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A Quality-Assurance guide for the evaluation of mathematical models used to calculate the consequences of Major Hazards

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Abstract

This paper presents a Quality-Assurance-based technique for evaluating the quality of a Mathematical Model used to calculate the consequences of Major Hazards. It starts by considering that the diversity of, and the discrepancies between, mathematical models today, in addition to the diversity of user categories, makes it necessary to seek clarification from modellers on the quality procedures adopted at the different stages of model development. Too often, these procedures are not sufficiently described, leading to obscurity and the possibility of misuse of the model or over-confidence in its predictions. We intend to offer the community of end-users in a broad sense, a structure for eliciting information from modellers which would enable the users to judge the quality of an environmental software without having to invest too much in the different facets of its realisation: the scientific and the algorithmic background, its computerisation, its validation and its sensitivity to internal parameters and, finally the quality of its user interface. If it is quite natural to accept the wide gulf between fundamental research prototypes and industrially oriented codes, it is, however, necessary to get reliable and robust measurement tools capable of judging their maturity, their domain of applicability and their limitations. Although the questionnaire-based technique presented in this work is applicable to a wider area than just the Major Hazard Environmental software, we preferred, as a start, to stick to this particularly important topic.

Keywords: Major hazard; Mathematical model; Quality assurance

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1. Introduction

Mathematical modelling is becoming increasingly used as a method for quantification, both in industry and among local authorities and specialised consultants.

In the field of Major Hazards, it is common knowledge that the quality of models, including both their fitness for purpose and their fitness for use, has not always been clearly established. The relatively large numbers of models developed on the market to date in universities and industries means it is vital to assess the quality of each model individually, and compare their respective performances.

This handbook draws its information broadly from the document issued by Dr. R.E. Britter [1] for the Directorate General (DG) XII of the European Commission. In this document, he stresses the need for methods and tools to evaluate and improve the quality of models. He also sets out the basis for an evaluation protocol allowing the end-user to grasp the objectives, field(s) of application and limitations of the models unambiguously. We can point out at this point that a working group, funded by DG XII (Model Evaluation Group), has been set up to look into this issue further [2,3].

We have formalised this step, intending to provide users with industrial-type simulation tools, a straightforward procedure to evaluate the quality of calculation models of Major Hazard Consequences. This procedural step naturally covers the following fields:

- Evaluation of the scientific rigour of the mathematical model.
- Validation of the model in terms of all available techniques: analysis of sensitivity to physical parameters, comparison with experimental results, comparisons with other models and 'benchmark exercises'.
- Computation and algorithmic aspects requiring qualities of reliability, robustness and ease of maintenance.
- User-friendliness and fitness of the Man-Machine Interface to the users' needs.
- Scientific and technical documentation for the model and its computerisation.

2. The context of the problem

The mathematical modelling, considered as a tool helping the decision-making process or communication tool, deserves its place in the quantitative evaluation of Major Hazards, especially since the Seveso Directive (82/501/EEC) requires certain industries to evaluate the hazards and anticipate measures to be taken whenever a disaster occurs. The legal authorities are also concerned with setting in place Emergency Plans in the case of accidents. Besides the Public Authorities and Industries, other interested parties include Insurance Firms, Consultants, Public Administrations and Researchers in a range of disciplines.

Today, we can confirm that the quality of answers provided by various situation analyses will depend to a great extent on the quality of results of simulations based upon mathematical models. However, the number of computerised models is rather impressive and it covers various aspects of risk analysis; the quality of these models varies and their reliability and field of application are not always well-defined.

To ensure that hazard studies remain as relevant and reliable as possible, it has become vital to be able to judge the quality of computerised models, the quality of each model individually and the quality of a model when compared with others. This harmonisation of the quality of technical data which safety studies rely upon represents an essential step which we have decided to take regarding different projects we are or we were involved in:

- the EURO_CHLOR project [4–6] which was funded by the European Chlorine Producers Association (formerly BITC) and developed in cooperation with the von Karman Institute;
- the SEVEX project which is still under way, funded by the Walloon Region (the Southern Part of Belgium) [7–9] and developed in cooperation with 3 Belgian Universities: the Université Catholique de Louvain (UCL), the Faculté Polytechnique de Mons (FPMs) and the Université de Liège (ULG);
- the DISCO project [10–13] internal to SOLVAY, which aims at replacing the Euro_Chlor code in the medium term, allowing for a better description of the atmospheric turbulence based on a k-ε model and being full 3-D.

