SMEDIS: scientific model evaluation of dense gas dispersion models

N.C. Daish, R.E. Britter and P.F. Linden

Cambridge Environmental Research Consultants Ltd., 3 King's Parade, Cambridge CB2 1SJ, UK

S.F. Jagger

Fire Safety Section, Health & Safety Laboratory, Harpur Hill, Buxton, Derbyshire SK17 9IN, UK

B. Carissimo

Electricité de France, Direction des Etudes et Recherches, 6 Quai Watier, 78401 Chatou CEDEX, France

Abstract: SMEDIS is a project currently in progress to develop a protocol for the scientific evaluation of dense gas dispersion (DGD) models, with particular emphasis on the complex effects of obstacles, terrain and aerosols often found in real situations, and then to apply this protocol to DGD models currently in use in Europe. This paper describes the general features of a model evaluation project and then outlines the implementation in the specific case of SMEDIS. The paper concludes with some experiences from the project to date.

Keywords: complex effects, dense gas dispersion, model evaluation, model validation.

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Introduction

Following a number of major incidents involving the accidental release of hazardous materials, such as those at Flixborough, UK in 1974 and Seveso, Italy in 1976, a regulatory regime has developed, particularly in Europe, which requires operators of chemical and process plants to produce a 'safety case' to demonstrate safe operation of their plant. Such a safety case involves identifying possible accident scenarios and calculating the consequences of the hazards associated with those scenarios by use of predictive mathematical models.

Users of these models — developers, consultants, safety personnel or regulators —

apply them to inform safety-critical decisions and, in doing so, often face questions regarding both the accuracy and applicability of a given model in the given situation(s).

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To respond to such questions, it would be helpful to users if they could refer to an (independent) examination of the model which had already addressed these issues.

Such an examination should clearly include validation of the model, i.e. the quantitative comparison of the model predictions and experimental data. However, there is an increasing body of opinion that this alone is not enough. In addition, with equal weight there should be a scientific assessment of the model to judge objectively its scientific basis (physical processes included, how they are modelled, approximations employed, solution techniques, etc.), and appraisal of its user-orientated features (user interface, resources required, etc.). Thus the strengths and weaknesses of the model may be established and conclusions drawn on its range of applicability. Yet another element can be incorporated, namely the verification of the model, i.e. to establish that the algorithms of the mathematical model have been translated accurately into the (computer) implementation. Attention is often concentrated on the first two elements. The combination of all three elements is referred to as evaluation of the model; the term scientific model evaluation is sometimes used to emphasize that validation is not the sole concern. The procedure for carrying out the evaluations is documented in the evaluation protocol.

These considerations are relevant to all mathematical models but, at present, this type of examination has been carried out for only very few. Evaluation has so far concentrated on models relating to major accident hazards, primarily those describing fires, explosions and the dispersion of clouds of denser-than-air gases. In particular, dense gas dispersion models are of key importance, as they provide the input both to fire and explosion models (flammable releases) and to toxicity models (toxic releases). The importance of the dense gas problem is also reflected in the large number of different models which have been applied or developed specifically to address it.

In Europe, scientific model evaluation has been spearheaded by the Model Evaluation Group (MEG), which grew out of the Commission of the European Communities (CEC) programme on Major Industrial Hazards. The MEG developed a generic protocol for conducting model evaluations, and early efforts in this area were reported by Cole and Wicks. Following this, the REDIPHEM project, sponsored by the Commission, was a first attempt to set up an evaluation structure. This project collected data suitable for model validation, making judgements of quality and utility before inclusion in a database, and developed a protocol specific to dense gas dispersion models. A subgroup of the MEG, the Heavy Gas Dispersion Expert Group (HGDEG), continued this work by drawing up a list of heavy gas dispersion models, identifying further datasets, further developing the protocol and conducting an informal open exercise to test this protocol. This open exercise comprised the distribution of a limited number of suitable datasets to interested participants followed by a statistical analysis of returned model predictions. Details and experience of this limited exercise are given by Cole and Wicks; the work of the HGDEG is described by Duijm et al. 5 and a separate protocol is in Mercer et al. 6

There has been similar interest in the United States. Hanna et al.⁷ reviewed available field data and described both the setting up of the Modeler's Data Archive (MDA), a database containing a subset of the available data in a standard format, and its use in comparing quantitatively the performance of 15 dense gas dispersion models. This exercise was based on a statistical comparison of model prediction and experimental measurements alone, i.e. without assessment. More recently, Lazaro et al.⁸ addressed the need for scientific assessment, though they chose to run their models for realistic, non-experimental scenarios, i.e. without validation (in the sense defined above).

