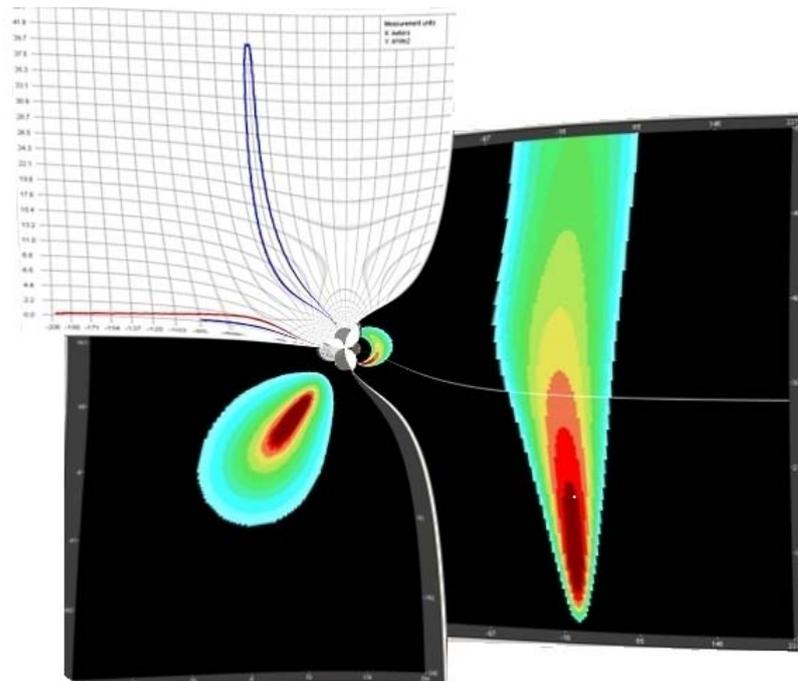


# On software interoperability for accident consequence assessment

A feasibility study for the definition of an XML data format to allow interoperability of software tools for accident consequence analysis

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## EXECUTIVE SUMMARY

The review of Safety Reports is one of the tasks of the National / Regional Competent Authorities responsible for the plant licensing according to the Seveso Directive. One task concerns the decision-making process about the acceptability of the consequences of the potential accidents and it involves the detailed analysis of the hypotheses made by the operator for the consequence estimation and the results of the models applied. This involves the needs to re-analyse (at least part of) the accident scenarios and to compare the results. This activity is straightforward if it is performed by applying the same software tools used by the operator. Unfortunately, the more common situation is that the tools are different, since the operator may use any model considered as acceptable by the scientific community; this makes the activity rather expensive in terms of time and resources.

In this context, in order to contribute simplifying the work of the authorities, a project was set up at the JRC to investigate about the feasibility of facilitating the data exchange between different software through the definition of a Common Data Exchange Format (CDEF). In this way the input data used by the operators and the accident consequences provided by using certain software tools could be suitably exported in a format compatible with the input format of the tools in use by the authority. Consequently the dialogue between the authority and the operators will be facilitated, which in turn will help the consensus building. A suitable CDEF would be of great benefit also to model developers and software developers, since it would foster the comparison of the results obtained using other models and tools; not to mention the advantages to the operator when dealing with the periodic update of the safety report.

The present document provides the main findings of the feasibility study. In particular it describes the structure of data exchange that has been developed in XML and applied for data exchange amongst different available consequence-related models. Few application examples were executed on a selected number of accident scenarios (i.e. fires, explosions and toxic releases).

Besides the interoperability issue, the feasibility study also addressed the problem of comparing the results of different software, e.g. the “operator tool” and the “authority tool”. Since the consequences of an accident are normally described by the physical damage that can occur on the ground, the comparison of two models that provide results for different points on the ground involves the solution of the problem of interpolating data on a common grid. The interpolation process was fully explored in this study with reference to the typical effect contours of industrial accidents. The interpolation and models’ comparison methods have been implemented in the software CEM (Comparison Effects Models).

The CDEF prototype was finally used to import into ARIPAR – a GIS-based software for area risk analysis and control - the results of accident consequences obtained by using some well known consequences assessment software: PHAST, EFFECTS, and ALHOA.



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# 1. INTRODUCTION

The Seveso Directive, in introducing the concept of the safety report, has formally obliged upper-tier operator to describe and defend the risk assessment report and in particular the measures adopted to prevent, control and limit the consequences of major accidents. The Competent Authorities responsible for the implementation of the Seveso Directive in their countries have the task, among others, of reviewing the report. In this context they are in charge of deciding about the acceptability of the consequences of the potential accidents identified and evaluated by the plant operator. This activity involves the examination of e.g. the source terms data used, the hypotheses adopted for the calculation, and the results of the consequence models applied.

Local authorities are also confronted with the risk analysis and management for those areas where the concentration of activities concerning the storage, process and transportation of dangerous substances take place in highly populated areas. These places pose indeed problems of risk control, land use planning, emergency planning and response. It is clear that the decision-making process requires the analysis of a large amount of accident scenarios. A valuable source of information is the safety reports for Seveso-type installations. For all other risk sources the collection and analysis of relevant data are followed by the assessment of the consequences of accidents and the estimation of their occurrence frequencies.

By considering the large number of models and software tools available on the market, and the fact that the operator has always the possibility to make use of any model considered as acceptable by the scientific community, the review activity of the impact of accident scenarios might become a long and expensive task. Indeed, authorities have their own preferred reference models and tools, which may differ from those used by the operator. On the other hand, in order to conduct this verification activity, the models used by the competent authority have to be run by using the same set of input data selected by the operator.

In this context, in order to simplify the work of Competent Authorities, it was decided to launch a feasibility study aiming at defining a suitable data exchange format between different consequence assessment software tools. Such a format will be referred to as Common Data Exchange Format (CDEF). In other words, this study was addressed to clarify how the input data and the accident consequence results provided by the Operator could be suitably exported in a format that is compatible with the tools in use by the Competent Authority. In this way the comparison of the calculated accident consequences would be straightforward and it would make the overall verification activity quicker and cheaper. The dialogue between the authority and the operator would be consequently facilitated and the consensus building would be accelerated. More precisely, a common data exchange format would give the possibility:

1. to easily import data and results of consequence analysis submitted by the operator;
2. to run the authority's reference model with the same input data of the operator;
3. to rapidly compare the results of two or more models on the same map or plotting system.
4. to run different models for the analysis of the same scenario, thus increasing the confidence in the results; and finally
5. to reduce the cost of the verification activity of the safety report.

The usefulness and relevance of the interoperability of these software tools becomes fundamental when area risk analysis is of concern due to the large number of scenarios to be analysed.

A CDEF would also be of benefit for the Operators. Safety reports have to be periodically reviewed to account for possible modifications within the plant (e.g. substances and related quantities, process), or

in the external environment (e.g. population distribution, new constructions). The existence of a CDEF would not oblige the operator to use the software applied in the past or to re-input all the necessary data if new models are used, but rather it would allow the re-use of the previously applied data.

Moreover a CDEF would offer the possibility to rapidly develop packages addressing accident scenarios that can be simulated by using different models, e.g. outflow, pool evaporation, dispersion. Indeed if each single model conforms to the common format the interoperability would be assured. Hence any single model could be substituted with a better one without programming effort.

Finally, a common data format would also be of great benefit to model and software developers, since it would foster the comparison of results obtained using different models and tools. As a spin-off, it could result possible development of new ideas, exchange of experiences and suggestions for further improvements/studies.

For all the above considerations the definition of a common format of data exchange to improve interoperability amongst different models has been considered as a challenging activity at the Major Accident Hazard Bureau (MAHB) of the European Commission of the Joint Research Centre. This activity is also in line with the institutional role of MAHB and its mandate to provide technical and scientific support to EC DG Environment and to the Competent Authorities of the Member States.

For this reason an internal activity was launched with the objectives summarised hereunder:

1. to study the feasibility of a common data exchange format for accident consequence models, by focusing on typical accidents that could develop from a Seveso-type establishment, i.e. fires, explosions and toxic releases;
2. to develop a specific software tool to compare the results of different consequence models for the same accident type. Since the consequences of an accident are normally described by the physical damage that can occur on the ground (thermal radiation, overpressure, toxic concentration), the comparison of two models that provide results for different points on the ground involves the solution of the problem of interpolating data on a common grid;
3. to apply the data exchange format to interface different software tools (e.g. by adapting an area risk assessment tool such as ARIPAR to import data from commercially available accident consequence packages).

It is important to highlight that a study for a common data exchange format is already underway in the nuclear field through the OPEN-PSA initiative (<http://open-psa.org>). This initiative aims at achieving several interesting objectives among which the definition of a common data exchange format for the Probabilistic Safety Assessment of nuclear power plants. The first level of nuclear PSA requires the plant modelling using fault trees and event trees i.e. two methodologies that are also used to a certain extent also in the chemical-petrochemical sector. The fault tree analysis is indeed applied to determine the occurrence probability of dangerous plant states associated with significant undesired consequences, as resulting from HAZOP studies; event trees are used to describe accident scenarios' development, which are triggered by the occurrence of an initiating event and other plant conditions.

The idea of extending a common data exchange format to the accident consequence assessment tools is particularly important by considering that, for all dangerous plant states, frequencies and related consequences allow determining the risk associated with the facility under study.

In the framework of the OPEN-PSA initiative and with regard to the implementation of the data exchange format, it was decided to use the Extensible Mark-up Language (XML) due to its large

spread for this kind of applications i.e. being XML particularly targeted at the improvement of interoperability of different systems. The same choice has been adopted for the accident consequence application described in this report.

Clearly, the results obtained in this study are merely intended to present the general concept and to explore all the possible technical problems that can be associated with this process. *A common data format suitable to all consequence assessment models available in the market can only be established after consultation and with the consensus of all relevant stakeholders* (i.e. European Committee for Standardization, EU safety authorities, industry representatives, software and model developers, etc). Only in this way it will be possible to build up a commonly agreed data exchange format to assure the interoperability of risk analysis tools.

The present report is intended to provide information about the main results of this feasibility study. Specifically Section 2 provides the basic information on the XLM structure proposed for data exchange amongst different commercially available consequence-related tools. It represents the synthesis of the results of the test cases considered during the study which allowed identifying the main problems to be solved to define a common format. Section 3 deals with the problem of interpolating the results of consequence analysis, expressed in terms of effect-contours, on a 2D grid. Different interpolation methods have been considered taking as reference data the results obtained by running a Gaussian model for each cell of the grid. Other experiments have been performed using PHAST and EFFECTS. An application is described in Section 4, where the ARIPAR software, for risk analysis calculation, has been interfaced with PHAST, EFFECTS and ALOHA, three well known software packages for consequence assessment. Section 5 presents the CEM software, developed within the present activity, for comparing the results provided by two different consequence assessment tools applied to the same scenario and interpolated on a common grid. Overall conclusions are given in Section 6.



## 2. PRELIMINARY CONSIDERATIONS ON THE INTEROPERABILITY OF ACCIDENT CONSEQUENCE ASSESSMENT TOOLS

In order to develop a common format for data exchange for consequence modelling, it is essential to clearly identify all aspects concerning the involved models and the whole set of parameters to be considered.

Within the OPEN-PSA initiative [1], the general requirements for a common data format have been identified. Some of them are:

- *Clarity*, to avoid misinterpretations leading to different implementations;
- *Completeness*, to cover data in all models;
- *Extensibility*, to leave the possibility to introduce new constructs, even if these are not recognised by all tools; however, any addition should be public to allow other software developers to implement them.

The present section describes the overall XML structure that was build up for the purpose of the present study and which represents a first prototype for a common data exchange format for accident consequence modelling. Clearly, the proposed structure does not claim to be exhaustive and to include all necessary elements of a common data format because it is based on the analysis conducted on a limited number of models and related software. However, it is a first attempt to create a comprehensive data structure, which is applicable for the transfer of data amongst a number of commercially available tools, broadly used for consequence assessment calculations. The Extensible Mark-up Language (XML) [2] was used due to its potential to improve the interoperability of systems for this type of applications.

XML is a mark-up language much like HTML, but it has a different objective. Whereas HTML was developed to display data, XML was designed to describe data. Both use tags to enclose data; however whereas in XML they can be defined by the user, in HTML this is not possible. Hence tags for consequence assessment can be defined describing the data used. XML uses a DTD (Document Type Definition) to formally describe the data. As for other XML documents, the proposed file format contains a tree-based data structure composed of units called *entities*. An entity may refer to other entities to cause their inclusion in the document.

In this report the description of the data exchange format will be focussed on the data structure rather than in the XML implementation.

### 2.1 Data structure to be exchanged

In the definition of the structure of the common data exchange format it is important to clearly address the following issues:

1. type of accident category under study (i.e. fire, explosion, or toxic release);
2. the specific accident outcome (e.g. for fire: pool fire, jet fire,...)
3. the considered type of model (e.g. 1D, 2D);
4. the input data and model's parameters to be considered;
5. the type of representation of results (e.g. 1D, 2D grid, effect-contours).

The first three points are necessary for documentation purposes and for checking the compatibility of data to be exchanged between two software tools. Point 4 is the most difficult to define, whereas point 5 is necessary for comparing models' results.

It is important to underline that it is not always possible to simply use the input data of one software tool, say A, to run another one, say B, when the two are based on different models for simulating a given accident scenario. In these cases it is indeed necessary to complement the data exported by A with extra data in order to run B.

For instance a 1D pool fire model does not have the same input data of a 2D pool fire model simply because models, applicable for the same accident type, have a different degree of complexity.

In other circumstances, together with the input data, it is necessary to incorporate part of the results of the second model to run the first one. This is the case when comparing tools that implement a single model (e.g. outflow, pool fire, UVCE, fireball) and other tools that automatically run, one after the other, all models necessary for the complete calculation of the impact of a given accident (e.g. from outflow to pool formation, pool evaporation, heavy gas dispersion, transition to neutral conditions and Gaussian dispersion). To simplify the discussion we will indicate the first type as “single model, SM” tools, and the second type as “multi-model, MM” tools. An MM tool may also be seen as of SM type for those types of accidents that require the use of a single model (typically fire and explosions). When an MM tool is involved, the output of all models (intermediate results) must be available, since some output data may become input data for another tool. For instance, for calculating the toxic concentration of a heavy gas release, PHAST can be classified as an MM tool, whereas SLAB as an SM tool. PHAST starts indeed the simulation from the storage conditions and determines the outflow, whereas SLAB requires the outflow as input data. Thus, both input and output data are to be part of the XML format.

The data to be exchanged between accident consequence tools can be organised in a tree-like structure as schematically shown in the following figure.

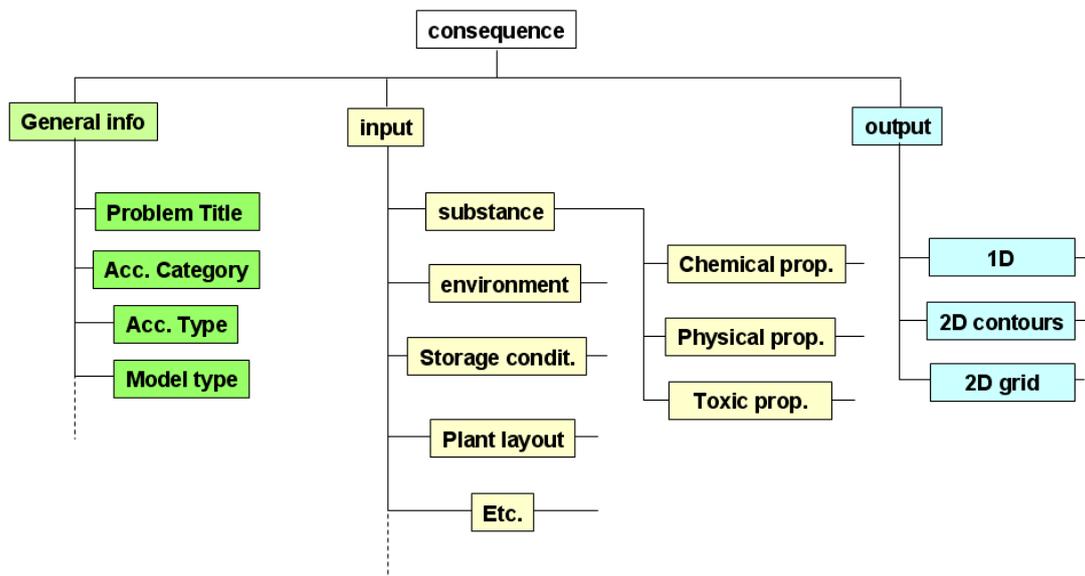


Figure 1. Tree-like structure of the data to be exchanged

In Figure 1, three sections can be identified:

- *General information section* containing the minimum set of information necessary to univocally identify the type of problem and model; this information is used for compatibility checks.
- The *Input section* is the most complex section containing all data necessary to run a model; these data can be organised in sub-sections to improve readability.