A further reason for having definitely placed our present approach in the Quality-Assurance framework is that safety engineers are facing a wide panel of either commercial or non-commercial software, amongst which it is rather difficult to navigate. Within SOLVAY, for example, they are offered 7 different codes: WAZAN, PHAST, TRACE, SAFER, EFFECT, HEGADAS, EURO_CHLOR and DISP; due to the fact that it is hard for them to see clearly the limitations or the discrepancies between these models, the tendency is not to invest in the understanding of models but to prefer the user-friendly PC 'black boxes'.

A final but no less important reason is that Industries and Public Authorities are more and more discussing Major Hazard issues in quantitative model-based terms. The absence of a good model evaluation tool often makes it more difficult to come to an agreement.

In this study, we will focus on considering Mathematical Models involved in studying the consequences of Major Hazards, which particularly means, from the outset, that the fields covered should not include:

- Techniques of risk identification.
- Probability techniques aimed at associating probabilities of occurrence with accident scenarios.
- Models connected to company management.
- Qualitative models.

The Mathematical Model terminology covers 3 main categories of models:

1. Empirical Mathematical Models which can be boiled down to:
   - either smoothing experimental results with the aim of making them easier to interpret,
   - or statistical correlations between characteristic sizes of physical phenomena.
   - Empirical Mathematical Models should not be confused with correlation models used to estimate the physical and chemical properties of chemical products likely to play a part in accident scenarios.
2. Analytical Mathematical Models, exact or approximate solutions of simplified models.

3. Numerical Mathematical Models (computational models) which require a numerical algorithm and computation. These models are broadly practised at different levels of sophistication and complexity.

We will concentrate particularly on the latter in this work as the former 2 categories can be regarded as particular cases from the quality-assurance viewpoint.

On this matter, we have already mentioned the diversity, not to say the discrepancy, between mathematical models available today; to this should be added the diversity of user categories which differ in the approach of analysing the consequences of an accident. Thus, in addition to the problem of technical quality of a model, its fitness for use must also be judged. Models based on similar scientific foundations may behave very differently; for example:

- Models aimed at meeting emergency situations requiring real-time measures and swift access to pre-calculated data.
- Models aimed at planning or establishing emergency plans usually requiring large numbers of tests covering a broad spectrum of scenarios.
- Models used in the most accurate calculations possible of the consequences of accidents which rely on advanced research and which are not normally concerned with constraints in calculation time or hardware resources in general.

3. The quality approach in the evaluation of quantitative models

We can see only too clearly that the field of application, the limitations and even the use of models are very often poorly understood by end-users. The fact that this kind of tool is based on non-trivial scientific considerations may represent a considerable obstacle when making it available to users spread over a range of different activities or unable to acquire a thorough understanding of complex systems.

There is a wide gulf between the scientific community, at the heart of developments and research, and the industrial world. The first group which is well aware of the theoretical foundations of models and considerably underestimates the gap separating an academic prototype from validated industrial software, applicable in real cases. The second group often underestimates the need to invest in an understanding of models, or even how they are computerised, preferring to use 'black boxes' whose inescapable 'advantage' is to conceal the difficulties to users who do not have to worry about the relevance of the model.

A quality approach can be justified by the desire to clarify a field which is still blurred around the edges. In practical terms, this means:

1. Producing a structured measurement of the quality of a model which can be communicated to all the interested parties (Legal Authorities, Industries, Central and Local Administrations, Insurance Firms, Consultants and Research Groups).
2. Authorising an open audit, i.e., performed by an independent expert, on the use of the model by end-users. This audit should result in a written opinion as to the relevance of the results, the field of applicability of the model and the type of users it is aimed at.

3. Providing the end-user with clear documentation on the field of applicability of the model and the degree of accuracy of the results.

By means of these 3 initiatives, we should be able:

- firstly, to encourage and assist the development and maintenance of quality models satisfying the 'Fitness for purpose' criterion;
- secondly, to reduce any distortions existing between the models;
- next, to identify those improvements required for future models;
- finally, and especially, to satisfy the expectations of users by satisfying the 'Fitness for use' criterion.

