User's point of view in using software in risk analysis

Guy Mavrothalassitis, Philippe Pons

USER'S POINT OF VIEW IN USING SOFTWARE IN RISK ANALYSIS

G. Mavrothalassitis P. Pons
Institut National de l'Environnement industriel et des Risques (INERIS)
Parc Technologique ALATA - BP n°2 - F-60550 Verneuil en Halatte

Abstract

The first need of the risk analyst is the availability of pertinent software to assess, in a realistic way, the maximum effects of possible accidents such as pressure pulses, thermal fluxes, accidental missiles formation and projection and toxic releases of gases, vapours, mists, soots or dusts.

To be useful to risk management, this approach has to be quite simple but also as realistic as possible. An underestimation as well as a crude overestimation of the effects may prove dangerous.

A lot of softwares aim at this purpose. The analyst has to make sure he is using a suitable tool. This involves :

- The knowledge of how to use it (it is usually time consuming and depends on the aptness of the theory and the user's manual) ;
- The analysis of the tool according to its internal consistency ;
- Comparisons of the results with calculations that might otherwise be assessed ;
- Comparisons of the calculations with existing data when possible (experiments and/or investigations of past accidents).

This paper aims at describing the approach of INERIS which began five years ago, and still goes on, working for French Ministry of Environment, about testing the ability of software to assess consequences of given scenarios.

Our point of view is that of the user who intends to use a reliable tool.

Introduction

A number of works exist, that aim at assessing the reliability of software, by means of comparisons with existing data (especially results from experiments). For instance, S.R. Hanna (Earth Tech, USA) has been comparing well known experimental data (Burro, Coyote, Desert Tortoise, Goldfish...) for many years with a great number of softwares [1]. The European Authorities have taken such an initiative more recently, by means of European Projects (see [2]), dealing with the evaluation of effects from major industrial hazards, by constituting a large data base.

But it is not easy to realise a parametrized evaluation by means of experimental data. There are two reasons for that state of affair :

1) There is a need of data that were obtained under exactly the same protocol and ambient conditions. Such a requirement is very difficult to fulfil, because of the numerous various sources of data available, and the variation of ambient conditions from a day to another ;
2) There is a need for more data. But there are expensive to get (especially far field data from dispersion experiments).

That is why such useful experimental comparisons had to be completed by another approach, which is part of the Evaluation Model Protocol recently elaborated by the Model Evaluation Group on Heavy Gas Dispersion of the European Community [3]. This approach is named « Scientific Assessment », and is part of the approach which INERIS began five years ago with French Ministry of Environment.

The context of the need of such an evaluation approach at INERIS is described in the first part of this paper.

The second one deals with the methods used to assess a software in risk analysis.

The third one is an illustration of two points :

1) It shows the way INERIS works to evaluate software ;
2) It points out the evolution that can exist between the two versions of the same software.

1- Context of risk analysis

This context has been described in a previous paper [4]. For a long time, INERIS has been interested in prevention and protection against the effects of fires and explosions in industrial facilities in various sectors, as well as in accidents investigations.

When carrying out such an accident analysis, as well as in assessing hazards related to a process, it is essential to use different types of computation tools to calculate effects, in order to be quite simple but also as realistic as possible.

To perform such calculations of effects, INERIS developed and uses its own tools to calculate for instance explosion effects, projections of debris, or radiative effects of pool fires.

On the other hand, INERIS had to consider commercially available softwares.

In this case, one of the first cares of the analyst is to make sure he is using a suitable validated tool. That is why INERIS, with the French Ministry of Environment, initiated a methodology of assessment of softwares in risk analysis.

First of all, the point of view is that of a user who wants to be sure he is using a suitable tool. Thus, there is a need to consider the following questions :

* Easiness to use the software,
* Internal consistency of the tool,
* Consistency of the results as compared with calculations which might be otherwise assessed,

* Comparisons with available data (experiments, investigations of accidents).

One or a few versions of the following softwares : CAMEO, PAMPA, CHARM, TRACE, PHAST, WHAZAN have been considered since 1991 [5]. The methodology of assessment is described in the following part.