- The *Output section* is quite simple to define since the result of the available tools can be normally one of the following: centreline (typical of 1D model), effect contours and grid, typical of 2D models.

The structure in figure 1 has been developed on the basis of the software tools considered in this feasibility study. Since this structure is open, other data can be added when deemed necessary (*extensibility* requirement).

## 2.2 The structure of the XML data exchange format

The XML document for accident consequence assessment begins with a “root” or document entity that has been named “**consequence\_analysis**”. According to the structure described in Figure 1, the following relevant entities are “**general\_info**”, “**input**” and “**output**”, respectively. The last two refer to the groups of parameters associated with the input and output data. The high-level structure of the XML document is given in Figure 2:

```

<consequence_analysis>
  <general_info>
    List of entities describing information useful for describing the
    scenario and the tool used for calculations
  </general_info>
  <input>
    List of entities describing input variables and model parameters
  </input>
  <output attribute_name="attribute_value">
    <effect_data_1 attribute_name="attribute_value">
      List of entities describing results (data points) of group 1
    </effect_data_1>
    ...
    <effect_data_n attribute_name="attribute_value">
      List of entities describing results (data points) of group n
    </effect_data_n >
  </output>
</consequence_analysis>

```

**Figure 2: XML high-level data structure for consequence assessment**

### 2.2.1 General information section

The “**general\_info**” entity is characterised by a number of attributes as described in

Table 1.

In particular, the attributes define the category and type of accident, which the XML file is referred to. To run a model of a given accident type it is important to verify that the XML input-file contains the data related to that type of accident. Attributes are listed separated by one or more spaces. Information on the software is also provided for documentation purposes. The following example refers to a pool fire analysed by means of the EFFECTS package.

```

<consequence_analysis>
  <general_info>
    <problem_description> text </problem_description>
    <accident_category>fire</accident_category>
    < accident_type>poolfire </accident_type>
    <software_name>EFFECTS</software_name>
  </general_info>
  .....
  .....
</consequence_analysis>

```

**Table 1 a: List of attributes and corresponding values for the root entity**

General_info entity	
parameter_name	parameter_value
<i>problem_description</i>	free field for documentation purposes
<i>accident_category</i>	explosion fire dispersion ---
<i>accident_type</i>	UVCE fireball jetfire poolfire instantaneous_release continuous_release Gaussian_dispersion
<i>Software_name</i>	free field for documentation purposes

### 2.2.2 Input data section

The entity <input> provides information on all essential input data necessary to run the consequence models. This part of the format is the most complex since it contains the data necessary to use the different models for consequence assessment, e.g. data to calculate the outflow (source term), the different fire and explosion models; models to determine the air and water dispersion of dangerous substances. Due to the large number and complexity of these data, the format should be flexible enough to account of possible new variables to be included in a later stage.

In this feasibility study, a first list of parameters was created by considering some commercial software, among which PHAST [7], EFFECTS [9], and ALOHA [10]. The organised list of parameters is clearly incomplete and it represents only a first possible example. In this example, which was specifically tailored to heavy-gas dispersion, each parameter was described, when relevant, by the attribute UM, representing the measuring unit, which was defined according to the international standard nomenclature (SI units).

The input parameters can be subdivided into:

- Input variables of the model;
- Model editable parameters;
- Calculation parameters.

The first type can be grouped into separate sub-entities as for instance: substance, containment, storage conditions, source term, plant layout, environment, ..., and so on. The grouping of input data is useful only to enhance the legibility of the file. An important point to be further examined is the use 'editable models' parameters. These have to be considered in the XML file since they represent a specific choice made by the user and it is, therefore, information to be transmitted. It goes without saying that all calculation parameters must necessarily to be considered.

A simple example concerning the input data for a confined pool fire would be represented as follows:

```

<input>
  <substance>
    < name>Butane</ name>
    <CAS_number>106-97-8</CAS_number>
    <flame_emissive_power UM="kW/m2">165.0</flame_emissive_power>
    <flame_temperature UM="K">1400.0</flame_temperature>
    <substance_density_in_vapour_phase UM="kg/m3">5.8</substance_density_in_vapour_phase>
    <substance_boiling_temperature UM="K">272.660004</substance_boiling_temperature>
    <substance_specific_heat UM="kJ/(kg K)">2.3</substance_specific_heat>
    <substance_evaporation_heat UM="kJ/kg">363.0</substance_evaporation_heat>
    <substance_combustion_heat UM="kJ/kg">45860.0</substance_combustion_heat>
  </substance>
  <environmental_conditions>
    <wind_direction_from_N UM="rad">0.0</wind_direction_from_N>
    <wind_speed UM="m/s">3.0</wind_speed>
    <air_viscosity UM="Pa s">1.846e-005</air_viscosity>
    <vapor_water_pressure UM="Pa">2310.0</vapor_water_pressure>
    <ambient_air_density UM="kg/m3">1.196</ambient_air_density>
    <ambient_relative_humidity UM="%">50.0</ambient_relative_humidity>
    <ambient_temperature UM="K">293.0</ambient_temperature>
  </environmental_conditions >
  <source_term>
    <pool_diameter UM="m">10</pool_diameter>
  </source_term >
  <model_parameters>
    <angle_fire_target UM="rad">0.0</angle_fire_target>
    <correlation_flame_tilt >AGA</correlation_flame_tilt >
    ...
  </model_parameters>
  <calculation_parameters>
    <iteration_number>30</iteration_number>
    <points_in_contour>20</points_in_contour>
    ...
  </calculation_parameters>
</input>

```

### 2.2.3 Output data section

The entity **<output>** is intended to contain all data resulting as the outcome of the models and typically consequence effects' values (i.e. overpressure, thermal radiation, toxic concentration) as a function of distance from the release point. The attributes of this entity are: **output\_distance\_from** that represents the point from which the effects are calculated, and **number\_effect\_data**, which represents the number of sub-entities described below.

For instance the XML format representing an explosion, described by means of 5 contours (number\_effect\_data), is as follows:

```

<output distance_from="center_cloud" number_effect_data="5">
  ...
  Description of data in different forms depending on the type of representation of results
  ...
</output>

```

The definition of the different types of results of consequence models is quite simple. Indeed the possible representation of the outcome of models used in risk analysis can be of three types:

- 1D effect vs. distance
- 2D effect contours
- 2DGRID: generic grid

### 1D: effect vs. distance

If the results are given by a 1D model, then we have only one curve to be represented; hence between the tags `<number_effect_data_01>` and `</number_effect_data_01>` the set of points distance-effect are stored. The information contained in the output file is summarised in the following table.

**Table 1 b: List of attributes and corresponding values for 1D models output**

<b>Number_effect_data_n</b>	<b>Attributes</b>
	coordinate_system (Cartesian)
	UM_coordinate1: unit measure of the distance
	UM_coordinate2: unit measure of the effect
	number_points of the curve representation type
<b>point</b>	<b>Attributes</b>
	coordinate1, representing the distance from the source
	coordinate2, representing the effect

The following XML example refers to an explosion described by 18 over pressure values expressed in Pascal vs. distance expressed in meters.

```
<output distance_from="center_cloud" number_effect_data="1">
  <number_effect_data01 coordinate_system="cartesian" UM_coordinate1="m" UM_coordinate2="Pa" number_points="18"
  representation="1D">
    <point coordinate1="34.000000" coordinate2="390600.000000"/>
    <point coordinate1="42.000000" coordinate2="241300.000000"/>
    <point coordinate1="46.000000" coordinate2="197600.000000"/>
    <point coordinate1="80.000000" coordinate2="64900.000000"/>
    <point coordinate1="273.000000" coordinate2="9700.000000"/>
    ....
  </number_effect_data01>
</output>
```

### 2D: effect contours

In this case `<number_effect_data_01>` refers to the first contour, .... and `< number_effect_data_n>` refer to the n-th contour.

Some software gives also the centreline concentration; when it is available it is represented as 1D. The information contained in the output file is summarised in the following table.

**Table 1 c: List of attributes and corresponding values for 2D models output**

<b>Number_effect_data_n</b>	<b>Attributes</b>
	coordinate_system (Cartesian, Polar)
	Effect value of the contour
	UM : measuring unit of the effect
	UM_coordinate1: unit measure of the distance on the x axis (Cartesian) angle (Polar)
	UM_coordinate2: unit measure of the distance on the y axis (Cartesian) distance (Polar)
	number_points of the curve representation type
<b>point</b>	<b>Attributes</b>
	coordinate1, representing the distance on the x axis
	coordinate2, representing the distance on the y axis

The following example refers to a pool fire for which 5 effect contours are given. Note that in this example the coordinate system is Polar with distances measured from the edge of the pool:

```
<output distance_from="edge_pool" number_effect_data="5">
  <number_effect_data01 coordinate_system="polar" iso_value="40.0" UM="kW/m2"
    UM_coordinate1="rad" UM_coordinate2="m" number_points="20" representation="2D">
    <point coordinate1="-1.570800" coordinate2="6.317039"/>
      <point coordinate1="-1.256640" coordinate2="6.317039"/>
      <point coordinate1="-0.942480" coordinate2="6.317039"/>
      ....
  </number_effect_data01>
  ....
  <number_effect_data05 coordinate_system="polar" iso_value="1,60" ...>
  ....
  </number_effect_data05>
</output>
```

As previously mentioned besides the 2D contours also the centreline can be part of the output. In these cases the XML file will also contain the data in the format as described for the 1D case.

**2DGRID: generic grid**

For software that produces the results in the form of a grid (sparse or not) the representation of the value in a grid cell (point) is given as a triple: coordinate x, coordinate y and effect. The information contained in the output file is summarised in the Table 1 d.

The following example refers to the results provided by SLAB for the instantaneous release of chlorine. Note that the coordinate system in this case is Cartesian.

```
<output distance_from="0" number_effect_data="1">
  <number_effect_data01 coordinate_system="cartesian" UM="ppm" UM_coordinate1="m" UM_coordinate2="m"
    number_points="671" representation="2DGRID">
    <point coordinate1="-37.500000" coordinate2="0.000000" effect_value="0.000000"/>
    <point coordinate1="-30.000000" coordinate2="0.000000" effect_value="10.600000"/>
    <point coordinate1="-22.500000" coordinate2="0.000000" effect_value="14600.000000"/>
    ....
  </number_effect_data01>
</output>
```

**Table 1 d: List of attributes and corresponding values for 2DGRID models output**

<b>Number_effect_data_n</b>	<b>Attributes</b>
	coordinate_system (Cartesian, Polar)
	UM: measuring unit of the effect
	UM_coordinate1: unit measure of the distance on the x axis (Cartesian) or of the angle (Polar)
	UM_coordinate2: unit measure of the distance on the y axis (Cartesian) or distance (Polar)
	number_points of the grid representation type
<b>point</b>	<b>Attributes</b>
	coordinate1, representing the distance on the x axis (Cartesian) or the angle from x (Polar)
	coordinate2, representing the distance on the y axis (Cartesian) or the distance (Polar)
	effect_value

### ***IDS: threshold values***

Besides the three types of representation of results it is worth to consider also what it is also used in safety reports for consequence assessment representation: the threshold values. This particular type of representation is conceptually equivalent to the above described 1D but with a limited number of points, which are generally less than 5. In the present study the distinction was specifically made to take into account of the limited number of data and the problems associated with their interpolation. This point will be clearer after reading section 4.

## **2.3 Discussion about XML file dimensions**

For the interoperability of consequence assessment software, an important aspect that must be addressed is the dimension of the XML file: if it is too big the time to read it could be too long. It is not very easy to establish a-priori what the maximum dimension of an XML file should be in order to avoid any problem in the uploading phase.

The set of data that may increase the file dimensions is the output part, but generally problems should occur only in the 2DGRID case. Let's consider, for instance, the release of a toxic substance in the atmosphere. The effect may be spread over a few kilometres from the source and the grid cell dimension might be selected to a small value to increase the accuracy. In this case the number of points might be very high and some dimension problems of the corresponding XML-file could arise. In such a situation, there are two possibilities to reduce the dimension of the output file:

- 1) to export a sampled grid;
- 2) to export contours.

A simple numerical example helps describing the problem. Let's suppose that the (squared) grid cell dimension used for calculation is 4m and that the grid dimension is 4,000m x 2,000m; then the number of points (x,y, effect) is 500,000. If this grid is sampled with a cell size of 20m the number of points to be exported would be 20,000; if the sampling was done with a grid cell of 40m the number of points would be 5,000; and so on.

In the second case, the contours already represent a significant reduction of the number of calculated points with respect to the grid case. The dimension of the output file is determined by the number of contours and by the density of points on each contour, i.e. the distance between two points on each contour line.

It should be pointed out that, after reducing the number of points to be exported, there is always the need to reconstruct, within the importing tool, the original grid. This has to be done by applying suitable interpolation methods. The interpolation operation is also necessary when the result of two software / models must be compared for a given accident scenario. The results could be indeed represented in different ways: 1D, 2D contours, or 2D grid. The comparison can be performed by interpolating the results of models on a common grid.

The problem of interpolation also arises when accident consequences data must be imported by an area risk assessment tool, such as ARIPAR for instance. In this case a grid covering the geographical area of interest is generated on which the risk value is calculated by combining the results of the consequence assessment models with meteorological data, population distribution, and other relevant information. Also in this case, there could be the necessity to export the risk map, which can be done either using a sampling method or using risk contours. In both cases the comparison of risk maps (very useful to verify the risk variation in a given area over time) requires the use of interpolation methods.

Several interpolation methods can be found in the open literature. In the present study seven different methods have been tested and results are provided in section 3. The work was limited to the

interpolation of (risk, effect) contours, since the interpolation of sparse data on a grid are well known and commonly used in Geographic Information Systems.

## 2.4 Example of exchange data format between pool fire models

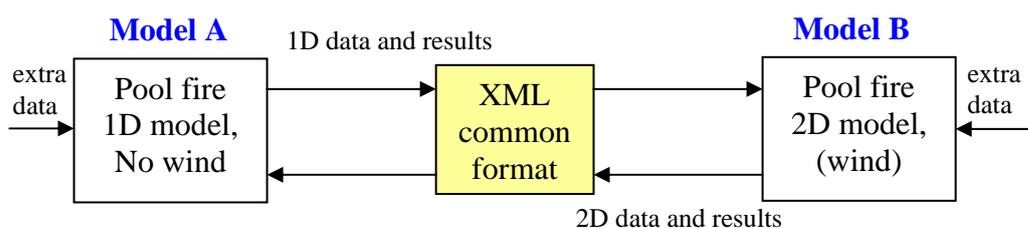
The XML format described above was applied to some test cases to show the feasibility of the proposed approach and to identify possible new problems. The first test concerned the interoperability between two different pool fire models. The availability of the source codes allowed us to perform a complete test, i.e. a two-way data exchange operations by implementing the import-export modules in XML.

