Application of an innovative risk dedicated procedure for both conventional and 3D atmospheric dispersion models evaluation

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APPLICATION OF AN INNOVATIVE RISK DEDICATED PROCEDURE FOR BOTH CONVENTIONAL AND 3D ATMOSPHERIC DISPERSION MODELS EVALUATION

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Abstract: In several contexts of risk assessment, prediction of safety distances is a key issue. Toxic or overpressure safety distances can be evaluated using both results from atmospheric 3D models (CFD, mass consistent, ...) and conventional approach results as Gaussian or integral models. Indeed, atmospheric dispersion of different types can be used in the same scope of application: hazardous materials, unobstructed environment, context of use (land use planning or emergency situation).
In this context, the SAPHEDRA project offers an innovative dedicated evaluation procedure for hazardous phenomena consequence modelling tools to be used for risk assessment studies.
The present paper describes the main steps of this procedure, the importance of defining the scope of application and the possible application to both above mentioned approaches with a view to increasing compatibility among atmospheric modelling evaluation. Based on a two-phase release example, which is much more complex than a gas release, this paper highligts different physics that both integral models and CFD tools evaluations have to adress to demonstrate the tools capability for a specific scenario.

Key words: *risk assessment, atmospheric dispersion modelling, safety distances.*

INTRODUCTION AND CONTEXT

In the risk assessment context of the European countries and particularly within the countries regulation for the land use planning in the industrial facilities neighbourhood, prediction of safety distances is a key issue. Toxic, thermal or overpressure safety distances due to hazardous phenomena can be evaluated using results from suitable consequence assessments tools in the case of accidents involving hazardous substance on an industrial site. Modelling tools are used within several contexts (see **Table 1**) to prevent accidents in the framework of Seveso-III-Directive (2012/18/EU) application, during emergency situation (Tognet et al., 2014) or in post accidental situation. Due to the large number of potential hazardous phenomena on human health, a wide variety of modelling models and tools are available to represent the possible effects that can be generated by an accident.

Table 1 : summary of risk assessement contexts and consequences modeling

Accident release modeling : when ?	Why ?	Type of Modeling
To prevent accidents - regulation for the land use planning: ▪ during industrial plant designing ▪ for existing plant facilities	• demonstrate control of risk • to optimize safety and to reduce cost • to give precise answers in a specific context	Predictive
During emergency situation	• support emergency responders • sensors / alarm equipment monitoring	Predictive / Diagnostic
Post accidental situation	• support to decision-makers • estimation of the impact on environment	Diagnostic

In this context, the SAPHEDRA project has been developed (Duplantier et al., 2016) to supply to decision-makers and model users relevant information to estimate consequences of industrial accidents.
The SAPHEDRA project offers an innovative evaluation procedure dedicated to hazardous phenomena consequence modelling tools to be used for risk assessment studies. The aims of the project are:

- to propose a procedure of impartial evaluation for consequences model within the most transparent way in order to publish the results of the evaluation to all the stakeholders involved,
- to offer elements to choose a valuable model when various models are available,
- to supply information to a broader public about the access to useful and relevant available model.

Moreover, for a specific hazardous phenomenon, such as toxic atmospheric dispersion, a large range of models were developed since 1970s. The range is extended from conventional approaches as Gaussian or integral models to atmospheric 3D models (CFD, mass consistent, tridimensional models means other than integral or Gaussian models). Whatever the category of model, several preliminary steps are required to demonstrate the modelling tool ability before using it for regulatory purposes. While this was achieved, in France, for the specific case of 3D models (Lacome and Truchot, 2013), such steps are required for all types of model. The objective of this paper is first to briefly describe a new methodology for this demonstration and then to give an example of application for a typical atmospheric dispersion problem.

GLOBAL APPROACH AND MAIN TASKS OF SAPHEDRA EVALUATION PROCEDURE

Preliminary work to demonstrate a modelling tool ability should be based on an evaluation protocol that commonly includes following stages:

- scientific assessment that aims at studying the limits of applicability of a model for a given scenario and hazardous phenomena,
- verification of the consistency of the computer implementation of the model with its mathematical basis,
- validation that aims at assessing how the input-output transformations generated by the model replicate those generated by the real world when compared to data (experimental, numerical data, past accident),
- sensitivity analysis that may be viewed as an initial test to find which model input parameters are important and their effect on output,
- user-oriented assessment that aims at addressing “ease of use” of the model.