4. The quality approach for calculation models

The Quality approach for Calculation Models of the Consequences of a Major Accident is based on 5 concepts:

- Scientific quality assurance,
- Algorithmic quality assurance,
- Computerisation quality assurance,
- Man-Machine Interface quality assurance,
- Model validation and analysis of sensitivity.

It presupposes 2 things:

1. a clear definition of the end-users' expectations including amongst others:
   - the scale of the problem,
   - the types of scenarios to be handled,
   - the nature and degree of accuracy of the results to be provided;
2. that the data used during the validation process are themselves subject to a certification process by those who have established the Databases in terms of the quality-assurance criteria.

4.1. Scientific quality assurance

This is based on a detailed presentation of the model, its underlying hypotheses and/or physical approximations, its limitations and duly motivated answers to the following questions:

- Is the mathematical modelling targeted at a given type of problem? Does it cover the physical nature of the problem? Totally or partially?
- Do the hypotheses and/or approximations correctly reflect the main physical effects, omitting any side effects if the case arises?
- Do they correctly take scale effects into consideration?
- Can the limitations of the model be justified, primarily with regard to the problem in question? Can they be removed and at what cost?
- Is there a guarantee that no non-scientific constraint, e.g. hardware type, is behind excessive simplifications of the model?

Scientific quality assurance should also be capable of addressing the experimentation if this proves necessary, notably to support any choices made or validate the hypotheses.

Finally, scientific quality assurance involves active participation in scientific events at the highest level as well as encounters with specialists. The same remark can be made for algorithmic quality assurance which we will be covering in the next paragraph.

4.2. Algorithmic quality assurance

This affects the numerical strand, i.e., the approximate formulation of the mathematical model to computer treatment. Algorithmic quality assurance is characterised by 3 concepts:

- the stability of the scheme,
- the convergence of the scheme, and,
- the accuracy of the scheme.

This strand of the modelling is very often hidden from the user for the obvious reason that (s)he is, in most cases, incompetent in this field, and questioning on numerical aspects may well perturb him (her).

We should remember that mathematical convergence is usually determined by stability and the numerical schemes used are supposed to be stable. By contrast, accuracy is closely linked to the grid, and it should be ensured that the code can converge towards the machine-zero, i.e., the residues do not stay and stagnate in terms of the number of iterations. In addition, the real accuracy involves defining the level of error as a function of the grid and verifying the slope (in a logarithmic graph).

Another major condition to be determined is the refinement threshold from which point the solution is independent of the grid. This is clearly a function of the kind of problem, but it is only in this case that the validation of the physical models and the study of sensitivity described in Section 4.5 can be estimated objectively.

4.3. Computerisation quality assurance

This paragraph deals with how the models and, in particular, their numerical approximations, have been computerised. At this stage, no consideration relating to the physical nature of the problem is included (other than those translating a direct influence of the physical nature on the calculation techniques being proposed), nor the algorithm itself.

We focus here on the quality (translation and performance) of the computer coding of numerical algorithms and relevant databases. In particular, the coding should either be an exact translation of the numerical algorithms and there should be no drift with regard to the analytical model.

In addition, the code's architecture should be modular and in particular the expert user should check experimentally the results announced in Section 4.2 by himself. The effort made in this field should also be considered at as early a stage as possible in the development of the computerised model for 2 reasons:

1. It is undesirable that, while the programme is being operated for practical purposes, questions which are of a purely mathematical nature should be considered.
2. The operating cost of the model, whether expressed as the number of operations (computational costs) or in currency (financial costs), depends crucially on the quality of the computerisation.

For the relevant Databases for the model, it must be carefully ensured that:
- they are structured according to a standardised format, if possible, and are portable;
- their content has been validated and certified by experts. This validation and certification work is crucial both regarding the physical/chemical and cartographic data, including land characteristics;
- their content is accessible to the expert user.

4.4. Man-machine interface quality assurance

The Man-Machine Interface (MMI) strand involves the computerised interface enabling the end-user to interact with the application programme, both in terms of acquiring data and interpreting results. The MMI must be designed to allow the user to carry out his task successfully, in a user-friendly way and with the provision of any help necessary.

