called 'Fractional Bias'). The MRB is defined as:

$$\mathrm{MRB} = \langle 2\frac{C_\mathrm{p} - C_\mathrm{o}}{C_\mathrm{p} + C_\mathrm{o}} \rangle$$

(here $\langle .. \rangle$ denotes averaging over all measurement locations, C_o is the observed concentration and C_p is the model prediction). It is noted that some of the sensors in the EC 55 data read zero concentrations. The MRB can be used here, whereas some other performance measures can not handle zero concentrations. For instantaneous releases, concentration C is replaced by dose D, the integrated value of concentration over time for the whole period of exposure between cloud arrival time t_0 and cloud departure time t_{end}: $D = \int_{t_0}^{t_{end}} C dt$. Dose was selected in order to avoid problems with the use of averaging time and definitions of maximum concentration. The explanatory note did not strictly define quantities like the period of cloud exposure, but requested that participants provided the definitions they used. No replies on this request were received.

The results of the evaluation exercise were presented at the Model Evaluation Group Seminar, held at Mol, Belgium, in November 1994. A detailed account of the Mol meeting is given by Cole and Wicks [5]. Only for sake of completeness and in order to show the amount of variability in the results we include the numerical results of the fractional bias for various models in Table 2. A MRB of $\pm 2/3$ corresponds to an average over- or underprediction with a factor of 2. We repeat that the purpose of the evaluation exercise was not to qualify or rank the models. In order to respect the agreed anonymity we do not identify the models nor model types. Although the data are too limited to draw valid conclusions, there did not seem to be a correlation between model complexity and performance.

We observe that all results agree broadly within a factor of two with the experimental data with a general tendency to overestimate. There seems not to be any correlation between model performance and the type of the experiment.

The participants were only required to supply a value for the MRB. One of the

Table 2
Values of Fractional Bias discussed during the open evaluation exercise in ascending numerical order

Trial EC 55 without fence (MRB based on concentration)
−0.53
+0.11
+0.13
+0.35
+0.47
+0.73
Trial EC 55 with fence (MRB based on concentration)
−0.58
−0.08
+0.13
+0.78
TNO wind-tunnel instantaneous release (MRB based on dose)
+0.01
+0.44
+0.79

participants complained about the lack of a variance measure (e.g., squared error). The participant claimed this would help to understand the model behaviour.

The main issues arising from the seminar are included in the discussion in Section 5.

5. Results and discussion

The evaluation protocol (which in final form can be found in the HGDEG final report [40]) divides the evaluation exercise into 6 steps:
1. description of the model (origin, type, documentation, etc.);
2. description of the database used for the validation (references, type, release conditions, etc.);
3. scientific assessment of the model (completeness of the description of the physical and chemical phenomena, assumptions made, use of model constants, solution techniques);
4. user oriented assessment of the model ('user-friendliness', guidance and assistance of the user, quality of user documentation, computer requirements);
5. verification of the code (software errors);
6. validation of the model by comparing model predictions with (experimental) observations.

The first two steps provide essential information. Steps 3 to 6 correspond to the essential activities leading to evaluation of the model as advised by the MEG: assessment, verification and validation (MEG [3]). All these 3 activities are of equal importance. However, the emphasis is too often put on the (statistical) validation. The Heavy Gas Dispersion Expert Group evaluation exercise paid much attention to this aspect also, but in view of the limited data and the complexity of the phenomena, the scientific assessment of the model should be much to the fore in any future evaluation exercise.

It is stated explicitly in the protocol that an evaluation can be performed by a model developer or (any) user. This implies that a model developer should provide sufficient documentation on the model to allow the scientific assessment to be performed by a third party. If the model developer is the evaluator, he/she is forced to provide an objective user-oriented assessment of the model. This may require assistance from a third party.

Hopefully the protocol requirements on the description of databases for validation will force experimentalists to present and document results carefully with validation in mind. Experimental data need also to be assessed. Calibration and averaging procedures need careful documentation and error measures on boundary and initial conditions like wind speed and source strength (used as input to dispersion models) should be provided. The utility of an experimental data-set increases with the amount of information on experimental conditions, such as turbulence levels in wind-tunnel data-sets, etc.