All these stages were used in previous evaluation procedures (CERC, 2000). To ensure such an evaluation relevance, it is important to ensure doing all those stages in the correct scope of application of the tool. Such a feature is an improvement proposed by SAPHEDRA (Duplantier et al., 2016). This new approach also relies on a two steps sequence. First, a writer or a model evaluator provides information, needed for a complete evaluation, in a standard report to make comparison for evaluations easier. The model evaluator should verify the availability of information needed for criteria evaluation with knowledge of the reading grid. This preliminary step requires a minimal level of information, in such way no lack of information can influence the final judgement. Secondly the model evaluator gives his opinion and judgement about the relevancy or the accuracy of the information presented in the description report.

THE IMPORTANCE OF DEFINING THE SCOPE OF APPLICATION

Whatever the risk assessment study context is (see **Table 1**), the concept of scenario is crucial on a plant site and it encompasses issues of different types such as human factors analysis or consequences on health effect study. This latter is directly related not only to material products involved but also to the initiating event and the direct environment of the industrial plant. Whenever a modelling study for the consequences is carried out all, those aspects should be considered. Therefore, it seems relevant to take it into account when evaluating a model intended for risk assessment study. All these aspects are gathered in *the scope of application* of a model which has been divided in the following 6 items:

- Release / Loss of containment scenario (e.g.: line rupture, catastrophic rupture, vessel burst);
- Material: chemical products involved, hazardous substances/materials;
- Environment, geometry (not targets definition but influencing factors on hazardous phenomena);

- Type of hazardous phenomena included (hazardous phenomena: explosion, fire, atmospheric dispersion,… and type of hazardous effects: toxic, overpressure, thermal,…);
- Context of use: risk assessment regulatory study, technical support for situation of emergency see **Table 1**);
- Evaluation of the damage on human health and life, environment or infrastructure.

The first five items (Release / Loss of containment scenario, Material, Environment/geometry, Type of hazardous phenomena, Context of use) take part of the input set or issues that are under the scope of the SAPHEDRA evaluation process. The last one is not to be considered, however the evaluated tool is expected to provide all the inputs necessary for the evaluation of damages. For each model evaluation, a scope of application has to be proposed by the evaluation demander in agreement with the model developer in order to avoid misunderstandings between model developers and model evaluator and prevent any use of the model out of the box. Once an agreement about the scope of application is obtained between the model developer and the model evaluator, the latter is in charge to carry out the evaluation process by adapting all the evaluation tasks (see below) according the scope of application for every model that could be included within a software dedicated to risk assessment modelling.

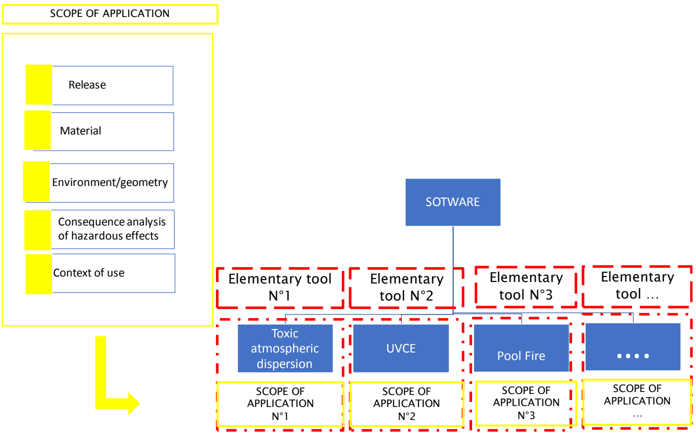

Figure 1: schematic description of a platform of elementary tools

HOW TO OBTAIN AN EFFICIENT EVALUATION FOR ATMOSPHERIC DISPERSION MODELING?

Based on the example of a two-phase flow release of a heavy product, as butane, this section describes the application of some stages of the evaluation protocol. This choice of a quite complex configuration is expected to provide enough specific difficulties to be pointed out. The work is done simultaneously for an integral tool and for a CFD one. For both approaches, the evaluation is not focussed on a specific tool but aims at highlighting main issues for each.

Scope of application

To define the scope of application, details about the scenario have first to be clarified. In the present example, a full line liquified butane release is considered and the objective is to evaluate the flammable mass and LFL distance in a land use planning regulatory study. It is then important to define the location of the release and the characteristics of the neighbourhood. In the present configuration, release is supposed to occur near the ground in an industrial facility with only some buildings in a quite free field configuration.

Scientific assessement

Based on the above defined scope of application, it is then possible to wonder about the compatibility of tools capability for the above defined scenario. This consists in checking that the whole set of models includes all the required physical phenomena required to evaluate the hazardous effects presented within the scope of application. For the present example, in terms of model this first means that tools must deal with two phase releases including droplet dispersion and evaporation, rain-out and thermodynamic of the release to be able to predict the correct temperature. Next, the configuration of the neighbourhood indicates that considering buildings does not appear as an important requirement.