In particular, the MMI must help a user to check whether the model is adequate for the scenario being offered and the model underlying the application programme; it should be designed so that the system is in the service of the user and not the other way around.

4.5. Model validation and analysis of sensitivity

The word validation is used in the strict sense of the term, as is the verification of closeness between those results predicted theoretically and experimental results. The term experimental results is used in the broad sense to mean:
- the results of real scale tests (field tests),
- the results of wind tunnel tests,
- the results of 'laboratory' or 'pilot' scale tests,
- results provided by other models,
- benchmarking exercises.

The validation of a computerised mathematical model involves the prerequisite of the existence of validated databases and accessibility to these databases. **The validation supposes that the experimental results have not been used when developing the model itself.**

This exercise is usually a complex one, costly in terms of time for thought and use of the computer; it is often accompanied by qualitative validations and an analysis of sensitivity to the physical parameters intervening in the model. It may even require experimentation itself!

Qualitative validations are often the only ones that can be considered in the hypothesis of very complicated scenarios.

Analyses of sensitivity are intended to study the variability of results in terms of the variability of the physical and mathematical parameters of the model. Analyses of sensitivity for physical parameters are used to characterise the level of uncertainty of the model; they must contribute to defining the validity ranges.

4.6. The quality-assurance questionnaire

The questionnaire-based methodology has been intensively studied and practised in at least 3 major projects within the European Strategic Programme for Research and Development into Information Technology (ESPRIT). These projects were: The Development of an Automated Flexible Assembly Cell and Associated Human Factors Study (Project No. 534, 1984–1988), Human-Centred CIM Systems (Project No. 1217/1199, 1986–1989) and Front-Ends for Open and Closed User Systems (Project No. 2620, 1989–1994) [14].

We were deeply involved in the last project whose goal was to develop generic methods and tools for constructing Knowledge-Based Front-Ends (KBFEs) for existing industrial and scientific software [15]. The interest of the questionnaire technique has been largely demonstrated both as a formative evaluation tool (used during the course of a project) and as a summative evaluation tool (used at the end of the project) [16,17].

The Quality-Assurance questionnaire below intends to cover the 5 issues described in Section 4.1, Section 4.2, Section 4.3, Section 4.4 and Section 4.5.

4.6.1. Questionnaire on scientific quality assurance

◇ Do you have the context in which the mathematical model was developed?

◇ Are the model's designers accessible?

- If yes:
  - where? [name(s), address(es)]
  - how? (e-mail)

◇ Do you have a detailed mathematical description of the model including:

- general equations for the model?
- the hypotheses and/or physical approximations leading to the operational model?
- the equations for the operational model?
- the initial conditions and/or boundary conditions?
- the internal parameterization of the equations?

◇ Is the mathematical description easily accessible?

- in the literature?
- from the model's designers?

◇ Does the model explicitly deal with instantaneous, short-term and/or continuous events?

If yes: is the dependence of the concentration on the averaging time explicitly stated when necessary?

◇ Are the limitations of the model:

- justified primarily from a physical reasoning?

If yes: which?

- directly related to a specific industrial problem?

If yes: which?

- independent of software constraints (SW)?
- independent of hardware constraints (HW)?

◇ Has the model been validated?
If yes: by whom?
where?
when?
in what context?
- with real scale tests (field tests)
- with wind tunnels
- with hydraulic tunnels
- by inter-model comparisons
- using laboratory or pilot experimentations.

◇ Has the model encountered the opinion of specialists in:
international conferences?
seminars or workshops?
peer-reviewed scientific press?
If yes:
where?
when?

◇ Has the model been submitted to the opinion of industrial experts?
If yes:
to whom?
where?
when?
how?

4.6.2. Questionnaire on algorithmic quality assurance

◇ What algorithm [1] is used to discretise the mathematical model?
◇ Who was responsible for this choice?
◇ What are the references for the proposed model?
◇ Has the stability of the numerical scheme been studied?
If yes:
by whom?
where?
when?
is the scheme unconditionally stable?
conditionally stable?

◇ Is the numerical scheme convergent?
If yes: who demonstrated this result?
where?

◇ What is the accuracy of the numerical scheme?
◇ Has a comparative study with other algorithms been made?