The two selected models were:

- First model: 1D model [3]
- Second model: 2D model [4]

The first model is much less sophisticated than the second, as it does not consider the influence of the wind on the flame tilt.

The scheme provided in Figure 2 shows that one model can be run by using the input data exported by the other model and vice-versa.



**Figure 3: Diagram showing the exchange of data between 1D and 2D pool fire models**

Table 2 contains the list of data used by the two models. Differences in input data must be addressed by the user. In this report, these types of data are referred to as “extra data” as shown in Figure 3.

The software created to implement this trial was linked to a specific database on substances. This was done in order to perform an automatic uploading of the substance data requested by the model. By selecting the substance, some associated data are extracted from the database and displayed in the model interface. Other data (e.g. CAS number, molecular weight), are also extracted from the database and stored in the XML input file without being displayed on the model interface.

The developed XML import module automatically converts data from the unit measure, say UMA, used in the first model, to the unit measure, say UMB, used in the second model. To this aim, the file UM\_Conversion.xml was prepared containing the conversion factors from two different systems.

In practice, the conversion is performed in two phases:

- Conversion from UMA to the International Standard System;
- Conversion (if any) from the International Standard System to UMB.

In Figure 4 an extract from the UM\_Conversion.xml file is provided to show its structure. The access to this XML file can be done either using the unit string (UM\_Engineering\_unit) or using the index. Figure 5 shows the user interface developed for the 1D model. The results of the 1D model are displayed on a plot giving the radiation intensity vs. distance from the edge of the pool. Due to the

difficulty to exactly match the data of different models, the possibility to enter extra data has been considered. In Figure 5 extra data are highlighted in green background colour (see e.g. radiation efficiency).

**Table 2: Data required in the 1D and 2D pool fire models**

Data	1D model	2D model
Substance	X	X
Heat of combustion [kJ/kg]	X	X
Heat of vaporization [kJ/kg]	X	X
Specific heat capacity (kJ/(kg K))	X	X
Boiling point temperature [K]	X	X
Ambient temperature [°K]	X	X
Density of ambient air [kg/m <sup>3</sup> ]	X	X
Relative humidity [%]	X	X
Pool diameter [m]	X	X
Radiation efficiency	X	
Combustible density in vapour phase (kg/m <sup>3</sup> )		X
Partial pressure of saturated water vapour (Pa)		X
Mass of air per unit mass of combustible		X
Emission power (kW/m <sup>2</sup> )		X
Air viscosity (Pa s)		X
Wind velocity (m/s)		X
Angle target - ground (rad)		X
Wind direction (rad)		X
Flame surface temperature (K)		X

The XML file exported by the 1D model containing both the input data set and the results of the calculations are represented in Figure 6.

```

<?xml version="1.0" ?>
- <UM_Conversion>
- <Length Engineering_unit="m" Conversion_factor="1." Index="5">
  <UM Engineering_unit="Å" Conversion_factor="1.e-10" Index="0" />
  <UM Engineering_unit="in." Conversion_factor="0.02540" Index="1" />
  <UM Engineering_unit="ft" Conversion_factor="0.3048" Index="2" />
  <UM Engineering_unit="yd" Conversion_factor="0.9144" Index="3" />
  <UM Engineering_unit="mi" Conversion_factor="1609." Index="4" />
</Length>
- <Area Engineering_unit="m2" Conversion_factor="1." Index="17">
  <UM Engineering_unit="barn" Conversion_factor="1.e-28" Index="10" />
  <UM Engineering_unit="in.2" Conversion_factor="6.452e-4" Index="11" />
  <UM Engineering_unit="ft2" Conversion_factor=".09290" Index="12" />
  <UM Engineering_unit="yd2" Conversion_factor=".8361" Index="13" />
  <UM Engineering_unit="acre" Conversion_factor="4047." Index="14" />
  <UM Engineering_unit="hectare" Conversion_factor="10000." Index="15" />
  <UM Engineering_unit="mi2" Conversion_factor="2.590e6" Index="16" />
</Area>
- <Volume Engineering_unit="m3" Conversion_factor="1." Index="29">
  <UM Engineering_unit="in.3" Conversion_factor="1.639e-5" Index="20" />
  <UM Engineering_unit="U.S. fluid ounce" Conversion_factor="2.957e-5" Index="21" />
  <UM Engineering_unit="quart" Conversion_factor="9.464e-4" Index="22" />
  <UM Engineering_unit="L" Conversion_factor="1.e-3" Index="23" />
  <UM Engineering_unit="U.S. gallon" Conversion_factor="3.785e-3" Index="24" />
  <UM Engineering_unit="ft3" Conversion_factor=".02832" Index="25" />
  <UM Engineering_unit="barrel" Conversion_factor=".1590" Index="26" />
  <UM Engineering_unit="yd3" Conversion_factor=".7646" Index="27" />
  <UM Engineering_unit="mi3" Conversion_factor="4.168e9" Index="28" />
</Volume>

```

**Figure 4: Extract from the UM\_Conversion.xml file.**

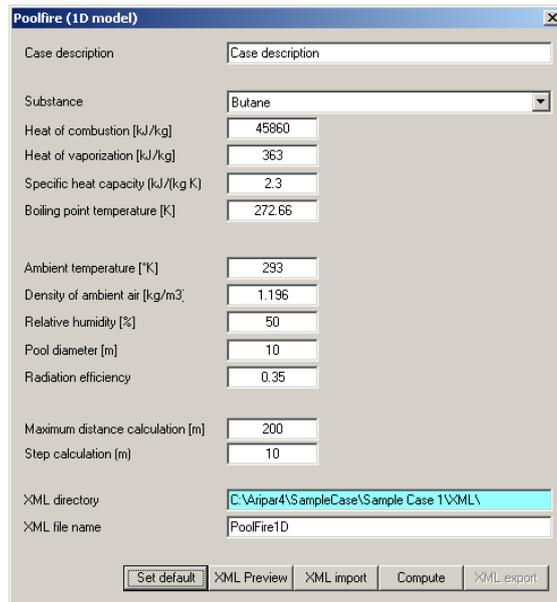


Figure 5: Interface of the 1D pool fire model-

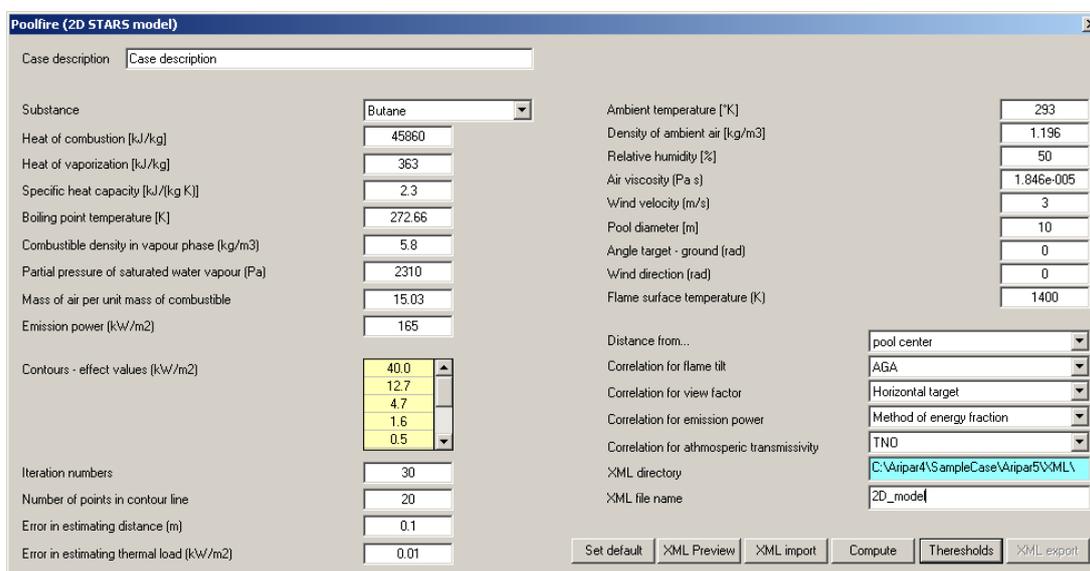
```

<?xml version="1.0" encoding="UTF-8" ?>
- <consequence_analysis accident_category="fire" accident_type="poolfire" software="PoolFireROTA">
- <input rev="1.0">
- <computing_data>
  <max_distance UM="m">200.000000</max_distance>
</computing_data>
- <chemical_physical_properties>
  <substance_boiling_temperature UM="K">272.660000</substance_boiling_temperature>
  <substance_specific_heat UM="kJ/(kg K)">2.300000</substance_specific_heat>
  <substance_evaporation_heat UM="kJ/kg">363.000000</substance_evaporation_heat>
  <substance_combustion_heat UM="kJ/kg">45860.000000</substance_combustion_heat>
</chemical_physical_properties>
- <source_terms>
  <fraction_combustion_heat_radiated UM="%">35.000000</fraction_combustion_heat_radiated>
  <pool_diameter UM="m">10.000000</pool_diameter>
</source_terms>
- <meteo_data>
  <ambient_air_density UM="kg/m3">1.196000</ambient_air_density>
  <ambient_relative_humidity UM="%">50.000000</ambient_relative_humidity>
  <ambient_temperature UM="K">293.000000</ambient_temperature>
</meteo_data>
- <substance_identification>
  <CAS_number>106-97-8</CAS_number>
  <substance_name>Butane</substance_name>
</substance_identification>
- <case_study_identification>
  <case_study_description>Case Description</case_study_description>
</case_study_identification>
</input>
- <output distance_from="edge_pool" number_effect_data="1">
- <number_effect_data01 coordinate_system="cartesian" UM_coordinate1="m" UM_coordinate2="kW/m2" number_points="21" representation="1D">
  <point coordinate1="0.000000" coordinate2="13.598477" />
  <point coordinate1="10.000000" coordinate2="10.892113" />
  <point coordinate1="20.000000" coordinate2="7.763642" />
  <point coordinate1="30.000000" coordinate2="5.401105" />
  <point coordinate1="40.000000" coordinate2="3.825262" />
  <point coordinate1="50.000000" coordinate2="2.792376" />
  <point coordinate1="60.000000" coordinate2="2.102373" />
  <point coordinate1="70.000000" coordinate2="1.627676" />
  <point coordinate1="80.000000" coordinate2="1.291028" />
  <point coordinate1="90.000000" coordinate2="1.045450" />
  <point coordinate1="100.000000" coordinate2="0.861732" />
  <point coordinate1="110.000000" coordinate2="0.721204" />
  <point coordinate1="120.000000" coordinate2="0.611596" />
  <point coordinate1="130.000000" coordinate2="0.524626" />
  <point coordinate1="140.000000" coordinate2="0.454568" />
  <point coordinate1="150.000000" coordinate2="0.397373" />
  <point coordinate1="160.000000" coordinate2="0.350118" />
  <point coordinate1="170.000000" coordinate2="0.310658" />
  <point coordinate1="180.000000" coordinate2="0.277390" />
  <point coordinate1="190.000000" coordinate2="0.249098" />
  <point coordinate1="200.000000" coordinate2="0.224848" />
</number_effect_data01>
</output>
</consequence_analysis>

```

Figure 6: XML file for the 1D pool fire model

In Figure 7 the user interface of the 2D pool fire model is presented. The XML file of the 2D model is given in Figure 8. Also in this case the results are given in the form of closed lines (contour) representing the same effect value for each point in a polar coordinates system. In this case, for the sake of simplicity, only part of the first contour is given.



**Figure 7: Interface of the 2D pool fire model**

In general, it is possible to run the 1D-model by using the input data from the 2D-model XML file, and vice versa as shown in the diagram reported in Figure 3. This first test was a first opportunity to draw our attention on several problems concerning the use of common data formats. Some of these problems were immediately addressed, whilst a few others required some extra efforts and dedicated study. For instance the problem of the choice of which model parameters are to be stored in the XML file is still an open issue.

Some other tests have been carried out using PHAST, EFFECTS and ALOHA, which are well know tools (commercial and freeware) in the field of consequence analysis. Unfortunately due to the unavailability of the source codes for these tools, it was not possible to carry out a two-way test.

For this reason it was decided to perform a one-way transfer of data from the output of these tools (i.e., consequence profiles) to another tool for risk analysis. In particular, the consequence damage curves calculated by the consequence analysis tools where suitably transformed in a XML format and used as input data for ARIPAR, an area risk assessment tool which makes use of consequence data. Such a test was successful as described in Section 4, where some more specific information is given.

As one of the necessary steps for the comparison between two different models is the transposition of their results into the same spatial grid, the next section addresses the problem of interpolating consequence assessment results and their representation on a 2D grid.

```

    <?xml version="1.0" encoding="UTF-8" ?>
- <consequence_analysis accident_category="fire" accident_type="poolfire" software="PoolFireSTARS">
- <input rev="1.0">
- <geometry>
  <angle_fire_target UM="rad">0.000000</angle_fire_target>
  </geometry>
- <parameters>
  <vapor_water_pressure UM="Pa">2310.000000</vapor_water_pressure>
  </parameters>
- <chemical_physical_properties>
  <substance_density_in_vapour_phase UM="kg/m3">5.800000</substance_density_in_vapour_phase>
  <substance_boiling_temperature UM="K">272.660004</substance_boiling_temperature>
  <substance_specific_heat UM="kJ/(kg K)">2.300000</substance_specific_heat>
  <substance_evaporation_heat UM="kJ/kg">363.000000</substance_evaporation_heat>
  <substance_combustion_heat UM="kJ/kg">45860.000000</substance_combustion_heat>
  </chemical_physical_properties>
- <source_terms>
  <flame_temperature UM="k">1400.000000</flame_temperature>
  <flame_emissive_power UM="kW/m2">165.000000</flame_emissive_power>
  <air_substance_mass_ratio>15.030000</air_substance_mass_ratio>
  <pool_diameter UM="m">10.000000</pool_diameter>
  </source_terms>
- <meteo_data>
  <wind_direction_from_N UM="rad">0.000000</wind_direction_from_N>
  <wind_speed UM="m/s">3.000000</wind_speed>
  <air_viscosity UM="Pa s">1.840000e-005</air_viscosity>
  <ambient_air_density UM="kg/m3">1.196000</ambient_air_density>
  <ambient_relative_humidity UM="%">50.000000</ambient_relative_humidity>
  <ambient_temperature UM="K">293.000000</ambient_temperature>
  </meteo_data>
- <substance_identification>
  <CAS_number>106-97-8</CAS_number>
  <substance_name>Butane</substance_name>
  </substance_identification>
- <case_study_identification>
  <case_study_description>Case description</case_study_description>
  </case_study_identification>
</input>
- <output distance_from="edge_pool" number_effect_data="5">
- <number_effect_data01 coordinate_system="polar" iso_value="40.000000" UM="kW/m2" UM_coordinate1="rad"
  UM_coordinate2="m" number_points="100" representation="2D">
  <point coordinate1="-1.570800" coordinate2="6.317039" />
  <point coordinate1="-1.507968" coordinate2="6.317039" />
  <point coordinate1="-1.445136" coordinate2="6.317039" />
  <point coordinate1="-1.382304" coordinate2="6.317039" />
  <point coordinate1="-1.319472" coordinate2="6.317039" />
  <point coordinate1="-1.256640" coordinate2="6.317039" />
  <point coordinate1="-1.193808" coordinate2="6.317039" />
  <point coordinate1="-1.130976" coordinate2="6.317039" />
  <point coordinate1="-1.068144" coordinate2="6.317039" />
  <point coordinate1="-1.005312" coordinate2="6.317039" />
  <point coordinate1="-0.942480" coordinate2="6.317039" />
  <point coordinate1="-0.879648" coordinate2="6.317039" />
  <point coordinate1="-0.816816" coordinate2="6.317039" />
  <point coordinate1="-0.753984" coordinate2="6.317039" />
  .....
  </number_effect_data01>

```

Figure 8: Part of the XML for the 2D pool fire model

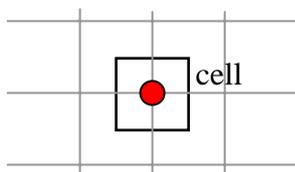


### 3. INTERPOLATION OF RESULTS OF CONSEQUENCE MODELS INTO A GRID

The comparison of the outcome of different models can be performed in different ways according to the type of output. For 1D-models, the comparison can be simply and directly performed on a Cartesian plan. The situation changes when 2D-models are involved. In this section, we consider the case in which two models, which outcome is expressed in the form of effect contours, have to be compared. These contours represent the points in the 2D area where the accident effect (i.e. thermal radiation, overpressure, toxic concentration) has the same value. The interpolation aims at determining the effect values in each cell of a grid that is supposed to represent the physical area where the accident effect takes place. In general, the grid dimension can be automatically determined from the maximum distance of the effects on the basis of the user defined grid cell dimension. Grid cells are squared.