This previous evaluation work dealt only with dispersion over flat open terrain. Real releases from process plants, on the other hand, can lead to widely different scenarios in many of which 'complex effects' are important: 9 releases may occur into regions confined by surrounding buildings and/or other obstructions; installations are often sited in areas with sloping terrain and releases may be complicated by the presence of evaporative two-phase aerosols, since they often result from loss of containment of pressurised liquefied gases.

Thus, there is a need to address these more realistic scenarios and combine this with use of real data for validation teamed equally with an in-depth scientific assessment of each model. ^{10, 11} The CEC sponsored project SMEDIS seeks to extend previous evaluation work concerning dense gas dispersion models in just this way.

Essential features of a model evaluation project

The aim of this section is to give a brief description of the features of a model evaluation project such as SMEDIS, covering all stages of the project from inception to dissemination of results. Four phases are identified, which take place in sequence. Many of the features are applicable in general, for example for use with a different group of models. Actual examples illustrating each stage are given in Section 3, where the application of this framework to SMEDIS is described.

2.1 Defining the project

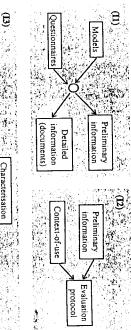
It is first necessary to define the scope of the project and its overall features. These will set the overall constraints of the project and will influence the stages that follow. The definition of the project is likely to be influenced by pragmatic constraints such as financial cost and available timescale.

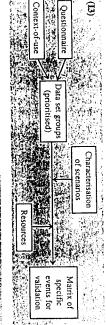
- List of models. An initial list of models that can simulate a certain type of problem
 must be compiled. Selection criteria may be applied for inclusion at this stage. A
 proponent/contact needs to be established for each model. It is also useful at this
 stage to identify different model types as a means of organizing the models in the
 rest of the project.
- Context-of-use. It is useful to highlight specific areas of application for the models; for example, inclusion of specific effects, ranges for the parameters specifying the problem. This context-of-use will, therefore, influence other aspects such as the data sets used in validation (see Section 2.2); it may also influence the choice of models.
- Active versus passive evaluation. Defining evaluation as a combination of
 assessment, validation and verification, it is possible to take either an active or a
 passive approach to each of these three parts. An active approach means actual use of
 the model, while passive means relying on pre-existing information on that aspect of
 the model. Clearly, an active approach will in general require greater effort than a
 passive one. In the rest of this paper it is assumed that, out of these three aspects,
 only validation is addressed in an active manner.

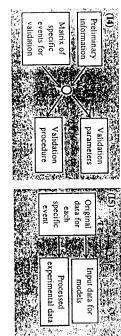
2.2 Input to evaluation

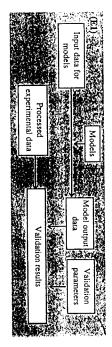
Having established the overall constraints, it is then necessary to compile the 'input' needed by the project, i.e. the various procedures and data which are used in the actual evaluations. Figure 1 illustrates the main elements of this input and how they relate to each other.

- Information on models. This is needed for two reasons. First, and most importantly, it is the 'raw material' used by the scientific assessments. However, summary information on the models is also useful at an early stage, for example, to gauge the range of capabilities of the models. Model information is conveniently gathered by means of questionnaires.
- Protocol. The evaluation protocol documents the stages of the evaluation in terms
 which are structured, unambiguous and objective. The protocol concentrates on
 explicit instructions for carrying out the scientific assessment; the other aspects
 (validation, verification) may be dealt with in separate documents, but the protocol
 should summarize these too.
- Datasets for validation. These datasets need to be carefully chosen to produce a
 meaningful validation. First, they need to cover as closely and completely as possible
 the context-of-use of the models. Secondly, they need to be of sufficient quality for
 model validation, meaning, for example, that there is no large uncertainty in
 meteorological conditions or in the source term.
- sets. It is then necessary to select for simulation a fixed number of specific cases, i.e. datasets corresponding to specific events. Representative scenarios should be identified; for example, by highlighting which are the most important physical processes and non-dimensional parameters of the problems being considered and using them to 'map' coverage of the context-of-use. The total number of cases depends on the types of model being used; resource constraints mean that an integral model can be validated for many more cases than a CFD model.
- Procedures for validation exercise. These procedures need to be prescribed in advance and agreed upon by all project participants. In particular, the procedures need to define:
- The input data that will be provided to the participants.
- The parameters which users will need to use when making validation comparisons between the observed data and their model predictions. These include both physical parameters, e.g. concentration at a fixed point and plume width, and statistical parameters, e.g. mean relative bias.
- Who will carry out the model runs and what control procedure will be in place
- Datasets for validation exercise. The input data for each case must be compiled and
 issued to participants. The observed data must also be compiled in a standardized
 way; they may or may not be issued to participants, depending on whether the
 validation exercise is to be conducted 'blind' one reason for allowing participants
 to see the observed values is so that they can improve their models as they proceed.









