Use of pertinent softwares in risk analysis

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ABSTRACT

The first need of the risk analyst is the availability of pertinent softwares 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 manuals)
- The analysis of the tool according to its internal consistency
- Comparisons of the results with calculations that might be otherwise assessed
- Comparisons of the calculations with existing data when possible (experiments and/or investigations of past accidents).

The paper aims at the first three above mentioned points, dealing with the comparisons of individual critical analyses of the following commercial softwares : CAMEO, CHARM 6.1, PAMPA 2.1, PHAST 3.0, TRACE 2.5.4.

When considering for example the physical consistency of models and submodels, the user-friendliness, the qualities of the data base and the explanations given in the documentation, it is possible to define an evaluation protocol for further studies.

To summarise, the use of pertinent softwares is an absolute prerequisite before determining criteria for acceptability of risks.

CONTEXT OF RISK ANALYSIS

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 : chemicals, oil, agri-foodstuffs, metals industry, energy, coal mines and more recently, the carriage by rail of dangerous goods. Studies have also concentrated on physical modelling and experimentation on the involved phenomena as well as on the definition and testing of detection, prevention and protective devices in order to suggest safer operational conditions.

Another aspect of the work performed by INERIS's experts is to deal with accident investigations such as fire in fertilizer storage plants, hydrocarbon fires, unconfined explosions following leaks of flammable gases, explosions of grain silos and in metal processing plants.

When carrying out such an accident analysis, it is essential to use different types of computation software to calculate effects.

The authors were also involved in safety cases, for which the use of these softwares was very important.

One of the purposes of risk analysis is to define the maximum effects of accident scenarios (eventually reduced by taking into account the technical measures of protection implemented by the manufacturer).

For all these tasks, the effects to be considered may be pressure pulses, thermal fluxes, accidental missile formation and projections and toxic releases of gases, vapours, mists, soots or dusts.

To perform such calculations of effects, INERIS developed and used its own tools (BIGEXP on explosion effects, MISSILE about projection of debris, JET on unconfined explosions from gaseous jets in atmospheric air, FNAP on radiative effects of poolfires...) or considered commercially available softwares.

But for plant managers, for insurance or control organizations and for competent authorities dealing with control of high-risk industrial sites, this approach has to be quite simple but as realistic as possible. An underestimation as well as a crude over estimation of the effects may be dangerous.

Thus, one of the first cares of the analyst is to make sure he is using a suitable validated tool.

The point of view taken into consideration is that of the user to make him sure he is using a suitable tool, when considering the following questions :

- Is it easy to use the software ? (It is usually time consuming and depends on the aptness of the theory and the user's manuals)
- Is the tool internally consistent ? (for instance may I calculate the same flow rate while considering a hole on the wall of a reservoir or considering a same size null length pipe ?)
- May I obtain the same results as those of calculations which might be otherwise assessed ?

- Are comparisons of the calculations of existing data available ? (These data may be drawn from experiments and/or investigations of past accidents).

This paper will deal successively with the following points related to :

- User friendliness of the software
- Quality of the data bases
- Internal consistency of the software
- Comparisons of the results against calculations.

The following versions of CAMEO, CHARM 6.1, PAMPA 2.1, PHAST 3.0 and TRACE 2.5.4 softwares were considered. These softwares are integral ones.

USER FRIENDLINESS OF THE SOFTWARE

Conditions of use of the software

This point first includes questions related to the conditions of use, such as :

- cost
- equipment needed (PC or workstation, graphical tools, size of RAM, ROM...)
- ease to install the software in the computer (are the steps of installation clearly defined in the Manual ? Is it possible to have an efficient help from the retailer or from the developer of the software ?)
- relevancy of answers (may the user ask questions directly to the developer or is there a retailer's interface ? Does the developer remain working on the same - or related - topics ?)

Use of the software

This point includes a lot of questions germane to the use itself :

1) *The product, we feel , is not only a software. It's a package which* includes both the software and the Manuals (Theory and User's Manual).

The quality of the manuals is a main feature of this package.

1.1 Is the user, after reading the so called "user's Manual", able to run the case he intends to assess ?

1.2 Are the results clearly explained ? Are relevant examples given, explaining the definition of messages, the significance of values... ?