2- Methodology of software assessment

This methodology can be illustrated by the following scheme (see figure 1 below) :

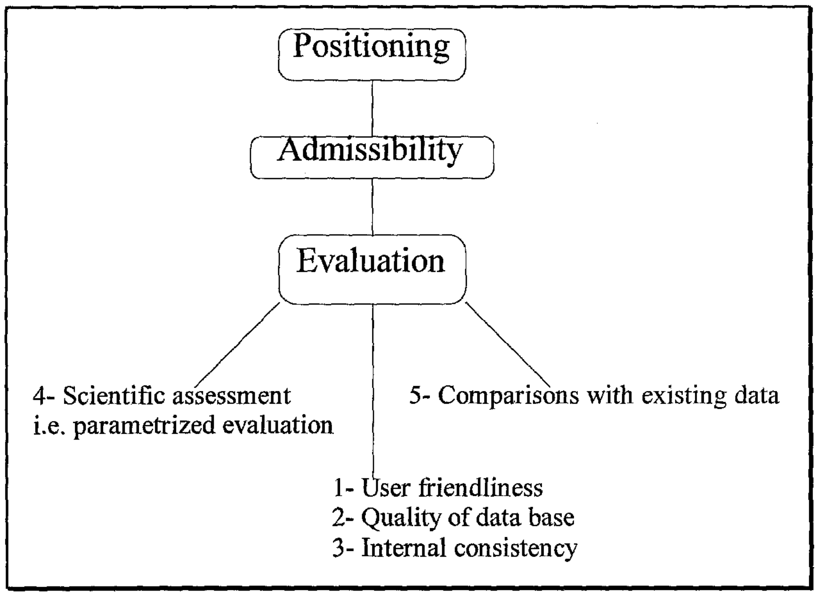

Fig.1 : This method for evaluating softwares concerns the whole package, that is the software itself + the user's manual + the theory guide.

The **positioning** allows to define the precise scope of risk analysis in which a software works. At the beginning of 1994, about 140 softwares were recorded in various areas : toxic releases in water and in air (the most numerous), gas explosions...(see [6]).

The **admissibility** allows us to choose quickly (within a month) a few softwares in a large market that may be assessed more completely.

Finally, the **evaluation** itself is performed within a few months, and concerns the whole package (software, user's manual and theory guide).

The following points are studied :

1) User friendliness of the package ;
2) Quality of the data base ;
3) Internal consistency of the software ;
4) comparisons with calculations that can be assessed independently. There are different ways to perform those comparisons. The risk analyst may either perform a scientific assessment (i.e.; a parametrized study) or compare the results with a few given scenarios of industrial accidents from which consequences are known (see [5 ; 7]) or compare the results with experimental data.

2.1- Positioning

The purpose for positioning softwares in risk analysis is that the user has a general view on a large market in a restricted area (see [6]). It also allows the user to know how many softwares are able to deal with the particular uses he or she intends.

That is why some information was sought at a given time on given versions of given softwares.

There are several criteria that allows the positioning of a tool.

2.1.1- BASIC CRITERIA

Before buying a software, the user must answer a few questions about the **origin** of the software and its first purpose. An other question related to the origin pertains to the relevancy of answers the user may obtain. The **age** as illustrated in figure 2 hereafter, the **cost** of the package and the hardware required to use the software (PC, Mac, Workstation,...,RAM, ROM,...) are interesting points too.