Whatever the context of risk assessment studies, the estimation of source term and its use as input for an atmospheric dispersion model to simulate the atmospheric dispersion of toxic and flammable substances is of first importance. For complex release scenario, as for pressurized liquefied gases, critical review (Britter et al., 2011) showed there is still a significant uncertainty in the overall modelling process. It is an open problem whatever the level of complexity of the dispersion model. Hence, the importance to evaluate a source term model in a standalone mode or included in a pool of models is of preliminary importance. The relevancy of source term implementation is tested during scientific assessment and validation task. Unfortunately, for releases more complex than pure gas ones, due to the lack of data at relevant scale and possibly significant substance dependence (Coldrick, 2016), experimental data may be scarce. In this case, feedback on previous protocol (Webber et a.l, 2009) showed that a greater emphasis is given to scientific assessment. Among the different complex physics to be considered in the model, the evaluation of the release mass flow rate, the thermodynamic and the capability of the model to predict the correct temperature field, the droplet size prediction, evaporation and displacement appears as key issues to be discussed. For both integral and CFD models it is, at this stage, important for the model user to go deeper in the model description to evaluate precisely the physical phenomena that are accounted for and those that are simplified. As an example, some CFD tools, that could appear as more complex does not include enough thermodynamics to provide a correct evaluation of the temperature field or droplet behaviour. On the opposite, such a CFD tool could include a physical model as very near field break-up to handle a droplet size distribution and/or a detailed thermodynamic model to calculate a coupled prediction of droplet evaporation and vapour temperature. The objective at this step is also to let the user be aware about the required details for the specific scenario.

Validation

Whatever the type of model, another important requirement of all the evaluation protocols is the validation procedure. It is important to highlight here that this requirement should be understood as the requirement for a user to show his capability to carry out himself validation studies and not relying only on validation performed by the developer. It is a way to ensure that a user controls himself the validation part to make the consistency clear between the modelling approach within validation studies and hazard analysis. It is required that the validation of a model contains several stages from fundamental cases up to representative large-scale cases. The model user will achieve a results comparison with different and analytical or experimental relevant cases for which the experimental data are available.

An example of key issue for this stage is the different choices required during the modelling process as sub models or constants etc. As for sophisticated model, some calibration constants exist for simpler models that should clearly be pointed out during scientific assessment and reviewed by literature data analysis. The validation task aims at testing the atmospheric flow and atmospheric dispersion module, ideally with multiple sets of data to allow comparison scores betwen model results and data and a global criticism analysis of score versus data set. It is then important that the constants or sub models are suitable for all relevant validation cases and not too specific. At the end of this stage, the user has demonstrated his own capability to use the dedicated tool for the target scenario to be modelled.

Sensitivity analysis

Due to a potentially great number of parameters for a scenario and possible lack of validation data, sensitivity analysis is required for an evaluation and is highly recommended during a regulatory study to make some results more robust. At this step, the model user is in charge of choosing a range of values for varying parameters in the scope of application to gain knowledge on physics trends of the tool to check if parametric sensitivity results indicate a physical behaviour of phenomena. For example, as evaporation rate is a crucial quantitative issue for two-phase releases, this step allows to analyse the relationships among the near field break-up, the droplets diameter and mass transfer evaporation. This analysis is required for any tool regardless of its level of sophistication.

User-oriented assessment

This task is often underestimated except for specific contexts such as emergency situations for which the user workload is carefully examined. However, there are also other ergonomic criteria. For example, the accessibility / traceability of the input data and parameters can be valuable for a regulatory study context. Indeed, the more complex physics is included in the release scenario, the more accessibility / traceability of the input data and parameters is helpful.

CONCLUSION

Predicting safety distances is a major issue in the field of land use planning. A large variety of models could be used in this context. While some papers were published about the requirements regarding the 3D models used in such a context, other assessment approaches should also be considered.

Based on existing evaluation protocoles, the recent SAPHEDRA one introduces the scope of application as a dimension which enables distinguishing the validity range of the different tools. The application of such an evaluation protocole to both integral models and 3D ones points out the key issue to be considered during the tool evaluation. It then appears through the complex example of a liquid release that not only the type of the model is important but the detail of the included physical models. The main conclusion of this analysis is that models do not have to be distinguished form a macroscopic view, 3D versus Gaussian, but in terms of their whole capability in a given precise scope of application.

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