[1] As for the notion of the model, the term 'algorithm' must be taken in the general sense and may actually cover several algorithms.

If yes:
by whom?
where?
when?
are the results of this study available?
◇ What justified the choice of the algorithm:
- its accuracy?
- its robustness?
- its ease of implementation?
◇ Can the algorithm be vectorised?
If yes: has it been vectorised?
◇ Can the algorithm be parallelised?
If yes: has it been parallelised?

4.6.3. Questionnaire on computerisation quality assurance

◇ In what language(s) has the software been coded?
◇ Are the source codes accessible?
If yes: where?
how?
If no: why not?
◇ Is it structured in functional modules?
◇ Is there a conceptual analysis file?
If yes: where is it accessible?
◇ Is there an organisational analysis file?
If yes: where is it accessible?
◇ Is the software documented?
If yes: in which language(s)?
◇ Is the user-interface functionally decoupled from the application modules?
◇ Is/are the computer language(s) used standardised?
If yes: is it the standardised version of the language(s) (without extension) that has been used?
◇ Is the code portable?
If not: what proportion of the code is not portable?
why hasn't it been designed to be portable?
◇ Is there an implementation procedure?
If yes: where is it accessible?
◇ Is there a user's manual?
If yes: where is it accessible?
◇ Is the software maintained?
If yes:
by whom?
where?
how?
If no: why not?

◇ On what computer platform(s) is the software available?
◇ If the software was to be run on several machines, do the software versions have the same release numbers?
◇ Is there a code version in single-length precision (32 bits)?
If no: why not?
If yes:
  is this precision enough?
  have comparisons with a double-length precision version of the code been made?
  If yes: by whom?
    where?
    on which machine(s)?
    have the results been included in an accessible report?
  If no: why not?
◇ Have the topographic data been structured to be portable where necessary?
If yes:
  by whom?
  how?
  are they available?
    If yes: where?
If no: why not?
◇ Have the results of the calculation (e.g. field of wind and/or field of concentration) been structured to be portable?
If yes:
  by whom?
  how?
    are they available?
    if yes: where?
If no: why not?
◇ Has a particular structure for files reserved for graphic designs been provided?
If yes: what is it?
If no: why not?
◇ Has the type of graphism used by the code been standardised (GKS, PHIGS, POSTSCRIPT, ...)?
If yes: what standard is it based on?
If no: why not?
  which solution has been adopted?
◇ Does the software require portions of code covered by external licences?
If yes: how much does it cost?
  can these portions of code be easily replaced (at low cost)?
◇ Is the supply of the code accompanied by training in its use?
◇ Is there a Help Desk in the case of difficulties?
If yes:
  where?
  accessible when?
  accessible how?

4.6.4. Questionnaire on the quality assurance of sensitivity analysis

4.6.4.1. Analysis of mathematical sensitivity.

◇ Are the results of the calculation independent of the mathematical parameterization? (*answer only if the question is pertinent to the model*)
- spatial grid?
- time steps?
- relaxation parameters?
- artificial viscosity coefficients?
- criteria for stopping in iterative procedures?
- initial conditions used in iterative procedures?

◇ Is the user capable of controlling these various points easily by himself?

4.6.4.2. Analysis of physical sensitivity.

◇ Did the variability studies of the calculation results concerning the physical parameterization of the model cover the following:
- the internal parameters of the model?
  If yes: what tests were made?
    by whom?
    where?
    The results: are they accessible?
      have they been published?
      have they been audited?
      If yes: which expertise?
        by whom?
        where?
- the physical data of the programme?
  If yes: what tests have been made?
    by whom?
    where?
    The results: are they accessible?
      have they been published?
      have they been audited?
      If yes: which expertise?
      by whom?
      where?

4.6.5. Questionnaire on validation quality assurance

◇ Have the results of the model been compared with those from real scale tests?
If no: why not?
If yes:
- Which ones?
- On what scenario platform?

- Did this platform have the consent of experts:
  - from Industry?
  - from the competent Legal Authorities?
  - from specialised Consultants?
- Have the data relating to the scenarios and the results of the simulations been published?
  If yes: by whom?
  where?
  when?
  If no: why not?
- Have the data and the results of the various scenarios been analyzed critically by external experts?
  If yes:
  by whom?
  where?
  when?
  how?
  If no: why not?