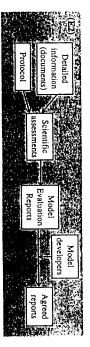


Figure 1 Stages in a model evaluation project such as SMEDIS. Input stages: (11) information gathering; (12) protocol development; (13) dataset selection; (14) development of validation parameters and procedure; (15) production of input and output data for each event. Evaluation stages: (E1) validation exercise; (E2) scientific assessments. Stages (11) and (12) relate mainly to the scientific assessments, while (13) to (15) relate to the validation exercise. Thus broadly the scientific assessments and the validation exercise can proceed in parallel.

2.3 Evaluation

summarizes the important elements of each one can begin. This consists of two main activities, which can run in parallel. Figure 1 again Once the necessary input has been either developed or obtained, evaluation of the models

- in place earlier are brought together in the validation exercise. cases and the procedures for running models and making validation comparisons put Validation exercise. The datasets (input and output) for the chosen experimental
- protocol and the results collated in a separate Model Evaluation Report Scientific assessments. Each model is assessed according to the categories in

2.4 Post-evaluation

results for each model. evaluations --- principally, the Model Evaluation Report and accompanying validation The final part of the project is concerned with what happens to the results of the

- developer for comment and, if possible, these comments incorporated in the final assessment with the developer of the model, as this will aid dissemination (see Consultation. It is helpful to seek agreement of the results of each scientific below). The Model Evaluation Report should, therefore, be passed to the model version of the report
- protocol for future use improvements could be made to the procedure, leading to a new version of the Refinement of protocol. Use of the protocol in actual evaluations highlights where
- available so that future potential users have this additional information. The Dissemination. If possible, the results of the evaluation should be made publicly Wide Web, say, would be an appropriate medium for this purpose

Implementation for SMEDIS

project was, essentially, completely determined at the proposal stage, while the remaining relevant to Section 3.4 to Section 3.11 inclusive. phases were carried out in the project itself. In the following description, Figure 1 is terms of the four phases identified in Section 2, the definition phase for the SMEDIS We now turn to the specific implementation of this evaluation procedure for SMEDIS. In

3.1 Models

The list includes a cross-section of different types of model: screening tools, integral A list was drawn up of models in use in Europe to study dense gas dispersion problems

models, shallow layer models and CFD models.

- Screening tools: Britter-McQuaid Workbook(H), VDI Guideline 3783 Part 2(U)
- $HAGAR^{(B)}$, $HGSystem^{(H)}$, $OHRAT^{(D)}$, $PHAST/UDM^{(D)}$, $SLAM^{(R)}$, $SLUMP^{(W)}$, Integral models: AERCLOUD(F), DRIFT(H), EOLE(G), ESCAPE(F), GASTAR(H) WHAZAN(D)
- Shallow layer models: DISPLAY-1(I), DISPLAY-2(I), GReAT(R), SLAB(T) $TWODEE^{(H)}$
- CFD models: ADREA-HF $^{(N)}$, CFX $^{(H)}$, COBRA $^{(B)}$, MERCURE $^{(E,G)}$, STAR-CD $^{(W)}$

open call was issued both in Europe (via the CEC CORDIS Focus bulletin) and in the evaluation. FLACS, KAMELEON and FLUENT (CFD) - have been accepted to undergo this and proposals from partners, four additional models - DEGADIS (integral) and United States (via the Forum for Hazard Assessment Research newsletter). As a result of Inclusion of further models was also allowed during the initial stages of the project. An

allowing evolution of models to occur, i.e. model developers can tune their models (see whether they are using the same version that has been evaluated. Second, SMEDIS is important for two reasons. First, prospective users of the evaluation results need to know Section 3.8) so version numbers are vital in making model evolution auditable Note that in all cases a specified version of each model is to be evaluated. This is