* To give an example, we had to study a software dealing with atmospheric dispersion, the snapshots of which were not clearly defined. Thus, a crude reading of the results could bring the analyst to think the severity of a permanent emission increases with time. This is obviously not true after the regime is established at the point under consideration. The lack of information in this case was related to the algorithm used to represent the permanent emission as a succession of equal puffs.

* Another example is related to the interpretation of results. Another software reports the results as if it was only possible to consider permanent emissions. Thus the information given as "cloud radius", "cloud height", "mean concentration"... have different meanings :

When the emission is instantaneous the meaning of the words is correct : the software describes the evolution of the cloud while it is advected and it vanishes.

When the emission is permanent, the cloud is represented by means of windows, the height of which is reported as "cloud height", and the semi-width as "cloud radius".

1.3 Are the hypothesis and ways of modelling accurately described in the Theory Manual ?

For instance, the Theory Manual has to describe the way chosen to assess aerosol formation.

Is it by way of Weber's number ? Is it possible to take account of mechanical tearing ? Is it only assuming empirical approaches ?

To be efficient, the Theory Manual has to be clear, complete and to show completely the limitation to modelling.

2) *Do the results include reference marks* to allow the analyst to be able to recognize the case he is dealing with ?

If the case is not referenced on the listings and on the graphs, the use of the software may be tedious for it is not possible to run a succession of cases without having to stand around the machine.

This practical point is very important when the user wishes to analyse the consequence of the variation of a given parameter.

Among the softwares we examined, only a few reference the cases studied.

3) *Is it possible to store in memory the cases studied ?* This is useful when studying a given plant and analysing different cases around the same topic. Such a study, if no storage is possible, is tedious and time consuming.

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.

For instance on dispersion :

- Are vertical and horizontal cross-sections of the cloud available as a function of time ?
- Is it possible to have the history of concentration at each point ? Is it possible to choose only points on the downwind axis ? Is it possible to calculate directly the dose ($\int C^n$ dt, in which C is the calculated concentration at the point under consideration. C is a function of time t. n is related to a toxical effect according to the relation $C^n t$=cte, t being the time of exposure) received at these points ?

We had to examine a version of a software which could only give calculated concentrations at the points of a universaly settled logarithmic grid. Such a version does not fit closely the requirements of the analyst.

- Are the listings complete with size, position of the cloud, concentration, temperature, time, description of pools formed by rain-out ?...

Error messages and guard-rails

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.

Our work underlined versions of softwares in which it was possible to calculate gaseous explosions of solids, or to consider a hole diameter greater than the diameter of the tank, or a reservoir containing liquid at atmospheric temperature in the ceiling of which pressure may be different from the saturated one !

Limitations of the model

The last point with regard to user-friendliness of the version examined is related to a clear description in the Theory Manual of limitations of the software. This has never been encountered in the Manuals of the examined softwares versions. However, it is very important. To give an example : assuming 1 kg of chlorine is dispersed downwind, what is the reliability of a result giving 30 ppm of this gas at more than 1850 m downwind when you do know that the mechanisms of dispersion have been calibrated from experiments where tons of chlorine were released ?

It is important for the analyst to know the minimum order of magnitude he can consider to carry out significant calculations.

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.

Usually, these properties are stored in one or several files. For the analyst, the main features of the data base are :

- The number of species involved, and their nature. The best is obviously to have as many species as possible. Practically, we noted that softwares designed by chemists do not usually include a lot of species used in oil plants. For instance, consideration of hexane is not sufficient when studying an oil storage. On the other hand, a data base that includes a lot of aromatic and aliphatic species does not necessarily include other products, such as T.F.M.A (Metatrifluoromethylaniline)
- The ease with which to create a mix of the species of the base, to add new species or to modify a property. We noted it was sometimes possible to add a new species without difficulty but without analysis of the consistency of the properties introduced.
- The capacity of the data base for constituting a library of physical properties. One may quote that the PHAST data base gives an analysis of all the properties as a function of temperature and pressure. This aspect is very useful for thermodynamic calculations and constitutes, in itself, a useful tool.
- The completeness of the base concerning toxicity. Are there values given about n ? (n being related to an effect according to the relation $C^n.t$= cte where t is the time of exposure).

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 rise about several topics.

Consistency in the software architecture

These questions are linked to the architecture of the software and can be summarized in the following one :

"If several ways exist to deal with the same case, are the results in every way the same ?"