Note that for the sake of simplicity the generic interpolated effect value will be represented on the intersection of horizontal and vertical lines, which is considered as the centre of the cells, as shown in the following figure.



Several interpolation methods are available in the open literature. However, by considering the typical distribution of accident consequence data as effect-contours, only a selected number of methods have been tested. In particular:

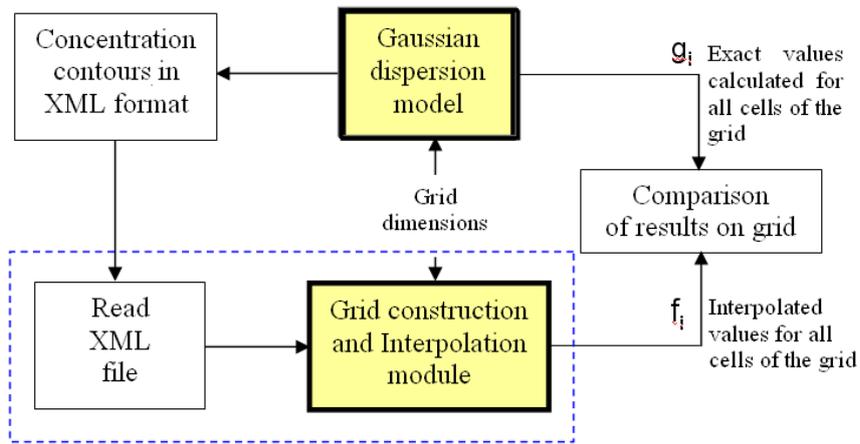
- 1 Inverse Distance to a Power;
  - 2 Linear;
  - 3 Cubic Spline.
1. The Inverse Distance to Power is very much appropriate to interpolate data on a sparse array, typical of environmental-related problems, risk mapping included. The extent to which they are also suitable to interpolate consequence assessment data has been verified and the results are hereunder presented.
  2. Linear interpolation is always applicable independently of the number of known points. In particular this method gives always conservative results: the entity of the error introduced depends on the number of known points and on their distribution in the range of interest.

3. Cubic Spline is a method that allows representing the interpolation between points by means of a 3<sup>rd</sup> order polynomial. Due to the monotonic behaviour of consequence data some abnormal behaviour of the Cubic spline must be avoided; for this reason a variation of the cubic spline, referred to as Constrained Cubic Spline, was also considered in the study.

A special test was designed to analyse the effectiveness and appropriateness of the above methods on a practical case. In general, the values produced by the accident consequence models are either distributed on a downwind central line (1D-model) or as contour lines (2D-model). The former can always be seen as a 2D-model with concentric contours. For this reason both types of models can be treated in the same way. The grids constructed for such an application were characterised by squared-cells. The original data, representing effect contours were contained in the XML file. Specifically, these data consisted of the position of the contours' points expressed by their coordinates: Polar or Cartesian.

For the test purpose, the reference accident scenario was an Ammonia release. The applied procedure is depicted in

Figure 9. A Gaussian analytical dispersion model was applied to determine the Ammonia ground concentration. The model output, which is exported in XML format, was represented as a number of contour lines for different effect values (concentration in mg/m<sup>3</sup>). These data were uploaded to the Grid-interpolation module to generate the reference grid and to compute the concentration values in each cell by interpolating the contour values. Finally, the interpolated values in each cell were compared with the exact values obtained by running the Gaussian model for all cells of the grid.



**Figure 9: Diagram showing the experimental phases to verify the suitability of the selected interpolation methods.**

In order to check the accuracy of the interpolation method applied, the following coefficients were calculated:

$$D^+ = \sum_{i=1}^N \frac{f_i - g_i}{g_i} 100 \quad (\text{if } f_i > g_i) \quad (1)$$

$$D^- = \sum_{i=1}^N \frac{g_i - f_i}{g_i} 100 \quad (\text{if } f_i < g_i) \quad (2)$$

$$D = D^+ + D^- \quad (3)$$

where  $f_i$  is the interpolated value in the  $i$ -th cell,  $g_i$  is the exact value obtained analytically and  $N$  is the total number of cells of the grid. Eq. (3) is equivalent to take the absolute values of the difference between  $f_i$  and  $g_i$ . The values  $D^+$  and  $D^-$  are separately calculated to allow judging the degree of conservativeness of the interpolation method applied.

### 3.1 Gaussian Model

As previously mentioned, the test was conducted using a Gaussian dispersion model. For this specific purpose, a special module for Gaussian gas dispersion [4] was built. Figure 10 shows the user interface of this module. The module was constructed in such a way that the user can define different effect values, i.e. different contours. In addition the user can select the distance between two consecutive points on each contour, which provides a measure of the density of the known points. The module allows also calculating the centreline concentration in the down-wind direction. The input data and the output results are exported as an XML file according to the format previously described.

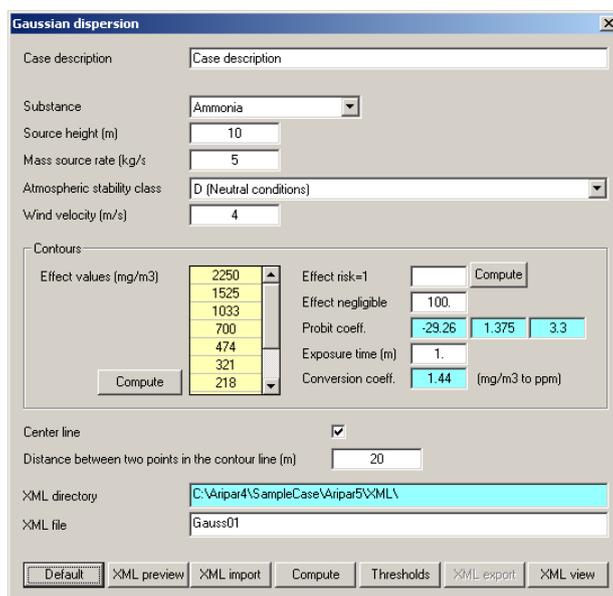


Figure 10: User interface of the Gaussian model

### 3.2 Reference Scenario

The accident scenario selected for assessing the different interpolation methods is a continuous release of Ammonia at a rate of 5 kg/s, from a height of 10m. The atmospheric parameters used for the calculations are as follows:

- Pasquill atmospheric stability: D (neutral)
- wind velocity of 4 m/s.

Nine different concentration contours were considered for calculation:

- 2250 mg/m<sup>3</sup>
- 1525 mg/m<sup>3</sup>
- 1033 mg/m<sup>3</sup>
- 700 mg/m<sup>3</sup>
- 474 mg/m<sup>3</sup>
- 321 mg/m<sup>3</sup>
- 218 mg/m<sup>3</sup>
- 148 mg/m<sup>3</sup>
- 100 mg/m<sup>3</sup>

These contour values have been selected by dividing the two extreme values, namely the maximum threshold value of 2250 mg/m<sup>3</sup> and the minimum threshold value of 100 mg/m<sup>3</sup>, as equidistant points on a logarithmic scale. The maximum concentration corresponds to risk 1, i.e. to 100% lethality. This value can be automatically calculated by using the Probit for the selected substance or manually given in the input data set.

### 3.3 Grid Generation and Interpolation Module

At this stage of the feasibility study it was decided to develop a specific software module intended to import data from a generic consequence assessment tool, generate the reference grid, and interpolate the model results on the grid. In particular, this module was created with the following objectives:

- 1) to read the XML file with the input/output of the consequence analysis,
- 2) to generate the grid,
- 3) to interpolate the concentration contours on a 2D grid using one of the above listed methods.

The grid with the interpolated values was exported as a binary file to minimise the memory requirements for the comparison phase.

The user interface of this module is shown in Figure 11, where the user can insert the main grid data and select one of the seven interpolation methods, four of which are variations of the Inverse Distance to a Power method. In particular the following input information can be edited:

- the source directory containing the XML input file;
- the XML file to be converted;
- the destination directory containing the output file (grid with interpolated values);
- the cell dimension.

The buttons “XML preview”, “Generate grid” and “Show grid” are self explaining

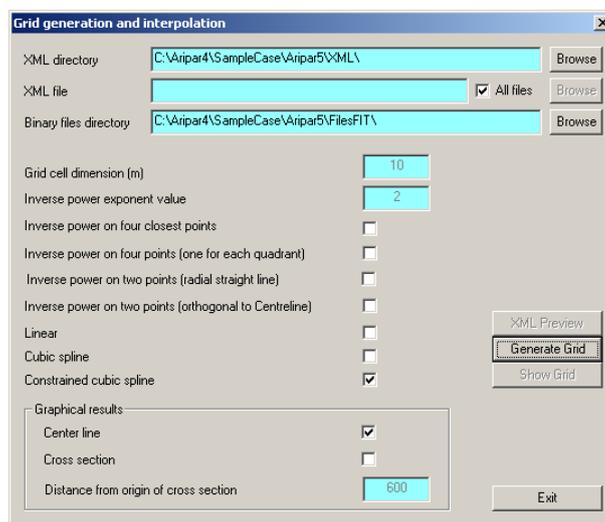
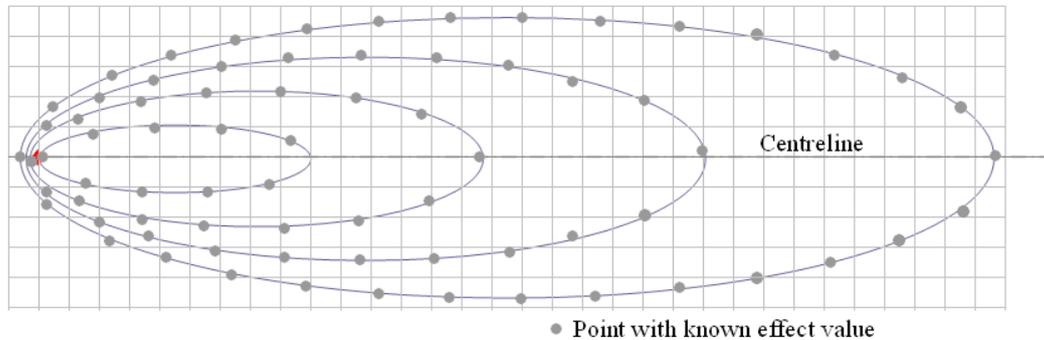


Figure 11: User interface of the grid generation and interpolation module

Very often the output of the tools for accident consequence calculations is represented as points distributed on *n* contours. An example is given in the figure below, which shows the simple case of four contours without data on the centreline. Data are equally spaced on contours. Each point is characterised by its x, y coordinates and, by definition, their associated value for the effect depend on the contour to which they belong, i.e. points located on the same contour have the same effect value.

The aim of the interpolation routine is to assign an effect value to each cell of the grid. The accuracy of the fitting operation is measured by the cumulative error quantified in terms of the parameters  $D^+$ ,  $D^-$  and  $D$ , previously defined in equations 1-3.



From a first analysis of the distribution of data as shown in the above figure, the following general considerations can be drawn:

- interpolation is strongly influenced by the number of available contours and the distance between *known points* in a contour, which define the density of points available (the distance between point is an input parameter);
- the available values that constitute the model output (“known points”) are not necessarily positioned at the centre of grid cells;
- the concentration of known points is denser in proximity to the accident source and, therefore, the number of unknown points to be interpolated increases with the distance from the accident source;
- known points are always positioned on contours; points belonging to the same contour have same effect value;
- the availability of data on the centreline generally reduces the interpolation error.

In order to visually compare  $f$  (interpolated values) and  $g$  (true values), a routine has been developed to graphically display the centreline and cross sections at different distances from the accident source’s position. In the present test, the selected distance values were: 100m, 200m, 300m, 600m and 900m. To be noted that, in the present example, the minimum concentration on the centreline is at 1,100m.

### 3.4 Inverse Distance to a Power

The inverse distance to a power (IDP) is a well known interpolation method which is typically used for GIS related application to interpolate 2D sparse data. It is used here to see to what extent it could be applied to interpolate grid data from effect-contours.

The basic procedure for determining the value at an unknown point (centre of a cell of the grid) given  $m$  data spatially distributed is as follows:

$$E_x = \frac{\sum_{i=1}^m \frac{E_i}{d_{ix}^\alpha}}{\sum_{i=1}^m \frac{1}{d_{ix}^\alpha}} \quad (4)$$

where:

$E_x$  is the interpolated grid node value;  
 $E_i$  is the neighbourhood  $i$ -th known value;  
 $d_{ix}$  is the geometric distance between the node  $x$  and the  $i$ -th known value;  
 $\alpha$  is the weighting power parameter;  
 $m$  is the number of considered neighbourhood points.

The value to assign to the parameters  $\alpha$  and  $m$  depends on the specific problem, on the distribution of known values, etc. The higher is  $m$  the more accurate is the interpolated value, but at the same time the higher is the computation time. Typical values are  $\alpha = 2$  and  $2 \leq m \leq 4$ .

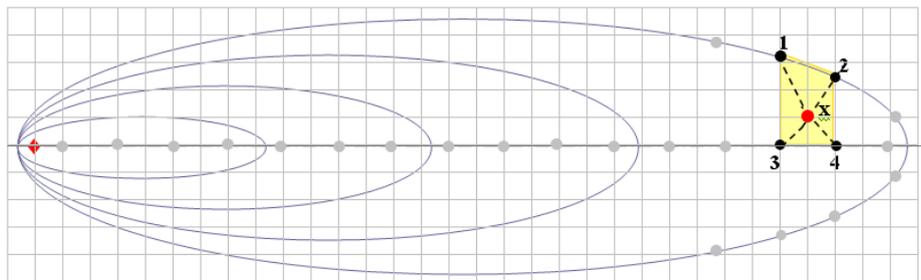
It can easily be seen from eq. (4) that, independently of the values  $d$ ,  $\alpha$  and  $m$ , if the values  $E_i$  are all equal, i.e. if  $E_i = E$  for any  $i$ , then  $E_x = E$ . This will be clearly explained in the examples described in this section.

### 3.4.1 Inverse distance from 4 closest points (ID4)

In this method equation (4) is applied with  $n = 4$  and  $\alpha = 2$  to all unknown points. Note that in what follows generally the known points represented in figures are only those necessary to explain the interpolation methods.

Depending on the position of the four closest points and the availability of data on the centreline, the interpolated results can be greater than or less than the exact value. Some examples are described below.