Context-of-use for models

3.5) and datasets for validation (see Section 3.6). areas in its context-of-use: (1) aerosol releases; (2) terrain; and (3) obstacles. These In the current terminology, and as noted in the Introduction, SMEDIS includes three main requirements affect other parts of the procedure, in particular the protocol (see Section

3 Active versus passive evaluation

through pre-existing information. simulate various experiments, but the assessment and verification are handled passively element of evaluation to the validation of each model, i.e. models are actively run to Because so many models are being considered, it has been necessary to restrict the active

Information on models

By means of questionnaires, two sets of information have been obtained for each model.

U = University of Hamburg Meteorological Institute; W = W.S. Atkins Safety & Reliability (UK) * The superscripts refer to the SMEDIS partner assigned to each model (responsible for supplying information and running the model — see Sections 3.4 and 3.10 respectively):

H = Health & Safety Laboratory (UK); E = Electricité de France; B = BG Technology (UK); J = Joint Research Centre, Ispra (Italy); N = National Centre for Scientific Research D = Det Norske Veritas (Norway); F = Finnish Meteorological Institute; G = Gaz de France; 'DEMOKRITOS' (Greece); R = Risø National Laboratory (Denmark); T = TNO (Netherlands);

The first is the preliminary information giving a summary of the capabilities of the model and the main characteristics of its (computer) implementation. This was useful in choosing datasets (see Section 3.6) and developing the validation procedures (see Section 3.8). The second set is the detailed information required for the scientific assessments (see 3.9). This latter information is handled by means of documents describing the different aspects of the model; the information suppliers provide copies of the documents and cross-reference them with the required aspects. All information is supplied by the responsible partner.

3.5 Protocol

A protocol was developed specifically for SMEDIS. It is consistent with the MEG protocol and has made use of the HGDEG protocol. However, it gives much more specific detail then either of these, and includes the specific context-of-use (see Section 3.2) by means of specific categories. It requires the scientific assessment to be carried out using six main headings: (1) General model description; (2) Scientific basis; (3) User-orientated aspects; (4) Verification performed; (5) Validation performed; (6) Conclusions.

There are a number of sub-categories under each heading. For example, under (2) the main sub-categories include 'Specification of the source', 'Model physics and formulation' and 'Limits of applicability', and up to two further levels are used. The protocol contains instructions on what should be assessed under each category; it also summarizes other parts of the evaluation procedure, such as the gathering of information, datasets for model runs and validation procedure. At the end of this stage, a 'working version' of the protocol is available with which to start the scientific assessments.

'.6 Datasets for validation

Identification of suitable datasets for the model validation was carried out with input from all participants. First, a preliminary list of over 40 datasets and corresponding references was prepared by collecting information from partners. Based on this preliminary list, a detailed questionnaire was sent to all partners to obtain information about the datasets, including their previous use for model validation, availability of data and an opinion of the user on the dataset's quality in several areas, for example, its source specification and concentration measurements. The replies were then analysed to produce a priority list of eight datasets which had been previously used for the validation of a range of models, including integral and CFD models, and which were judged of sufficient quality by the participants, that is, they rated highly according to the categories used in the dataset questionnaire.

There turned out to be relatively few high quality datasets available for validation in these complex situations: Burro, ¹² Desert Tortoise, ¹³ FLADIS, ¹⁴ BA-Propane, ¹⁵ BA-Hamburg, ¹⁶ BA-TNO, ¹⁷ Thorney Island ¹⁸ and EMU-Enflo. ¹⁹ The majority of these datasets are to be found in the REDIPHEM database, ²⁰ which therefore serves as the primary basis of the dataset selection, including quality issues (see Section 1). A summary of a number of these datasets, which were sponsored by the CEC, is given by Britter. ²¹

A provision was made to include more recent datasets, which had not already been used for validation, as the project progressed. Unfortunately, these did not become

available in time for use by SMEDIS. In addition, data sets for which near-field effects are important, either through strong gravitational slumping, e.g. low wind, or confinement of the flow, e.g. obstacles near the source, have also been sought and will be included in some measure in the course of the project.