For instance, when studying the outflow from a definite reservoir containing liquid, are the initial gaseous outflow the same :

- when calculated through a hole in the top of the gaseous part,

- when calculated from an equivalent reservoir which contains only gas ?

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 of dispersion.

1) *In a phenomenon itself*

To give an example, one may quote a monophasic gaseous flow from a hole in a reservoir. According to the pressure inside it, the flow may be hyper or sub critical; the critical pressure is a function of γ (rates of the heat contents Cp/Cv). Physically, flow rates are to be very close when the pressures inside the tank are very close on both sides of the critical pressure.

This may not be true in the calculation, owing to the mechanism chosen to calculate the value of C_d (constriction coefficient).

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

For instance, around the saturation curve, there may be a domain of (P, T) for which calculations can't be done. This may be related to the equation chosen (virial coefficients,...).

3) *When the different conditions vary continuously*

For instance, when everything about the reservoir and temperature (of reservoir, atmosphere and ground) is set as well as a given wind velocity, one has to obtain a continuous trend when passing from stability class C to F.

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

For instance, two gaseous leaks, the first of CO, the second of ethane, from the same reservoir at atmospheric temperatures have to lead to very close dispersion calculations.

In certain softwares, this may not be true for the continuity at the boundary of domains heavy gas - passive dispersion is not fulfilled.

Related to the same topic is the distinction between an instantaneous and a quick continuous emission. Are the results slightly different when the release is instantaneous or when the same amount of species is released over a few seconds ?

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

This happens for instance in some softwares where the extension of the pool may be not limited. This happens also when a software does distinguish between different physical cases : for instance, when pouring CS_2 on water, it is possible to calculate an important extension of the pool though CS_2, heavier than water, sinks to the bottom of the dyke.

COMPARISONS OF RESULTS WITH CALCULATIONS THAT MIGHT BE OTHERWISE ASSESSED

After examining user-friendliness, quality of the data base and internal consistency of software, the next step consists in comparing the results with calculations that might be otherwise assessed using physical modelling of the phenomena.

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 (Cf table 1).
- Pressure drop for the same flow through a pipe, as a function of the length of this pipe. Does the software take into account viscosity ?
- Calculation of a liquid flow rate through an orifice.
- Some flow through a pipe. Are pressure drops function of viscosity ?
- Discharge velocity related to phase. Flashing fraction and temperature of release.
- Formation of aerosols. Is potential condensation considered ?
- Are there calculations of diphasic flow ? When ? Empirical formulas ?
- Rain out and mass balance between flash, rain out and aerosols.
- Emptying the reservoir as a function of time. Do the results lie between results obtained for an isothermal or a adiabatic discharge ?
- Pool formation, extension and evaporation. (table 2 and 3).

Dispersion

- Influence of wind speed,
- Influence of density (Cf table 4 and 5),
- 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 (Cf table 6).

CONCLUSION

In the analysis of the various softwares we investigated, user friendliness was examined by reference to conditions of use, the use itself, the quality of tools to assess the evolution of the phenomenon, error messages and the presence of guard-rails and limitations. With the exception of one software, user friendliness was rather poor.

With regard to the quality of data base, only one of the investigated softwares showed an ability to constitute a complete library.

The internal consistency of a software is related to its architecture and to the boundary problems. It would be desirable to improve this aspect, even if one of the investigated softwares was rather consistent.

The calculations we performed emphasized great discrepancies when comparisons were possible. Flammable properties were very poor as regard explosion effects and accidental missiles.

Further developements of such a work on software evaluation requires the definition of an accurate protocol. Nevertheless it is very important not to use only integral models in order to assess the phenomena more accurately with methods such as 2D or 3D finite differences or finite elements hydrodynamic models.

Naturally, the physical aspects have to be integrated in the purely computerized requirements such as graphical outputs of results in connexion with intermediate results.

Further developments will deal with other commercially available softwares, using funding from the French Ministry of Environment.