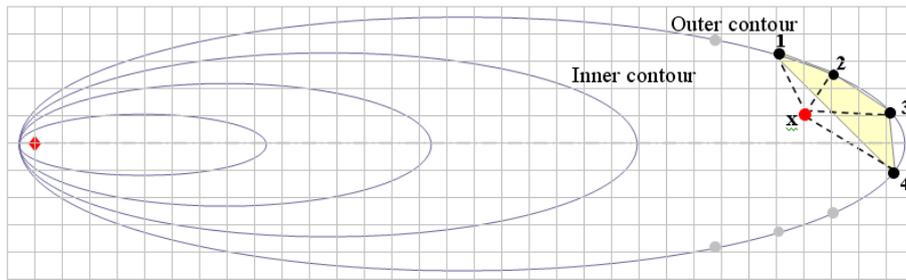
Let's consider first the case in which the centreline data are available, as shown in Figure 12 and suppose that the value at point  $x$  has to be determined from the values of the four closest points. Two out of four points closest to  $x$  are on the centreline in which the effect is higher than the effect on the contour. The value for  $x$  is obtained from equation (4) resulting in a value that is smaller than the value at points 3-4 and greater than the values at points 1-2, i.e.  $E_3 = E_4 > E_1 = E_2 \Rightarrow E_2 < E_x < E_3$



**Figure 12: Centreline available, interpolation based on the closed 4 points**

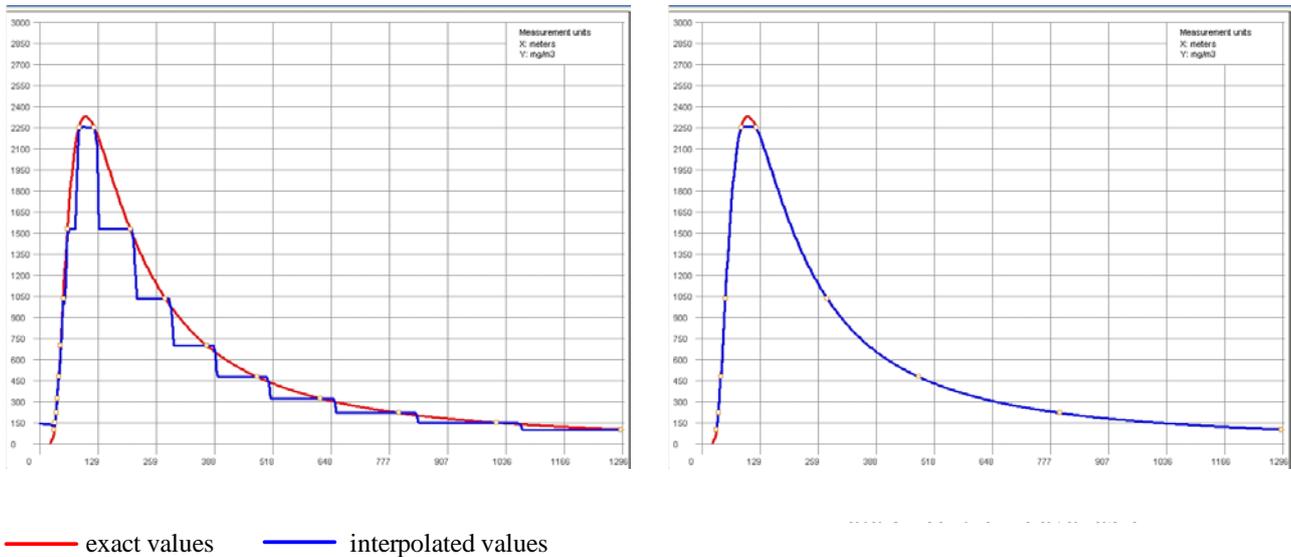
Let's suppose now that the centreline is missing (Figure 13). In this case the four points closest to  $x$  are 1-2-3-4. As they are on the same contour they have the same value. Hence the value on  $x$  will be equal to the contour line value, i.e.  $E_1 = E_2 = E_3 = E_4 = E \Rightarrow E_x = E$

Consequently, all  $x$  points whose distance from the inner contour points is greater than the points on the outer contour have the same value. In this case the interpolated grid shows a flat area, i.e. non conservative values. The extension of the flat area becomes larger as the number of contours decreases and the distance between points on contours increases.



**Figure 13: Centreline not available, interpolation from the closed 4 points**

The following figures show the interpolated and the exact values on the centreline when the data to be interpolated contain the known points on the centreline (right) and when such points are not available (left). The flat areas are visible in the latter case only.



**Figure 13: Representation of the interpolated values on the centre line using the ID4 interpolation method. Left: data on centreline not available; Right: data on centreline available**

This interpolation method has been applied to the following cases:

- Number of contours: 9; distance between points: 4m
- Number of contours: 9; distance between points: 20m
- Number of contours: 5; distance between points: 4m
- Number of contours: 5; distance between points: 20m

Due to the poor results that were obtained for the case of absence of data on the centreline, the tests were completed only for the cases in which data on the centreline were available. Table 3 shows the results of these tests in terms of  $D$ ,  $D^+$  and  $D^-$  for the above listed cases.

**Table 3. Comparison of the D-parameters for different cases using the ID4 method**

Number of Contours(n)-Data Points Distance (m)			
9-4	9-20	5-4	5-20
$D^+ = 1.79 \%$ ;	$D^+ = 1.70 \%$ ;	$D^+ = 3.71 \%$ ;	$D^+ = 2.47 \%$ ;
$D^- = 3.33 \%$ ;	$D^- = 3.46 \%$ ;	$D^- = 6.79 \%$ ;	$D^- = 4.32 \%$ ;
$D = 5.12 \%$	$D = 5.16 \%$	$D = 10.50 \%$	$D = 6.79 \%$

Looking at the results it can be noticed that the maximum absolute error is about 10%, which is sufficiently small for practical applications. However the  $D^-$  value is too high compared with  $D^+$ , which means that the resulting concentration grid is not conservative. For this reason the ID4 method cannot be considered as suitable for interpolating contour lines.

### 3.4.2 Inverse distance from 4 points located in a local Cartesian plane (ID4X)

Inverse distance from 4 points located in a local Cartesian plan is similar to the previous method but differs from it for the selection criteria of the 4 points. More precisely, given a point  $x$  where the interpolation has to be calculated, instead of selecting the four closest points,  $x$  is taken as the origin of a hypothetical Cartesian plan and the four closest points are taken one from each quadrant.

In the previous section it was verified that the presence of the centreline reduces significantly the interpolation error. The tests carried out with the current method led to the same conclusion: without the centreline the interpolated values are not acceptable. Consequently, also for this case only the tests with data on the centreline are here presented. Figure 14 a) shows the four points taken from the four different quadrants, which are used to determine the value to assign to  $x$ .

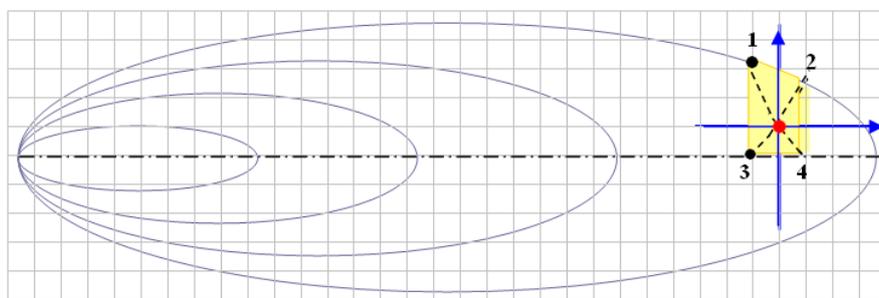


Figure 14 a): Interpolation from the closed 4 points belonging to different Cartesian quadrants

It may happen that for points close to the largest contour (i.e. with the lowest concentration value) one of the quadrant falls outside the contour area, where the effect is considered nil. In these cases only three points are used for determining the value at the  $x$  location, as shown in Figure 14 b).

It may also happen that one axis crosses a known point: in this case the point is considered as belonging to both quadrants. See for instance in Figure 14 b) the point 3-4 for the determination of the effect at point  $y$ .

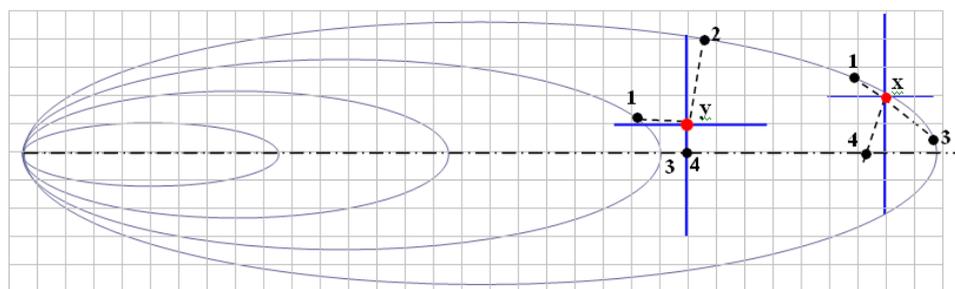


Figure 14 b): Special cases.  $x$  with no points in one of the four quadrants;  $y$  with same point in both quadrants

The results of the test for this interpolation method are summarised in the following Table.

**Table 4. Comparison of the D-parameters for different cases using the ID4X method**

Number of Contours(n)-Data Points Distance (m)			
9-4	9-20	5-4	5-20
$D^+ = 0.65 \%$ ;	$D^+ = 1.39 \%$ ;	$D^+ = 1.08 \%$ ;	$D^+ = 1.40 \%$ ;
$D^- = 2.29 \%$ ;	$D^- = 2.86 \%$ ;	$D^- = 4.31 \%$ ;	$D^- = 3.98 \%$ ;
$D = 2.95 \%$	$D = 4.25 \%$	$D = 5.39 \%$	$D = 5.38 \%$

By comparing the results obtained with those of the previous method, it is clear that the current approach is noticeably more accurate. This is probably due to the typical spatial distribution under analysis (plume-type), which can be better interpolated by considering neighbouring data which have better symmetry with respect to the point to be interpolated.

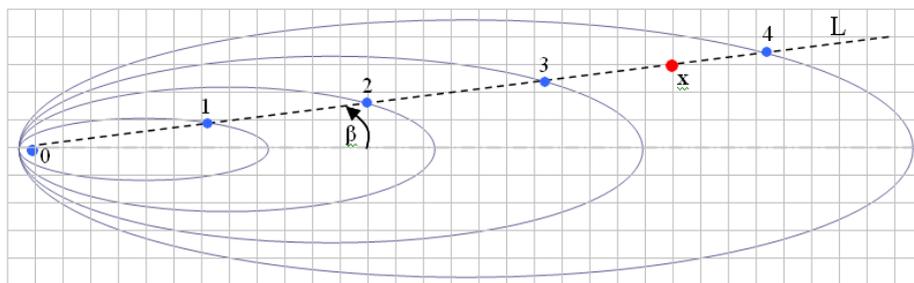
Unfortunately,  $D^-$  error values are still higher than  $D^+$  values, which make also this method not perfectly suitable for this type of applications.

### 3.4.3 Inverse distance with 2 points on a radial straight line (ID2R)

In this method equation (4) is applied to two points only. A straight L line starting from the source of the accident and passing from x is generated, as shown in

Figure 15. The angle  $\beta$  measured between the straight line and the centreline ranges between 0 and 90° because of the symmetry of the contours. The line L intersects all contours. The value at x is obtained applying equation (4) to points 3 and 4.

Differently from the two previous methods, the presence of data on the centreline is not that relevant for interpolation purposes. Indeed this is nothing but the line at  $\beta = 0$ .



**Figure 15: Inverse power with two points on a radial straight line**

Also in this case, the combinations of 9 and 5 contours together with variable density of data points (i.e. 4m and 20m distant) were considered. The results are summarised in the following Table.

**Table 5. Comparison of the D-parameters for different cases using the ID2P method**

Number of Contours(n)-Data Points Distance (m)			
9-4	9-20	5-4	5-20
$D^+ = 2.93 \%$ ;	$D^+ = 5.22 \%$ ;	$D^+ = 7.35 \%$ ;	$D^+ = 9.07 \%$ ;
$D^- = 1.30 \%$	$D^- = 1.41 \%$	$D^- = 1.89 \%$	$D^- = 1.85 \%$
$D = 4.23 \%$	$D = 6.64 \%$	$D = 9.24 \%$	$D = 10.92 \%$

During the tests it was noticed that the present method gives good conservative results especially when the interpolated point lies between two contours which are at a certain distance from each other. In order to support this statement, the following test was performed. It consisted of removing two contours from the 9-4 case. In particular the 7<sup>th</sup> (218 mg/m<sup>3</sup>) and the 8<sup>th</sup> (148 mg/m<sup>3</sup>) contours were

removed. This produced a situation in which the last two contours (i.e. 6<sup>th</sup> and 9<sup>th</sup>) were very much spread apart. The interpolation resulted in a conservative behaviour for the cross sections in the range 700-900m. This fact also appeared for the centreline. The overall results provided in Table 5 show certain regularity amongst the different combinations, which was not evident in the previous methods. The error  $D^-$  is also limited to acceptable values (from 17% to 30% of  $D$ ). Definitely this method is more conservative than the previous two as it can be noticed by comparing the corresponding  $D^+$  and  $D^-$  values.

In general this method is less accurate than the ID4X method; nevertheless it represents a more interesting alternative when data on the centreline are not available.

### 3.4.4 Inverse power with 2 points orthogonal to the centreline (ID2O)

Also in this method equation (4) is applied to two points only. In this case, however, a straight L line orthogonal to the centreline and passing from  $x$  is generated, as shown in Figure 16. The line L intersects one or more contours at given points; the value at  $x$  is obtained by applying equation (4) to points 1 and 2.

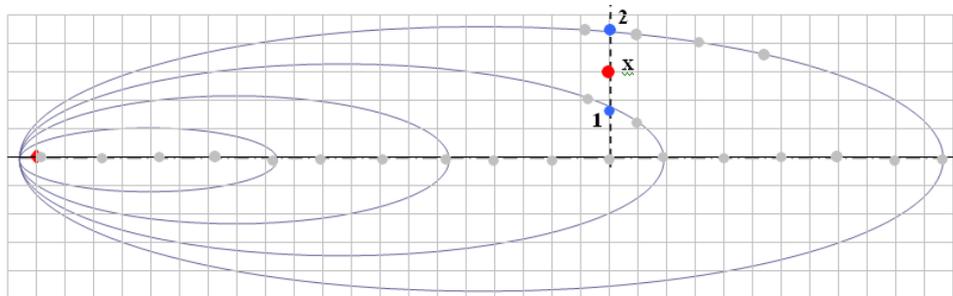


Figure 16: Interpolation using inverse power with 2 points orthogonal to the centre line

It is clear that, for this method, the availability of data on the centreline is essential to obtain acceptable results. The lack of such data would indeed result in large flat areas between the two adjacent contours.

The test was performed for combinations of 9 and 5 contours with 4, 20, 40 and 100m distance points. The results are summarised in the following Table.

Table 6. Comparison of the D-parameters for different cases using the ID2O method

Number of Contours(n)-Data Points Distance (m)					
9-4	9-20	5-4	5-20	5-40	5-100
$D^+ = 0.87 \%$ ;	$D^+ = 4.49 \%$ ;	$D^+ = 1.86 \%$ ;	$D^+ = 5.27 \%$ ;	$D^+ = 11.31 \%$ ;	$D^+ = 42.93 \%$ ;
$D^- = 0.73 \%$ ;	$D^- = 1.59 \%$ ;	$D^- = 0.83 \%$ ;	$D^- = 1.62 \%$ ;	$D^- = 2.09 \%$ ;	$D^- = 2.81 \%$ ;
$D = 1.60 \%$	$D = 6.08 \%$	$D = 2.69 \%$	$D = 6.89 \%$	$D = 13.40 \%$	$D = 45.74 \%$

In general, the absolute values of the interpolation errors ( $D$ ) are even better than previously. As the present method appeared to behave very well for this type of applications, it was decided to explore its accuracy to extreme situations. For this reason it was executed the test with 5 contours also for situations with very low density of data points on the contours (i.e. up to 100m distance between adjacent points). Although the overall absolute error was relatively high for these extreme situations, the low values of  $D^-$  make this method promising for consequence-related applications when the distance between known points is few meters only and the data on the centreline are available.

### 3.5 Linear interpolation

In this method the value at point x to be interpolated is determined by drawing a straight line L connecting the source of the accident to x in a similar way as for the ID2R method. Hence L intersects all contours and the point x will be between two contours.