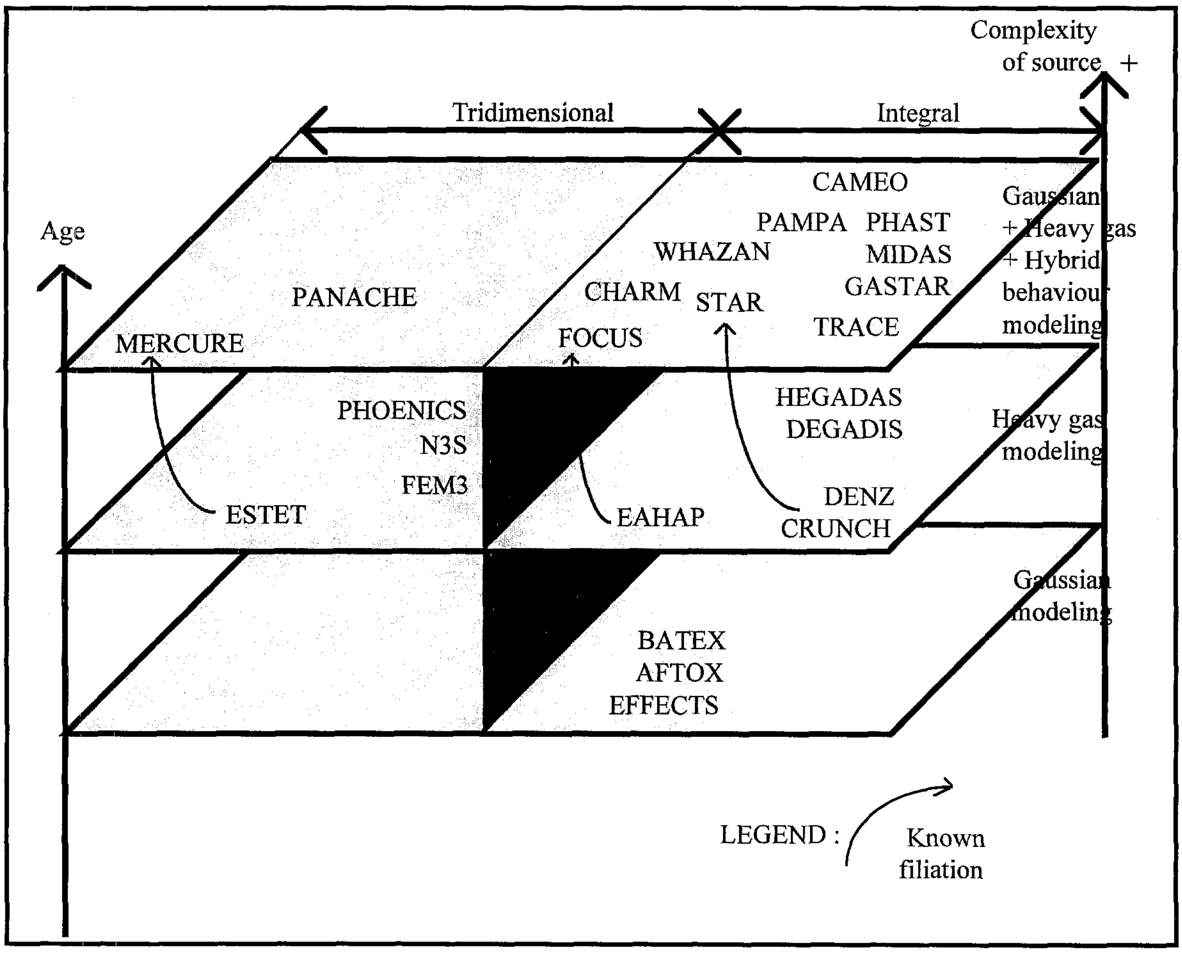

Fig.2 : Scheme illustrating different possible classifications in families of softwares.

2.1.2- SUBJECTIVE CRITERIA

They are difficult to define precisely. But some questions seem to be interesting to consider systematically. For instance, the user can wonder whether the aftersales services are competitive or not. In particular, does a hot line exist ?

2.1.3- SPECIFIC CRITERIA ABOUT SOFTWARES ON GAS DISPERSION

The points to be looked at are :

* The models used (Gaussian, box, Lagrangian),
* The source term definition,
* The number of chemicals in the data base.

2.2- Admissibility

2.2.1- MAIN ASPECTS OF ADMISSIBILITY

Admissibility is made of three indissociable parts :

The Theory Guide, which has to be considered under the following points:

* Its pertinency related to the version of the software that is evaluated,
* The accurate description of the hypothesis and ways of modelling,
* The definition of the limitations and of the areas of competence of the models,
* The quotation of the sources and references.