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* CAMEO (April 1993)
* CHARM 6.1 (August 1991)
* PHAST 3.0 (November 1991)
* TRACE 2.5.4 (August 1992)

TABLE 1

GASEOUS LEAK : CALCULATION OF INITIAL MASS RATE			
INITIAL CONDITIONS : Subritical flow Release of CO (γ_{Co} = 1.404) Pres = 1.5 bar Vres = 100 m3 Tamb = 293 K Ø hole = 50 mm			
	Velocity of release v eject m/s	Release Mass rate kg/s	Constriction coefficient (Cd)
Reference calculation	258.1	0.663	1
Software 1	256.6	0.447	0.67
Software 2	- *	0.455	0.69
Software 3	7129.7	0.650	1
Software 4	- *	0.71	- *

* A dash means it is not possible to deal with the proposed case, using the given software.

TABLE 2

POOL EVAPORATION : INFLUENCE OF AMBIENT TEMPERATURE				
INITIAL CONDITIONS : Instantaneous release of 10 tons of vinyl chloride Pres = Patm Tres = 230 K Meteo D3 Ground : concrete Tamb = Tground				
Calculated mass flow rate $kg/m^2\ s$				
Softwares	T ground 283 K	293 K	303 K	313 K
1	$2.67\ 10^{-2}$	$3.59\ 10^{-2}$	$4.39\ 10^{-2}$	$5.08\ 10^{-2}$
2	0.15	0.22	0.28	0.34
3	$2.6\ 10^{-2}$	$3.6\ 10^{-2}$	$4.6\ 10^{-2}$	$5.6\ 10^{-2}$
4	$1.38\ 10^{-2}$	$1.42\ 10^{-2}$	$1.48\ 10^{-2}$	$1.54\ 10^{-2}$

TABLE 3

POOL EVAPORATION : INFLUENCE OF GROUND NATURE			
INITIAL CONDITIONS Mass of release 10000 kg of liquid CS_2 Pres = Patm Tres = 293 K = Tamb = Tground Mean rugosity of ground Meteo D3			
Calculated mass flow rate $kg/m^2.s$			
Softwares	Gravels Thermal conductivity λ = 2.5 W/m.K	Concrete λ = 1.5 W/m.K	Water λ = 0.6 W/m.K
1	$5.42\ 10^{-3}$	$4.66\ 10^{-3}$	$4.66\ 10^{-3}$ *
2	$8.92\ 10^{-3}$	$8.92\ 10^{-3}$	-
3	$3.37\ 10^{-3}$	$2.88\ 10^{-3}$	-
4	-	-	-

* Remember that CS2 sinks under water. Dashes have the same signification than in table 1

TABLE 4

INSTANTANEOUS RELEASE : INFLUENCE OF GAS DENSITY							
INITIAL CONDITIONS : Mass of release 50000 moles of gas Pres = 0.1 barg Tres = 298 K = Tamb = Tground Mean roughness of the ground Meteo D3							
Downwind distance (m) where a 50 ppm concentration is calculated							
Softwares	H_2 2g/mole	NH_3 17g/mole	N_2 28g/mole	C_2H_6 30g/mole	CO_2 44g/mole	Cl_2 71g/mole	$COCl_2$ 99g/mole
1	2582	2739	2770	3056	3200	2641	2527
2	-	2350	2300	-	2300	2425	2250
3	2485	2445	2452	2447	3754	3754	3754
4	3300	3360	3360	3240	3080	2910	2840

Dashes have the same signification than in table 1

TABLE 5

CONTINUOUS HORIZONTAL RELEASES : INFLUENCE OF GAS DENSITY				
INITIAL CONDITIONS Molar flow rate 50 mole/s Pres = 0.1 barg Tres = 298 K = Tamb = Tground Mean roughness of ground Meteo D3				
Concentrations (ppm) calculated 500 m downwind from the source				
Softwares	H_2 2g/mole	CO_2 28g/mole	C_2H_6 30g/mole	Cl_2
1	140	140	147	261
2	-	144	-	240
3	8	115	-	-
4	805	772	800	535

Dashes have the same signification than in table 1

TABLE 6

UNCONFINED VAPOUR CLOUD EXPLOSION	
INITIAL CONDITIONS Instantaneous release of 250 tons of n Butane contained in a saturated liquid vessel at ambient temperature 293 K Early ignition.	
Distance where an overpressure of 140 mb is calculated	
TNT equivalent	630 m
Software 1	530 m
Software 2	-
Software 3	-
Software 4	990 m

Dashes have the same signification than in table 1