Let 3 and 4 be the two points as shown in Figure 17. Independently of the fact that 3 and 4 are actual data points or not, their effect value is the same as the value at the contour they belong to. The effect  $E_x$  at point x is then obtained by using the following linear approximation:

$$E_x = E_3 + \frac{E_3 - E_4}{d_3 + d_4} d_3 \tag{5}$$

where  $d_3$  and  $d_4$  are respectively the distances between points 3-x and x-4 and  $E_3, E_4$  are the concentration values on the considered contours. The linear interpolation is schematically shown below.

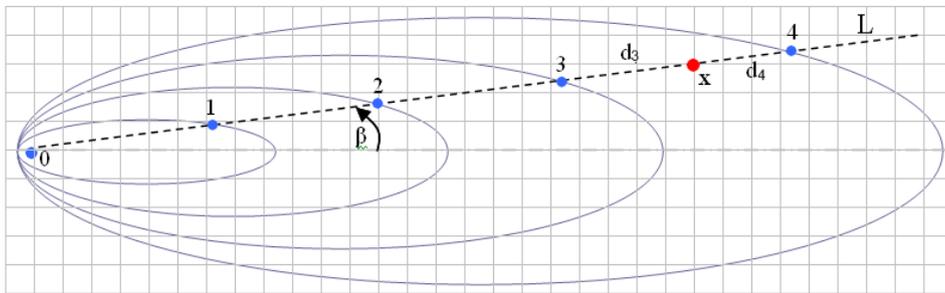


Figure 17: Scheme for Linear Interpolation

The results of the test for different values of the number of contours and density of points show that the linear interpolation is good enough for these applications. As shown in Table 7 also for the 5-40 and 5-100 cases the results are acceptable.

Table 7. Comparison of the D-parameters for different cases using the Linear method

Contours(n)-Data Points Distance (m)					
9-4	9-20	5-4	5-20	5-40	5-100
$D^+ = 2.08 \%$ ;	$D^+ = 2.72 \%$ ;	$D^+ = 7.14 \%$ ;	$D^+ = 7.81 \%$ ;	$D^+ = 9.01 \%$ ;	$D^+ = 14.68 \%$ ;
$D^- = 0.10 \%$ ;	$D^- = 0.15 \%$ ;	$D^- = 0.23 \%$ ;	$D^- = 0.18 \%$ ;	$D^- = 0.13 \%$ ;	$D^- = 0.22 \%$ ;
$D = 2.19 \%$	$D = 2.87 \%$	$D = 7.37 \%$	$D = 7.99 \%$	$D = 9.14 \%$	$D = 14.90 \%$

### 3.6 Cubic Spline and Constrained Cubic Spline interpolation

Similarly to the linear interpolation, in this method the interpolated values are also determined on a straight line L from the source to the point x to be interpolated as shown in Figure 18. The values at the intersection between contours and straight line L determine the known of interest for the application of the Cubic spline method [5].

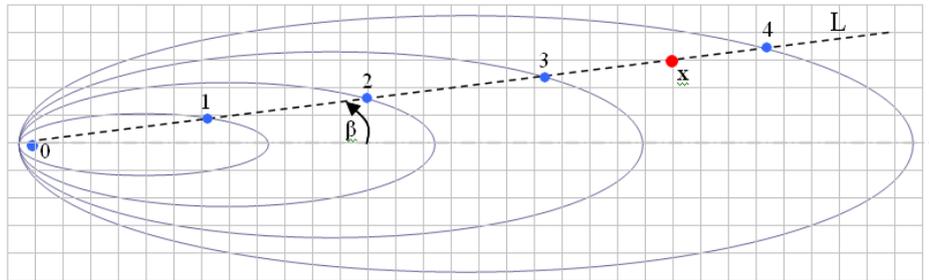
If n is the number of contours, a third order polynomial is constructed for each of the n intervals:

- $x_0 \leq x < x_1$
- $x_1 \leq x < x_2$
- .....
- $x_{n-1} \leq x < x_n$

where  $x_0$  is the accident source point,  $x_1, x_2, \dots, x_n$  are the points in which the line L intersects the contours (e.g. in the figure  $x_0, x_1, x_2, x_3, x, x_4$ )

Points  $x_1, x_2, \dots, x_{n-1}$  are internal points;  $x_0, x_n$  are the end points.

As usually values assigned to points  $x_k$  ( $k > 1$ ) are given by the value on the corresponding contour.

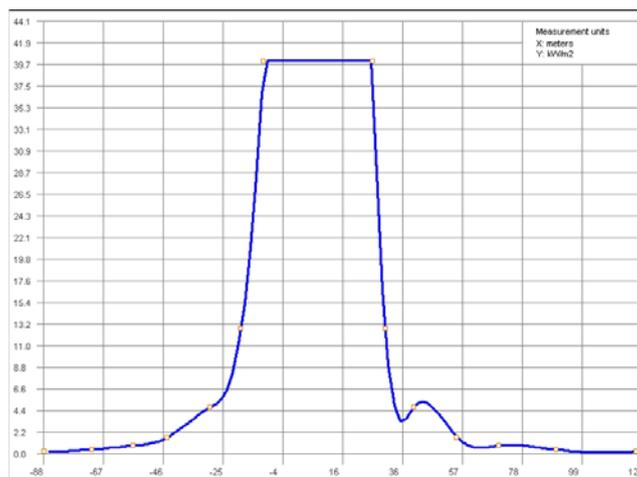


**Figure 18: Interpolation by Cubic Spline**

The Cubic Spline functions fit the  $n$  points with a third degree polynomial satisfying the following conditions:

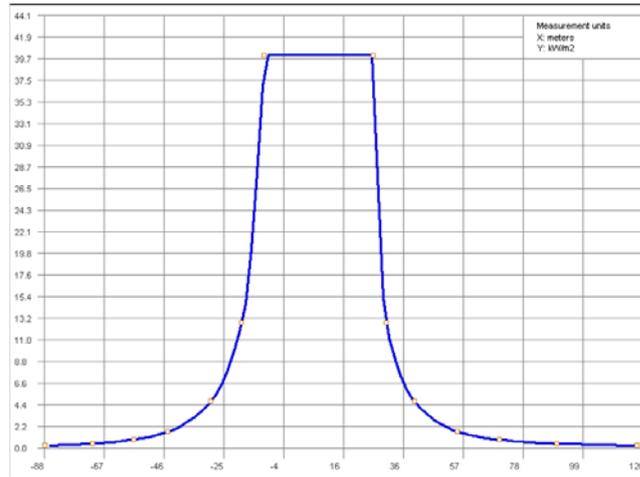
- the polynomial cross all selected points.
- continuity of first and second derivative at all points;
- the first order derivative is the same for functions on the two side of an internal point;
- the second order derivative is the same for functions on the two side of an internal point;
- at the end points the second order derivative is assumed to be zero (Natural spline).

The Cubic Spline method in certain situations may introduce some distortion, e.g. when the first derivative at the extreme points is not selected appropriately. For instance in Figure 19, which represents the downwind cross section of a pool fire, contains some relative minimum points. This behaviour is not followed by the real physical effect of the fire radiation intensity. This is due to the deep slope of the curve and the distance between known points.



**Figure 19: Cubic Spline: pool fire interpolated data showing the typical case of “overshooting”;**

In order to correctly interpolate the known points the “optimum” first order derivative was calculated at the end points. This method, known as “Constrained cubic spline” [6] is particularly suitable for our applications. For instance, Figures 20 show the result of the constrained spline method applied to the pool fire case described above. In this case, the interpolation is very good.



**Figure 20: Constrained Cubic Spline interpolation applied to the pool fire in Figure 19.**

The following Table contains the results of the constrained cubic spline for different cases applied to the Gaussian dispersion data. As can be seen the error is very small also for the extreme case of 5 contours with 100m between points.

**Table 8. Comparison of the D-parameters for different cases using the Constrained Cubic Spline method**

Contours(n)-Data Points Distance (m)					
9-4	9-20	5-4	5-20	5-40	5-100
$D^+ = 0.59 \%$ ;	$D^+ = 1.28 \%$ ;	$D^+ = 1.57 \%$ ;	$D^+ = 2.13 \%$ ;	$D^+ = 3.59 \%$ ;	$D^+ = 10.14 \%$ ;
$D^- = 0.11 \%$ ;	$D^- = 0.23 \%$ ;	$D^- = 0.34 \%$ ;	$D^- = 0.28 \%$ ;	$D^- = 0.34 \%$ ;	$D^- = 0.66 \%$ ;
$D = 0.70 \%$	$D = 1.52 \%$	$D = 1.91 \%$	$D = 2.42 \%$	$D = 3.93 \%$	$D = 10.79 \%$

### 3.7 Comparison of the examined interpolation methods

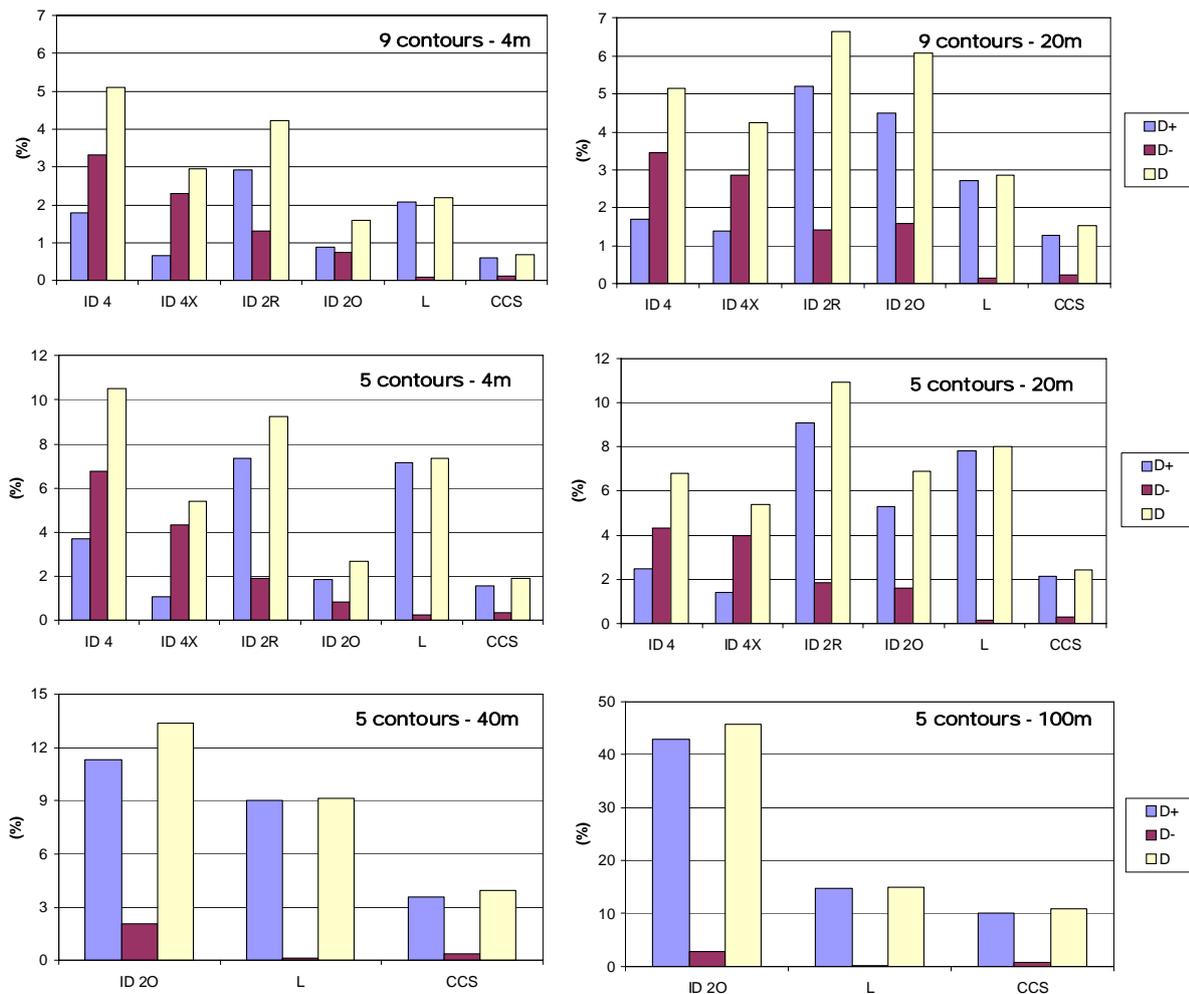
The present section summarises the results of all interpolation tests performed using the different methods applied to the Gaussian dispersion scenario. These results are summarised and graphically represented in Figure 21. Note the different scale of the histograms.

As it is evident from the Figure, methods ID4, ID4X, and ID2R are not applicable to interpolate consequence effect contours because of the high non-conservative error  $D^-$ .

Method ID2O gives acceptable results provided that the distance between points on the effect contours is lower than 5-10 meters. Since usually not all software packages available for consequence calculations satisfy this condition the ID2O method has to be discarded.

The linear method is always applicable even though it could be too conservative when the curve shape is deep and the number of points or contours is limited.

The Constrained cubic spline (CCS) method is the best amongst those submitted to test provided that the number of contours is greater than 5-6 and equally spaced on the logarithmic scale within the range between the maximum and the minimum values of the consequence effect.



**Figure 21. Summary of the results of the interpolation methods applied to the Gaussian dispersion model.**

To further investigate the potential of the CCS interpolation method it was decided to perform another test on a different accident scenario. This consisted of instantaneous heavy gas dispersion, whose consequence effects were calculated by using the commercial software PHAST [7].

Due to the unavailability of the specific format for reading the binary output data produced by PHAST, the test required the development of an ad-hoc software programme designed with the purpose of generating the output file in the proper XML format. This was done by extracting all necessary information from the printout file of PHAST. This XML file was then read by the interpolation module to generate the 2D rectangular grid containing the interpolated values.

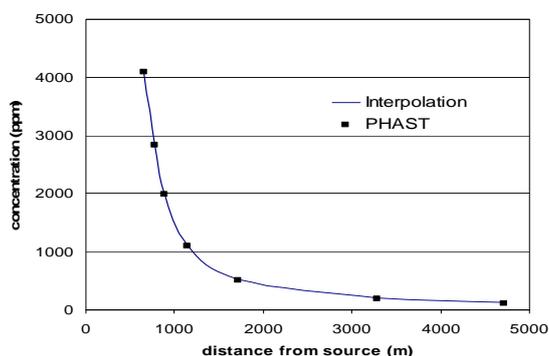
Table 9 contains the centreline concentration values along downwind distance from the source, whereas Table 10 is a sample of concentrations along a cross section at 380m from the source of the release.

In order to check the goodness of fit, the interpolated values have been compared manually with the results of PHAST given in the printout file. This implied the need to read the concentration values on the plot of PHAST; therefore the relative error is also affected by the “imprecise” reading. In spite of this it can be seen that the error is very limited even at larger distances. More specifically, the error is lower at higher concentrations because of the higher amount of data available, whereas it increases with the distance from the source because of the increasing distance between two contours. Indeed the

greater is the distance the greater is the error. However, the error is relatively larger (a few %) at low concentrations, i.e. at distances where the risk values are negligible.