The user's manual, which has to be read bearing in mind the following points:

* Precise descriptions of all the parameters,
* Relevancy and pedagogical features of the examples,
* Exhaustiveness of the explanations of the available functions,
* Completeness of the informations to enable the user to run the case he intends to assess.

The software itself, which is considered under 150 tests performed by INERIS. These tests aim at assessing the physical consistency of the software. They are about source term, dispersion and flammable properties, and aim at comparing results from software with theory. Their contents and philosophy are described and illustrated in the next.

Generally speaking, the software is considered as admissible when :

a) the answers related to the manuals are generally positive ;

b) the tests don't point out a lot of inconsistencies.

Then, if admissible, the software is fully evaluated.

2.2.2- EXAMPLE RELATED TO ADMISSIBILITY

The hereafter example is source term test n°18. The aim of this test is to make sure the results related to mass flow rate, discharge velocity and temperature are close when considering a saturated tank or a padded one, the pressure in the gaseous part of which is equal to the saturated pressure.

<table>
<tr><td>Test n°18
***
Continuous release of gas
***
Leak through an orifice
Consistency related to the type of reservoir</td><td colspan="3">Theory
***
Results (flow mass rate, discharge velocity, temperature) are to be nearly the same.</td></tr>
<tr><td rowspan="6">Initial conditions
***
Product : Cl_2
Tank head :10 m
Height of leakage : 0 m
Φ orifice : 500 mm
Patm : 1 bar
Amount released : 1 Ton</td><td colspan="3"></td></tr>
<tr><td>Reservoir</td><td>1</td><td>2</td></tr>
<tr><td>Mass Flow rate (kg/s)</td><td>229.1</td><td>228.7</td></tr>
<tr><td>Discharge velocity (m/s)</td><td>183.1</td><td>183.1</td></tr>
<tr><td>Temperature (K)</td><td>Teb</td><td>Teb</td></tr>
<tr><td colspan="3"></td></tr>
<tr><td>Reservoir 1 : "Saturated"
P = 2.66 barg T = 273 K</td><td colspan="3" rowspan="2">Results
***
Results are nearly the same</td></tr>
<tr><td>Reservoir 2 : "Padded"
P = 2.66 barg T = 273 K</td></tr>
</table>

2.3- Evaluation

This step is in fact a full development of the work performed during the admissibility phases. All the following points are thoroughly considered (A to D), and a dialogue is held with the seller of the software on the aspects on which the package seems to be inconsistent.

The final report of the evaluation takes into account the positioning and admissibility parts, under the following scheme :

A- USER FRIENDLINESS OF THE SOFTWARE

Use of the software

The steps of installation must be clearly defined in the manuals, and it is necessary to have an efficient help from the retailer.

The user must be interested in the conditions of use : see the basic criteria for positioning a software. This point includes also a question related to the ease to install the software in the computer.

The software itself must be clearly built, and the results have to be clearly explained and referenced. Also convenient is the possibility for the user to store in memory the cases studied. We could illustrate these points in a previous paper [4].

Quality of tools to assess phenomenon evolution

Another point of concern in user-friendliness of the examined version of the software is related to the quality of tools available to assess phenomenon evolution.

Error messages, guard-rails and limitations of the models

Another point with regard to the user-friendliness of the version examined is related to the error messages and the presence of guard-rails testing the physical consistency of the data introduced to calculate a case, in relation with the description of the limitations of the models.

B - QUALITY OF DATA BASE

One function of the softwares used is to give the physical properties of species involved in the study, in order to allow calculations.

For the analyst, the main features of the data base are the number of species involved and their nature, the ease with which to create a mix of species of the base, to add new species or to modify a property, the capacity of the data base for constituting a library of physical properties, and, finally, the completeness of the base concerning toxicity.

C - INTERNAL CONSISTENCY OF SOFTWARE

The purpose of this part of the examination is to make sure the tool the analyst uses is consistent. Problems of consistency may arise about several topics.

Consistency in the software architecture

These pertains to the results that have to be the same - or nearly the same - whatever the ways of dealing with the case are choosen.

These problems of consistency are mainly relevant when, for instance, flammable properties and modelling have been added on a software built initially to deal with dispersion.