3.7 Specific cases

Selection of specific cases from the above list of datasets is the next stage of the process. This must be carried out in a structured way to ensure that all aspects of models in the context-of-use employed by SMEDIS are covered in the validation exercise. Therefore, a four-dimensional matrix of scenarios was constructed based on the context-of-use and the following four aspects:

- source type (instantaneous/continuous);
- gas density (strong/weak density effects):
- atmospheric conditions (stable/neutral/unstable);
- complex effects (aerosols/terrain/obstacles/none)

The alternatives for each aspect are given in parentheses. This gives 32 combinations of conditions or scenarios, which were then identified with specific cases as far as possible using the available datasets. For continuous releases, datasets are available for all combinations except for stable atmospheric conditions with terrain (any gas density); for instantaneous releases, this gap in coverage is repeated, together with no releases for which aerosol effects are important during the dense gas/passive regime.

3.8 Validation parameters and procedure

Before starting the model runs it was necessary to agree on the validation comparison parameters that would be used together with the procedure itself. As far as the physical parameters are concerned, two different approaches have been adopted:

- Point-wise comparisons. A comparison based on values at individual sensors. Timeaverage concentration for continuous releases, and dose and arrival/departure times for instantaneous releases are used.
- Arcwise comparisons. A comparison based on values taken over sensor arcs.
 Maximum concentration and plume width for continuous releases, maximum concentration and corresponding time for instantaneous releases are used.

These choices were made taking into account a number of factors, including the cloud properties of most importance, the range of models and their capabilities, and the limitations of the selected data sets.

Statistical comparison techniques are applied to these physical parameters for each case being simulated. The main parameters used are (see, for example, Duijm et al.³):

-) Mean Relative Bias, MRB = $< 2(\Psi_p \Psi_o)/(\Psi_p + \Psi_o)>$,
- ii) Mean Relative Square Error, MRSE = $<4\left(\Psi_{p}-\Psi_{o}\right)^{2}/\left(\Psi_{p}+\Psi_{o}\right)^{2}>$,

iii) Factor of n, FAn = (fraction of points where $1/n \le \Psi_p/\Psi_o \le n$), with n = 2, 5.

In the above, ψ_ρ, ψ_ρ are, respectively, the observed and predicted values of the physical parameter, for example the time-averaged concentration at a sensor location. <...> denotes an average over all points/arcs being considered.

For reasons of time and costs, it was decided from the outset that the model runs would be performed by the project partner responsible for a given model. In many cases the responsible partner is also the model developer; hence it was decided to exploit this and include a model improvement aspect in the project. Thus, model developers running their own models are allowed to tune parameters or make modifications to the algorithms provided all changes are documented and all the validation exercise cases are eventually run with a single defined version of the model.

3.9 Data for validation exercise

The datasets were then prepared and distributed to participants as spreadsheets containing the input necessary for the models (geometry, release conditions, etc.), together with the measured experimental values, such as concentration and temperature, both point-wise and arcwise values. Empty templates were also provided to return model results. This procedure allows automatic treatment of model results and the possibility of checking results and, therefore, also to tune a model (see Section 3.8). Although all datasets are circulated to all participants, the minimum number of cases which each model is expected to simulate depends on the type of model. For screening tools/integral models, shallow layer models and CFD models, the expected number of runs is approximately in the ratio 10:5:2, owing to the increased resource requirements over the different model types.

3.10 Validation exercise

The validation procedure (see Section 3.8) is applied to the relevant input and output datasets (see Section 3.9) for each model by the partner responsible. The output from this stage is a set of model predictions for each validation case attempted together with a set of values for the statistical comparison parameters and a record of the steps carried out to set up, run and produce the output for the model.

3.11 Scientific assessments

The SMEDIS protocol (developed under Section 3.5) is applied to the detailed information elicited on each model (see Section 3.4) from the partner responsible,[†] and the results recorded in the Model Evaluation Report for the model. Parts of the assessment for which there is insufficient information are noted. It is intended that the results from the validation exercise will be included in each report when they are available.