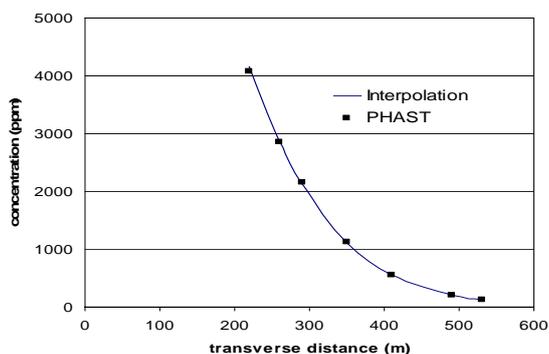
**Table9. Comparison of the interpolated and exact values of ground concentration for a heavy gas continuous release (Centreline).**

x	y	Interpolated concentration value (ppm)	Concentration read on the PHAST plot (ppm)	Relative error (approximated) (%)
660	0	4061.3	4100	-0.95%
770	0	2832.5	2832	0.02%
880	0	2010.1	1990	1.00%
1150	0	1113.0	1099	1.26%
1720	0	520.4	517	0.64%
3290	0	200.8	194	3.39%
4710	0	120.7	116	3.92%



**Table 10. Comparison of the interpolated and exact values of ground concentration for a heavy gas continuous release (Cross section at 380m).**

x	y	Interpolated concentration value (ppm)	Concentration read on the PHAST plot (ppm)	Relative error (approximated) (%)
380	220	4153.1	4075	1.88%
380	260	2877.5	2860	0.61%
380	290	2134.4	2160	-1.20%
380	350	1118.1	1125	-0.62%
380	410	562.0	562	0.01%
380	490	212.1	212	0.02%
380	530	128.3	127	1.02%





## 4. APPLICATION OF THE DATA EXCHANGE FORMAT IN RISK ANALYSIS

As a final test on the use of the XML exchange format, it was decided to develop an interface between the risk assessment tool ARIPAR and different software packages for consequence calculations. ARIPAR is a quantitative risk assessment package developed by the JRC in collaboration other organisations, namely the University of Bologna (DICMA) and the Civil Protection Dept. of the Emilia Romagna Region. ARIPAR is being used to evaluate the risk of major accidents in industrial areas where hazardous substances are stored, processed and transported. The application of ARIPAR requires the quantification in terms of frequency and consequence of all significant accident scenarios in fixed installations and for the transport of dangerous substances [8]. In particular, frequency and consequence data are assessed off-line and uploaded into ARIPAR. Consequence data are normally calculated by using external software and it is therefore necessary to upload these consequence data into ARIPAR by using the appropriate file format.

The present test for interfacing the consequence models with ARIPAR was based on the following procedure, applied to all accident scenarios:

- generation of the XML file from the consequence programs;
- interpolation of the results of effect-contours, thus generating ‘consequence grids’;
- uploading into ARIPAR of the ‘consequence grids’ and computation of the overall area risk.

A series of different commercial and freeware software for consequence assessment were used for this exercise. Specifically the following tools were used:

- PHAST: used to determine the effect of a heavy gas instantaneous release [7];
- EFFECTS: used to determine the effects of an explosion (UVCE) [9];
- ALOHA: applied to the continuous release of heavy gas dispersion [10];
- GAUSS: applied to Gaussian dispersion of continuous releases [4];
- STARS: used to determine the radiation effects of a pool fire (2D model) [4].

Again, in order to transform the different data output of the above models into the defined XML format, it was necessary to develop specific conversion modules, i.e. ad-hoc software programs. In such a way it was possible to generate for each tool an output file perfectly compatible with the uploading input module of ARIPAR, designed to read the XML-based format. The XML files were then transformed into the correspondent consequence effect grid and fed to ARIPAR for risk assessment calculations.

Clearly in order to execute risk calculations, other specific information had to be uploaded into ARIPAR (e.g. frequencies of accidents scenarios, Probit functions to convert the consequence effects to impact on human beings, zoning information (land use), population distribution, transport routes, meteorological data, vulnerability centres).

The overall procedure is schematically represented in Figure 22.

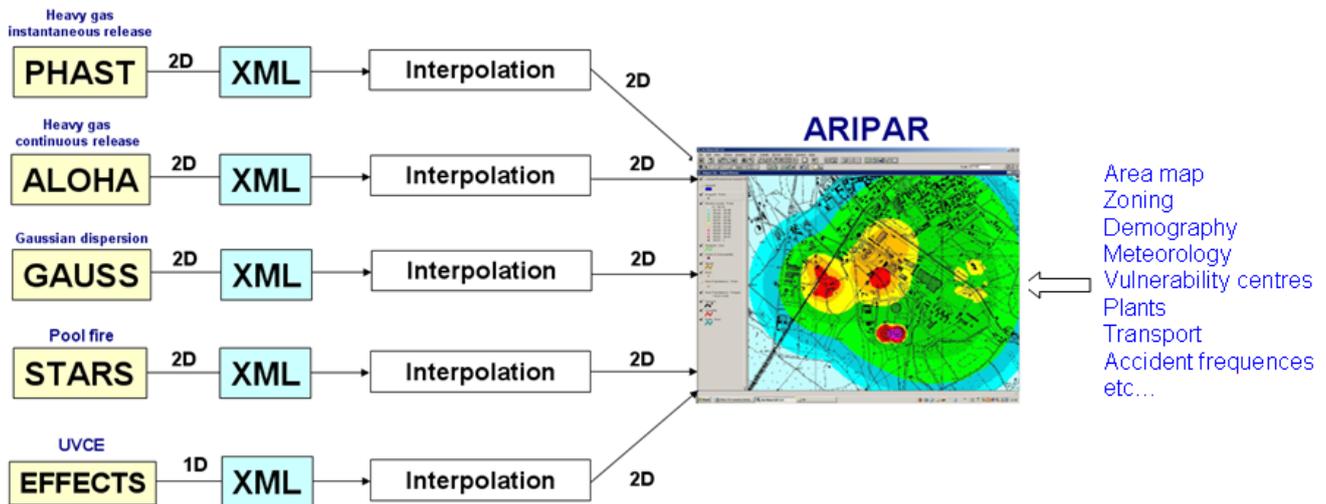


Figure 22: Schematic diagram for the experiment aiming to interface ARIPAR with accident consequence tools

Five different accident scenarios were uploaded into ARIPAR. The consequence effects of these scenarios were those calculated by using the above models, and particularly three toxics releases (heavy gas instantaneous release, heavy gas continuous releases, and Gaussian dispersion), a pool fire and an unconfined vapour cloud explosion. The risks of the different scenarios were calculated and suitably aggregated, and the overall result for individual risk is depicted in the risk map image of Figure 22.

The imported results of accident consequences can also be represented as a set of effect contours, which are calculated after assigning user-defined effect values. These contours are extracted from the interpolated grid and can be shown on the affected area. An example is given in Figure 23 for the dispersion of a toxic substance. This allows getting an overview of the impact of the accident consequences on the concerned area.

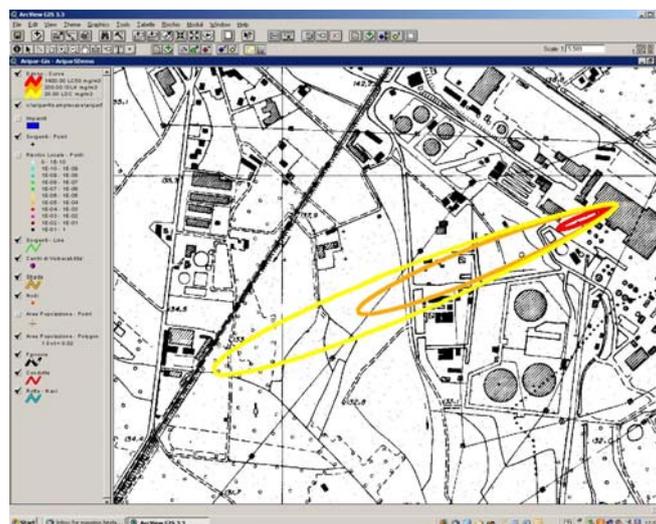


Figure 23. Effect contours extracted from the grid generated from the results of PHAST.

The present example demonstrated the importance of interoperability of different systems to facilitate data uploading in risk-based applications.

## 5. DATA EXCHANGE FORMAT AND INTERPOLATION TO COMPARE THE RESULTS OF DIFFERENT ACCIDENT CONSEQUENCE MODELS

Once the input and the output data of different consequence models are represented by a common data format (e.g. the proposed XML), interoperability amongst different systems is ensured. This chapter describes the tools developed, within the present feasibility study, to compare the results of different models or different interpolation methods applied to the same data.

Interoperability is very important when there is the necessity to perform a comparison of the consequence effects of the same accident as obtained by using different computation models. This situation is quite typical in the review activity performed by competent authorities. In this case it is indeed necessary to evaluate the risk assessment results produced by the plant operator, and normally the review process is conducted by using different models i.e. those that are actually preferred by the competent authority. One of the most critical steps of this review process is the estimate of the consequence effects, due to the large number of assumptions and parameters used for the calculation and the variety of tools and models available for this purpose.

The present section addresses exactly this situation and describes the procedure to compare consequence data for the same accident scenario. Specific software was also developed for the comparison of the different models' outcome. This software was tested on a number of practical cases, which can be grouped in the following categories:

1. comparison of results of 1D models;
2. comparison of results of a 1D model with a 2D model;
3. comparison of results of two 2D models.

In general it can be stated that if the amount of available data is sufficient to perform meaningful interpolations (i.e. sufficient number of contours and/or of points' density) then all the above cases can be addressed using the tools described in the following sections.

To practically perform a comparison of the output of two different models, the data (normally 2D) have to be distributed on a common grid. Once this is established, the comparison is done on each node of the grid (cell) that corresponds to a specific spatial location in which the effect values are known. It is therefore necessary to define a common grid and to interpolate the original data produced by the models on the newly established grid nodes. Section 3 has already addressed how to create the grid and to perform the interpolation of effect-contours. As a consequence of the results previously described, Linear and Constrained Cubic Spline were the selected method for contour interpolation.

### 5.1 MapViewer

In order to display the main outcome of an accident consequence model a specific package, named *MapViewer*, was developed. It allows displaying a 2D-map representation of the consequence effects given by a consequence analysis program. The 2D-grid may be the results of a consequence program or it may be generated through interpolation. Figure 23 shows the interface of *Map-Viewer*. A chromatic scale helps interpreting the variations of the accident consequence effects values. The maximum value of the effects calculated for the map is also numerically displayed. The main commands on the user interface menu are described in Table 11.

In particular, these commands are available to allow the user:

- to know the value of the effect in a selected point on the map;
- to visualise the profile of the effects along the centreline and on any cross section.

Figure 23 displays the results of a Gaussian model. The centreline concentration profile is given in Figure 24, whereas the concentration cross section at a distance of 187m from the source is represented in Figure 25.

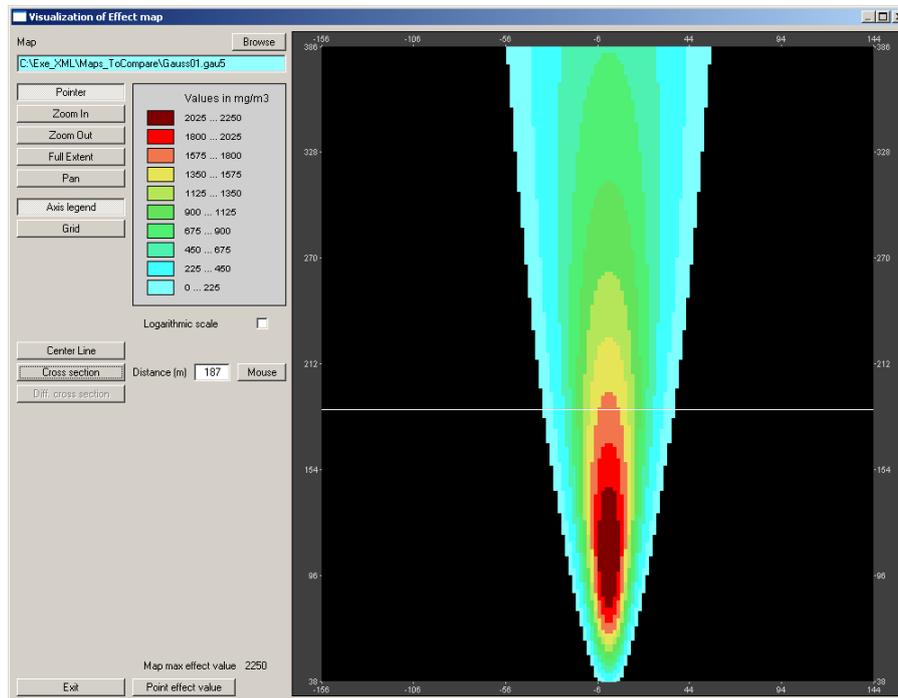
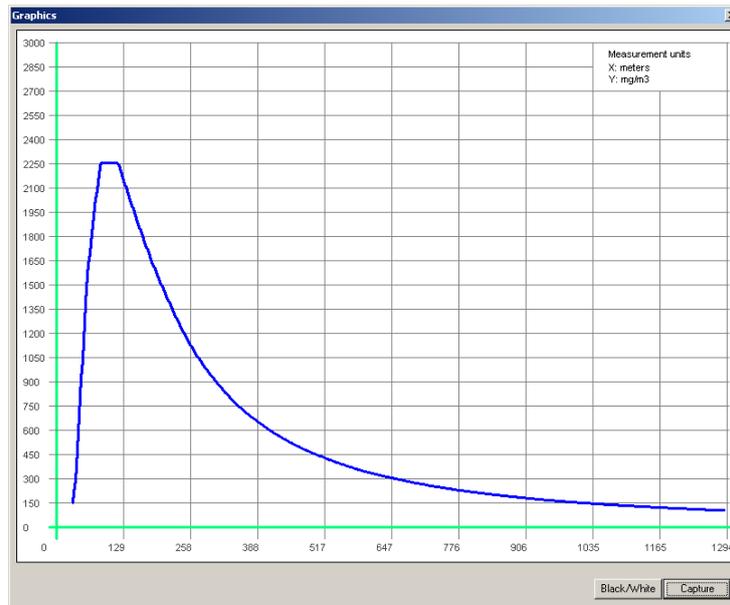


Figure 23: User interface of *MapViewer*

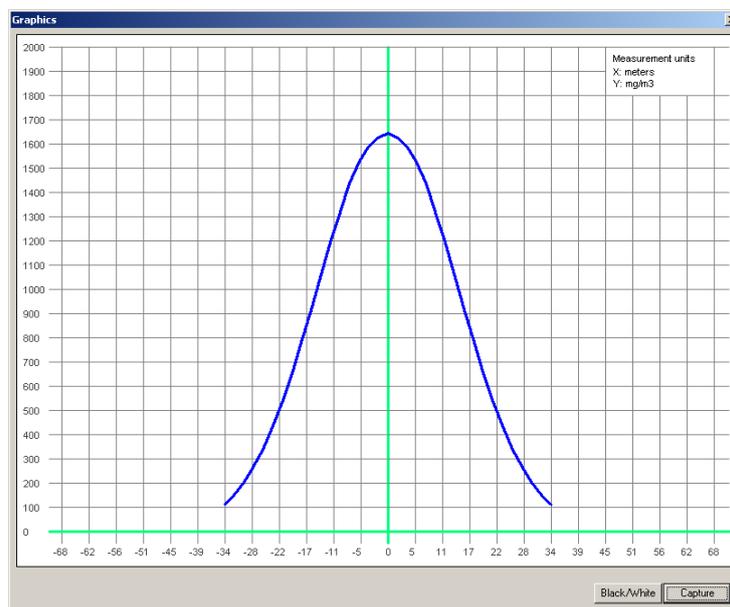
Table 11: List of commands of *MapViewer*

Command	Description
Browse	Browse to the map to be displayed
Pointer	Change current mouse pointer to arrow
Zoom in	Zoom in the displayed map
Zoom out	Zoom out the displayed map
Full extent	Represents the whole map on the display area
Pan	Change the mouse pointer to pan, to allow the user to drag the map
Axis legend	Displays the axis legend
Grid	Displays the grid on the display area
Centreline	Displays the Centreline distribution of the effects
Cross section	Makes the program ready to construct and display cross sections
Mouse Distance	Clicking the Mouse button and then a point on the display area generate the cross section plot and displays in the field "Distance" the real distance from the source. Inversely, entering the distance in the field and clicking the Return key the line on the Display area and the cross section plot appear.
Log scale	Displays the map taking Log-values of the effects
Point-effect-value	Clicking this button and then a point on the display area returns the value of the effect at the selected point.