Boundary problems

The main points of consistency arise at the boundary of domains where continuity must be fulfilled, according to the question «when physical conditions are very close, are the results close ?».

The problems may arise according to several boundaries and the results pertain mainly to calculation of source term and dispersion.

1) *In a phenomenon itself*

2) *When the conditions given are close to those of a change of state*

3) *When the different conditions vary continuously*

4) *When conditions are close to the boundary of different modelling domains*

5) *Lastly, when the conditions are close to an internal boundary of modelling which is unknown to the user.*

D - COMPARISONS OF RESULTS WITH CALCULATIONS THAT MIGHT BE OTHERWISE ASSESSED

For each software, comparisons are systematically made about a lot of calculations. Some examples are given related to source term, dispersion and flammable properties.

Source term

- Calculation of flow rate in a monophasic gaseous flow through an orifice as a function of pressure and temperature inside the reservoir.
- Pressure drop for the same flow through a pipe, as a function of the length of this pipe.
- Calculation of a liquid flow rate through an orifice.
- Calculation of a flow through a pipe.
- Discharge velocity related to phase. Flashing fraction and temperature of release.
- Formation of aerosols.
- Diphasic flow.
- Rain out and mass balance between flash, rain out and aerosols.
- Emptying the reservoir as a function of time.
- Pool formation, extension and evaporation.

Dispersion

- Influence of wind speed,
- Influence of density,
- Influence of air moisture,
- Influence of roughness,
- Jets,
- Transition from dense gas to passive dispersion.

Flammable properties

One has to note that the importance given to flammable properties depends on the main features of the software. The investigated softwares are very poor on flammable phenomena for their main purpose is source term and dispersion.

When the software includes flammable effects, comparisons are made considering :

- a given pool fire, various sizes and products involved (hydrocarbons, alcohol,...)
- BLEVEs of propane, butane, ethylene oxide...
- UVCE related to a given flammable mass of product, the concentration of which is between LIE and LSE.

3- An example : from PHAST 3.0 to PHAST 4.2

PHAST is a software from DNV Technica. Two non-Windows versions were evaluated (3.0 in 1991 and 4.2 in 1995 : see [5]). A Windows version exists, the number of which is 5.0.

Two illustrations of the work performed are given here. The first one is about a test that pointed out a slight lack of consistency. The second one gives an idea of the improvements performed on software between the two versions 3.0 and 4.2.

3.1. Example of a lack of physical consistency

This example highlights some features of the evaluation. Generally speaking, PHAST is one of the best among the evaluated softwares.

Let's assume a monophasic gaseous leak of chlorine from a vessel through a pipe (length = 0m, 1m, 10m, 100m), all other parameter fixed, let's vary the initial pressure in the vessel (Pres). The observed variable is the mass flow rate (m in kg/s).

We notified that the results are within the right order of magnitude, but we also observed a discontinuity around Pres = 1 barg (see figure3 below).
Such a discontinuity seems to be related to the connection between two different models, and is not always scarce in a software.
But experimentations do not produce continuous results either.
In that case, the order of magnitude for the mass flow rate as a function of Pres is correct. It is the same for its evolution. Therefore, the discontinuity that was pointed out is only a slight problem compared with the expected accuracy of results related to the existing models.