3.12 Post-evaluation

- Consultation. Agreement is being sought with model developers on the results of the scientific assessments by sending them the report for their model for comment.
- Refinement of protocol. The current 'working version' of the protocol is undergoing refinement as the scientific assessments proceed.
- Dissemination of results. It is intended that approved versions of the documentation
 will be issued; for example, the evaluation protocol, data sets used for validation,
 validation procedure, final report and Model Evaluation Reports and validation
 results where possible. A workshop will be held in 1999 to describe this project,
 possibly with other model evaluation work currently in progress. A SMEDIS website
 is being set up.

4 Summary and conclusion

In this paper, we have described the main aspects of SMEDIS, a project in progress to carry out a scientific evaluation of nearly 30 dense gas dispersion models in use across Europe. This paper is intended to summarize rather than to be exhaustive in its description. More details of the project will appear as the project concludes, with as many as possible of the documents and results produced by the project being available in the public domain.

In terms of the four phases described in Section 2, the first phase was completed as part of the work programme specification. The second phase, input development, has been completed, except where there has been a decision to stage some activities which overlap with the third (execution) phase, for example, the production of datasets for model runs. The third and fourth phases are in progress.

We have seen that there are two main strands to the evaluation project: scientific assessment and validation. The original plan for the scientific assessments was to develop the protocol, applying the resulting 'working version' to all the models and then carry out revisions to produce the final tested version of the protocol. However, it has proved more effective to consider a range of models and then review the adequacy of the protocol before proceeding with the remaining models. The result has been that the basic approach and the categories and instructions contained in the protocol have required relatively little modification, while the presentational aspects of the assessment (report) have undergone greater change. Summary information is included throughout each report so that an abbreviated version of the results of the assessment may be extracted if required.

The validation exercise has also been staged in order to identify potential problems with the procedure. Thus, an initial set of eleven data files was distributed to partners running the models, who then ran their models using the data provided and returned model output. The conclusions so far regarding the validation procedure are that it appears to be suitable for its purpose. The statistical comparison parameters chosen are simple and relatively robust, but they are subject to a common difficulty for the pointwise comparisons associated with the edge of the cloud (which can potentially dominate the values of the statistical parameters if there are insufficient points over which to average). Thresholds have been used to alleviate this problem. The validation exercise is viewed as testing a number of options and it is hoped that useful conclusions may be drawn concerning this type of exercise for future use. Preparing data for distribution was

[†] CERC Ltd. (UK) is responsible for the scientific assessment of each model.

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found to be very labour intensive so that fewer specific cases will be considered in the validation exercise than originally anticipated.

Even without resource constraints, there appears to be a limiting factor in the availability of high quality datasets for realistic release situations. SMEDIS has highlighted the paucity, even absence, of experimental data for many scenarios featuring complex effects, and this is currently one important area where improvements are needed. Nevertheless, the models are being tested over a much wider range of conditions featuring realistic effects than in any previous study.

One important aspect of SMEDIS is that it is intended to be constructive in its approach. Thus, there is an opportunity for model improvement to be carried out as the validation exercise proceeds. The validation results will not be used to rank the participating models; nevertheless, it would be a satisfying outcome of the project if all models gave acceptable predictions by the end. The scientific assessments will also be constructive, in that they will highlight both the strengths and the weaknesses of each model

It is intended to establish a simple SMEDIS website during the project. It would be highly advantageous if the website could be extended so that the protocol and the datasets used could be made accessible for future use, not only for future developments of the participating models but for other models as well. Such self evaluation should encourage the development of high quality models. In fact, with a network of 13 participants distributed across Europe, the Internet has already proved invaluable in this collaborative project for circulating information and documentation, in particular the questionnaires used in some input stages and the datasets used for the validation exercise. A survey of electronic mail capabilities of the participants was carried out at the start of the project to identify limitations at an early stage.

The aim of this project is to develop and test a framework for the scientific evaluation of models for dense gas dispersion in complex situations. It is intended that this will be of use not only to all who use such models but also to model developers, since it will provide a basis for assessing the weaknesses of models as well as their strengths. It is hoped that the project will raise awareness of the importance of model quality and the utility of model evaluation; that it will encourage further use of model evaluation by showing the evaluation process can be made auditable, i.e. open and well-documented, and that is will show it is possible to evaluate a wide range of models with the same protocol and produce information about them which is helpful to users faced with the task of applying them in given situations.

5 Acknowledgement

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