With respect to the statistical validation procedure, during preparation of the protocol and the evaluation exercise, the HGDEG considered that there was too little guidance available to recommend specific procedures or statistical techniques. Therefore, the evaluation protocol does not recommend such techniques. It is the responsibility of the evaluator to select the 'best' method for his/her particular situation. In view of the discussion at the Mol seminar of possible performance measures and manipulation of observed data it became clear that a general methodology that can be recommended does not (yet) exist. Comments, questions and suggestions at the Mol seminar covered such problems as:

- Should the validation be based on centreline maximum concentrations (or doses) or should one use measured and calculated data at fixed positions (instrument positions) in the field and for the same moment, i.e., use data 'paired in time and space'?
- In an open validation exercise, should the necessary analysis of source term data and atmospheric data be provided centrally or should this analysis be left to the participants themselves?
- How should one deal with situations that the model cannot explicitly cope with (e.g., obstacle effects, misalignment of the wind with the jet)?
- Should one use different weighting factors in a statistical performance measure for different types of application and for users or developers?
- Should data from wind-tunnel experiments first be scaled to field dimensions or not?

As stated before, the protocol still leaves freedom in these cases. Documentation of procedures, analysing techniques, etc. of any validation exercise is therefore vital for future use and reference. One should realise that, on the aspects of scientific assessment and user-oriented assessment, no experience on unified or generally applicable techniques is available, but that these techniques perhaps are more badly needed here than for the statistical validation. Keeping this in mind, we should not exclude future changes and improvements of the protocol.

6. Conclusions of the heavy gas dispersion expert group

(i) The work of MEG in heavy gas dispersion has reached its initial goals and is largely complete. The results of this activity are:

- a tested Heavy Gas Dispersion model evaluation protocol
- a list and classification of available models
- a list and classification of relevant data.

(ii) The Heavy Gas Dispersion Evaluation Protocol, with a few suggested improvements, was widely approved at the meeting in Mol in November 1994.

(iii) There is a great deal of interest in model evaluation in this field. There is an urgent need for guidance for;

- model users on how to use models,
- buyers of models in choosing the best model for their needs,
- model developers in developing models of high quality, which includes that models are easy to use and that model documentation allows an independent evaluation to be performed.

The HGDEG protocol can be considered a step forward in providing this guidance.

(iv) An independent evaluation exercise with adequate funding would be very worthwhile, However, the way in which it is conducted requires very careful thought. The exercise of Hanna et al. [39,43] in the US is widely appreciated as a serious attempt to address a very important need. Nevertheless, it has provoked a certain amount of criticism, e.g., on the use of centreline or 'arcwise maximum' concentrations only, and the selection of performance parameters (see e.g., Davies [45]).

In the terms used by the MEG, Hanna's exercise should be considered to be a validation. The work of the HGDEG has built on this while seeking to put in place a methodology for evaluation. This has a broader set of aims, like model improvement and understanding of weaknesses and gaps in data.

(v) The statistical validation tends to be over-emphasised in the evaluation process. The scientific assessment and the verification are as least as useful to determine the validity of a model for a certain application, whereas the user-oriented assessment helps to identify the overall utility of the model. There is a lack of general techniques to perform these parts of the evaluation process, especially when different models are compared.

7. Postscript—ongoing and future activities

Since the Expert Group completed their duties, some other activities were performed or initiated, following the discussions and conclusions described above.

Duijm et al. [44] elaborated on the question: "Should the validation be based on centreline maximum concentrations (or doses) or should one use measured and calculated data at fixed positions (instrument positions) in the field and for the same moment, i.e. use data 'paired in time and space'?". This exercise gained insight into the sensitivity of the statistical validation on the choice of the data-sets, the validation method ('paired in time and space' versus 'centreline concentrations') and resulted in recommendations on the use of performance parameters.

Following on from Section 6 (iv), an independent evaluation exercise is now to be carried out with funding from EC DG XII. This is the SMEDIS project, Scientific Model Evaluation of Dense Gas Dispersion Models, co-ordinated by the UK Health and Safety Executive. A crucial element of this project is the scientific assessment of a number of models currently in use throughout Europe. The project started June 1996 and will be completed in 1999.

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