◇ Have the results of the model been compared with those from wind tunnel tests?

- If no: why not?
- If yes:
  - Which ones?
  - On what platform of scenarios?
  - Has this platform had the consent of the experts:
    from Industry?
    from the competent Legal Authorities?
    from specialised Consultants?
  - Have the data relating to the scenarios and the results of the simulations been published?
    If yes: by whom?
    where?
    when?
    If no: why not?
  - Have the data and the results of the various scenarios been analyzed critically by external experts?
    If yes: by whom?
    where?
    when?
    how?
- If no: why not?

◇ Have the results of the model been compared with those coming from hydraulic tunnel tests?

If no: why not?
If yes:

- Which ones?

- On which scenario platform?
- Has this platform had the consent of experts:
  from Industry?
  from the competent Legal Authorities?
  from specialised Consultants?
- Have the data relating to scenarios and the results of the simulations been published?
  If yes: by whom?
  where?
  when?
  If no: why not?
- Have the data and the results of the various scenarios been analyzed critically by external experts?
  If yes: by whom?
  where?
  when?
  how?
  If no: why not?

◇ Have the results of the model been compared with those of laboratory and/or pilot installation tests?

If no: why not?

If yes:

- Which ones?
- On which scenario platform?
- Has this platform had the consent of experts:
  from Industry?
  from the competent Legal Authorities?
  from specialised Consultants?
- Have the data relating to scenarios and the results of the simulations been published?
  If yes: by whom?
  where?
  when?
  If no: why not?
- Have the data and the results of the various scenarios been critically analyzed by external experts?
  If yes: by whom?
  where?
  when?
  how?
  If no: why not?

◇ Have the results of the model been compared with those coming from other models?

If yes:

- With which models?
- On what scenario platform?

- Has this platform had the consent of experts:
  from Industry?
  from the competent Legal Authorities?
  from specialised Consultants?
- Have the data relating to scenarios and the results of the simulations been published?
  If yes: by whom?
    where?
    when?
  If no: why not?
- Have the data and the results of the various scenarios been critically analyzed by external experts?
  If yes: by whom?
    where?
    when?
    how?
  If no: why not?

◇ Have the results of the model been critically analyzed in a 'benchmark exercise'?
If yes:
  by whom?
  where?
  when?
  how?
  is a report available?

4.6.6. Questionnaire on the man-machine interface quality assurance

◇ What category of users is the code aimed at?
- a fluid mechanics expert?
- an atmospheric physics expert?
- an engineer responsible for Industrial Safety studies?
- an engineer responsible for Emergency Plans with Legal Authorities?
- a Consultant in the field of Major Hazards?

◇ Has the user-interface been developed with the help of end-users?
If yes:
  which ones?
  where?
  how?

- Has the user-interface been evaluated (usability assessment):
- by end-users?
  If yes: which ones?
    where?
    under what conditions?
    is a final report available?
      - if yes: where?
  If no: why not?

- by software engineering specialists?
  If yes: which ones?
    where?
    under what conditions?
    is a final report available?
      if yes: where?
  If no: why not?
- by cognition engineers?
  If yes: which ones?
    where?
    under what conditions?
    is a final report available?
      if yes: where?
  If no: why not?
- by ergonomists?
  If yes: which ones?
    where?
    under what conditions?
    is a final report available?
    if yes: where?
  If no: why not?

5. Conclusion

Starting from the observation that:

- an intensive use is made of the mathematical models as quantification tools for the consequences of Major Hazards,
- this use is going to increase,
- little has been done to formalise the evaluation of existing models and increase the transparency of the ins and outs of these models to the user,

we wanted, in a practical sense, to set out the basis for a strict quality assurance approach from our industrial experience.

The questionnaire technique used in this work has been structured in a 'task chain' approach, to be carried out by experts with different skills: modelling experts, physicists, chemists, engineers, mathematicians, computer experts, ergonomists and end-users. Each questionnaire has been drawn up in professional jargon to lighten the evaluation task.

Our methodology is currently being experimented with as part of a development project for evaluation software for risk zones around the SEVESO sites developed for the legal authorities of the Southern Region of Belgium (Région Wallonne).

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