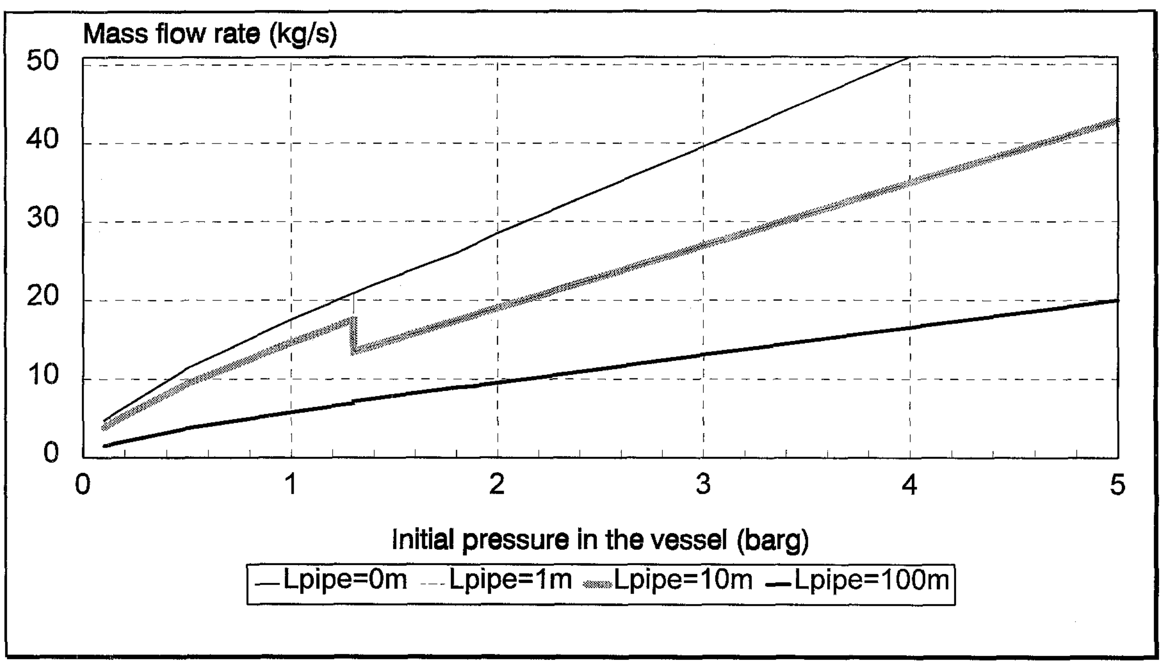

Fig.3 : Gas release through a pipe

3.2. Three examples of improvements between version 3.0 and version 4.2 of PHAST

1) Related to the documents

When INERIS has evaluated the version 3.0 of PHAST, the conclusions about the document were:

- Advantage: The two manuals fully describe the whole models used in the software;
- Limitation 1: The user's manual would be clearer if it was integrating schemes and explanations about generic terms like :
  «early ignition», «late ignition», «flash fire», ...
  Indeed, the user is not always a specialist in risk analysis, and doesn't necessarily know all the specific english terms.
- Limitation 2: The theory guide would be more complete if it was describing the model used more precisely.

In the new version (4.2) of PHAST, the first limitation is no longer present. A few schemes were added that help the user to understand the software better.

2) Related to the data base

- Advantage 1: It's a full and useful base that allows the user to calculate the consequences of the release of a product chosen amongst 59 toxic chemicals;
- Advantage 2: The first data base can be completed with another base that contains 900 chemicals;
- Limitation 1: Some data are missing related to the assessment of the effects of a human exposure to a toxic gas;
- Limitation 2: It's not possible to define a mixed substance made up with a few products.

In the new version, the second limitation does not remain.

3) Related to the source term

- Advantage1: The models related to a catastrophic rupture (instantaneous) are correct...
- Advantage 2 : The models related to a liquid pool development and evaporation are correct;
- Limitation 1: The models related to a release through a pipe perform results (speed of the flow, mass flow rate, liquid fraction) that might be inconsistent...
- Limitation 2: The option «Vent from vapour space» is not operational.

In the new version, all the advantages are still convenient, and limitation 2 is no longer present.

Conclusion

The methodology mainly dealing with positioning, admissibility and evaluation was applied to six softwares.

For such a work, the following restraints are to be considered:

1) The evaluation of a package is time consuming,
2) It is difficult to give synthetic results because of the complexity of the points to deal with (user friendliness, quality of data base, internal consistency and comparison with calculations are parts of the assesssment of the software),
3) Only a given version of a given software is evaluated. The conclusions that are drawn about that version are generally speaking no longer relevant concerning a further version,

4) The assessment is strongly depending upon the knowledge of the physical phenomena involved.

But the advantages of such a methodology for software assessment are mainly three:

1) Eliminate softwares the quality of which is not convenient,
2) Increase the quality of existing softwares,
3) Enable the software developer to take account of the risk analyst's needs.

Further developments will deal with other commercially available softwares.

Acknowledgement
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