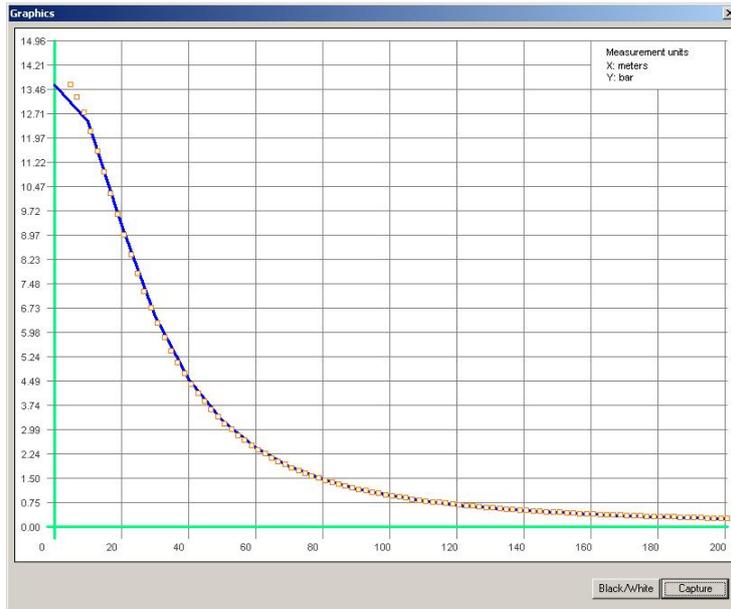
**Figure 24: Centreline profile of the cloud represented in Figure 23**

The max concentration value corresponding to the flat area (i.e. the innermost contour) is  $2250 \text{ mg/m}^3$ . This value is also reported on the bottom-left side of the user interface. The minimum value is about  $100 \text{ mg/m}^3$ . From the cross section at a given distance from the source both the highest concentration and the cloud width can be read.

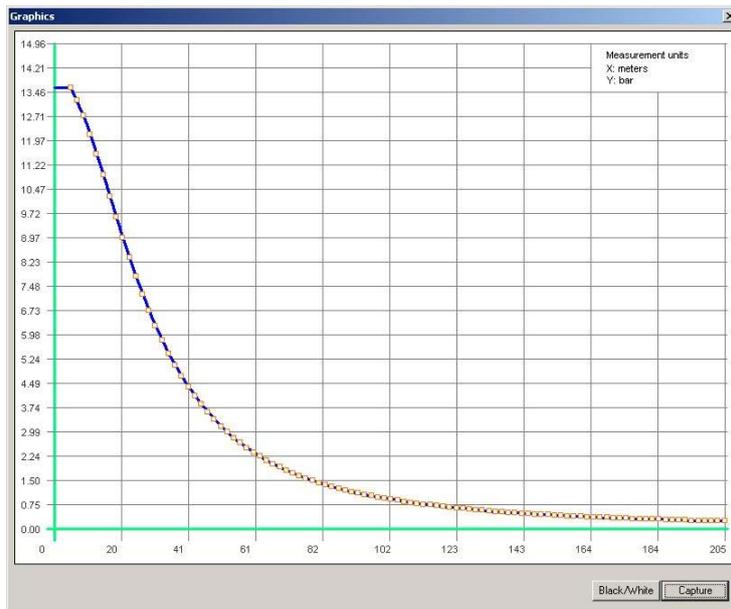


**Figure 25: Cross section at a distance of 187m from the source for the cloud represented in Figure 16**

Figure 26 shows the comparison of centreline concentration profile resulting from interpolation (blue curve) compared to the original data points (yellow circles). The two graphs refer to the situations in which the selected grid cell dimension is respectively of 10 m (Figure 26a) and 2 m (Figure 26b). It is worth to notice that in the first case the data very close to the source are not well fitted. This is due to the fact that the grid cell dimension (10 m) is larger than the distance between data points (2 m). In the second case (Figure 26b), the situation is generally improved, which demonstrate that whence the original data are very dense, it is better to select a comparable dense grid.



**Figure 26a): Interpolation of 2m distant data points on a grid with cell size of 10m**



**Figure 26b): Interpolation of 2m distant data points on a grid with cell size of 2m**

*Map Viewer* has been developed with the overall objective of incorporating it as a new module in the novel version of ARIPAR. It has also been used to develop the CEM tool described below.

## 5.2 The CEM program

In order to perform the comparison of two different consequence effect maps, and in turn, the outcome of two different consequence models/tools, specific software has been developed. This programme was called *CEM* (Comparison Effects Models), which was designed to import consequence effects data contained in an appropriate file with XML format.

The *CEM* program, integrates the different modules previously described for grid-generation and interpolation, and it incorporates *Map Viewer*. Its interface is given here below. Table 12 describes the general commands to import and compare the two maps.

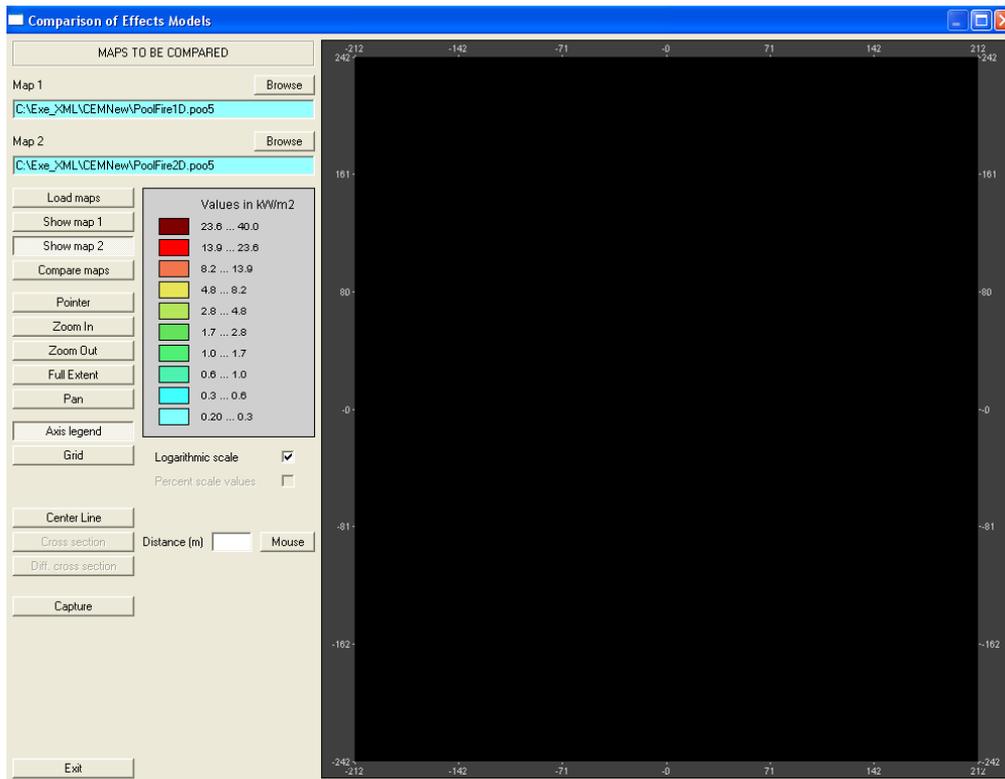


Figure 27: The *CEM* interface

Table 12: List of commands of CEM

Command	Description
Map 1	Loading the first map resulting from data interpolation
Map 2	Loading the second map resulting from data interpolation
Load maps	Load the two maps in memory from HD
Show map 1	Displays the first map
Show map 2	Displays the second map
Compare maps	Displays the map given by Map1-Map2

Since *CEM* uses the *Map Viewer* module, it contains also those commands previously described in Table 11.

Clearly *CEM* is designed to read XML files with the specific format presented in this report. However, the grid data that are generated by the interpolation module are normally stored as a binary file. The *CEM* program can also read this data format.

CEM can be used for two different purposes:

1. Comparison of the results of different accident consequence models/tools. In this case use is made of the same interpolation method;
2. Comparison of the results of different interpolation methods applied to a given accident consequence model. This is particularly relevant to test interpolation methods.

Figure 28 and Figure 29 show the schematic diagrams for these two possible applications:

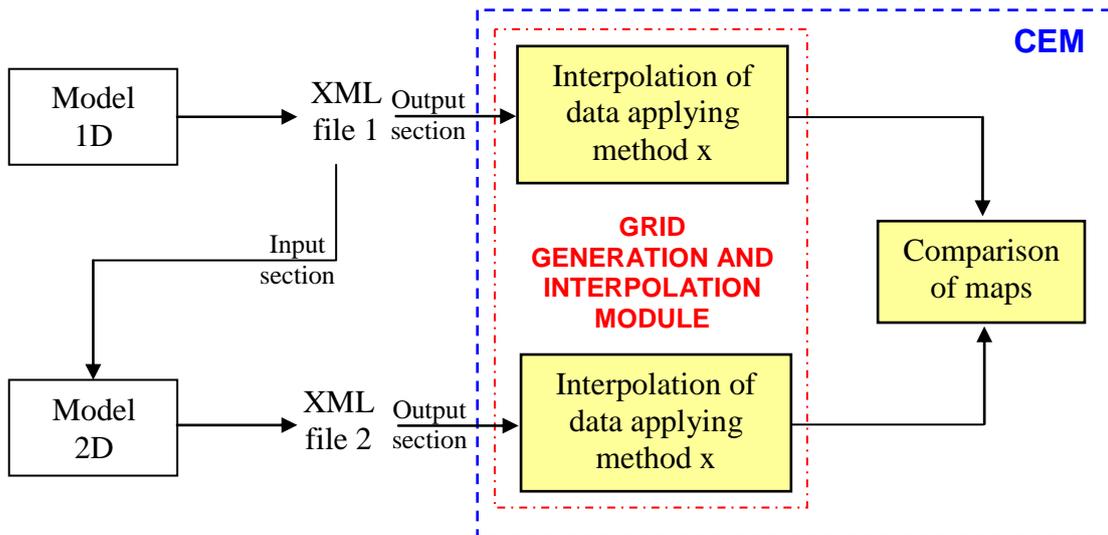


Figure 28: Functional diagram for the comparison of different consequence models

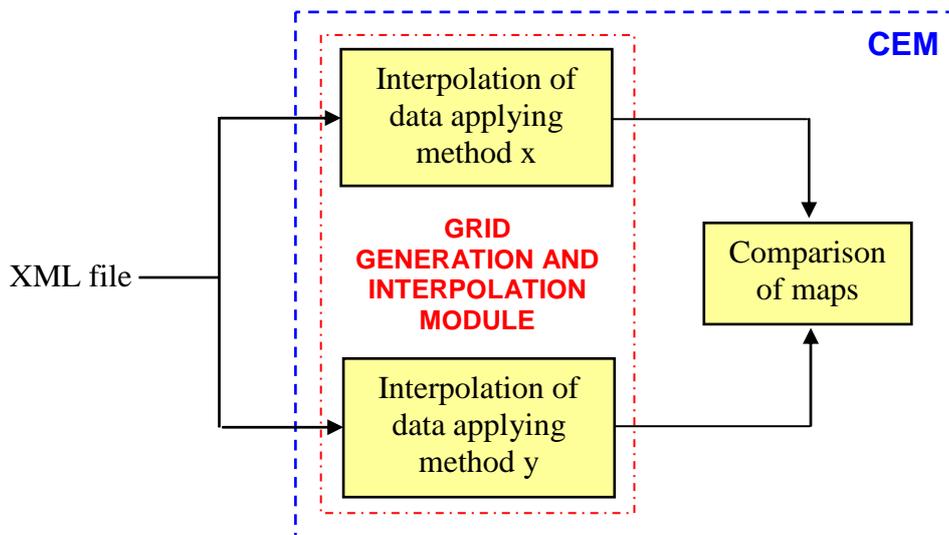


Figure 29: Functional diagram for the comparison of different interpolation methods

### 5.2.1 Comparison of the results of different models

With reference to Figure 28 the input consists of two XML files containing the data associated with the results of the same accident scenario analysed by means of two different consequence models. For illustration purposes it was considered the example given in Section 2.4, where the outcome of two different pool fire models (i.e. 1D and 2D models) was compared.

The result of the run of the 1D-model is stored in the associated XML file. The input section of this file is used to feed the 2D-model. The input data set of the 2D-model is completed with the addition of extra data, due to its greater complexity with respect to the input of the 1D-model.

The data in the output section of the generated XML files (1 and 2) are interpolated on a common grid using the same interpolation method and compared. *CEM* allows to separately display the radiation maps associated with each single model and also to show the differences between the two maps.

The procedure to use *CEM* consists of the following steps.

- i) Upload the files with consequence assessment data to be compared.

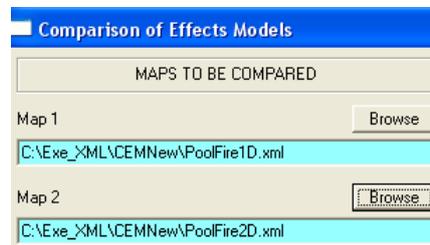


Figure 30: *CEM* Window for uploading the XML consequence files

The files to be uploaded are normally of the XML format designed and presented in this report. However the software accepts also binary files (grid maps) generated by the interpolation.

- ii) Run the Maps-Generation and Interpolation module for both XML files after having selected the interpolation method and the (square) grid cell dimension that must be the same for both maps. The generation/interpolation module is active for consequence files with XML format (see Figure 31a) whilst is inactive for those files in binary format, since these have already resulted from a generation/interpolation process (see parameter Map 2 in Figure 31b).

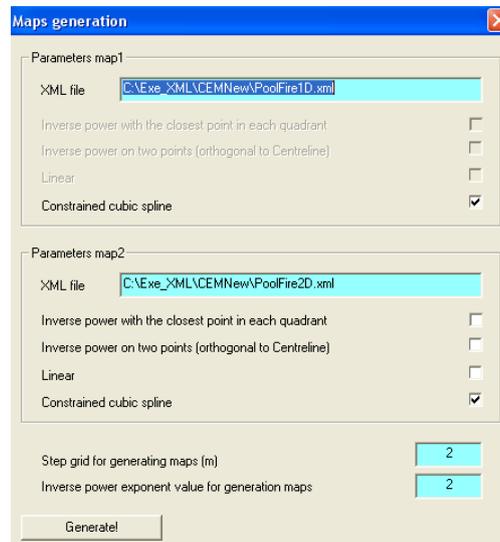
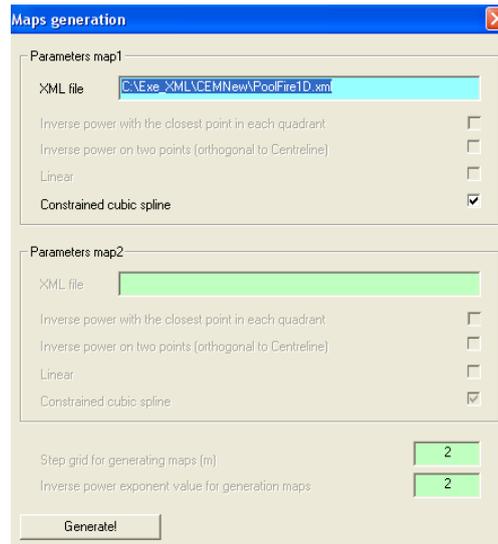


Figure 31a: *CEM* Window for map generation and interpolation (case with two XML files)



**Figure 31b: CEM Window for map generation and interpolation (case with a XML file and a binary file)**

iii) Click the “Map generation” button to generate the interpolated maps.

iv) Click the “Load maps” button and then “Show Map1” or “Show Map2” to display the generated maps. Click “Compare maps” to display the map resulting from the difference between Map1 and Map2.

All other commands are common to those of Map-viewer and are self explaining.

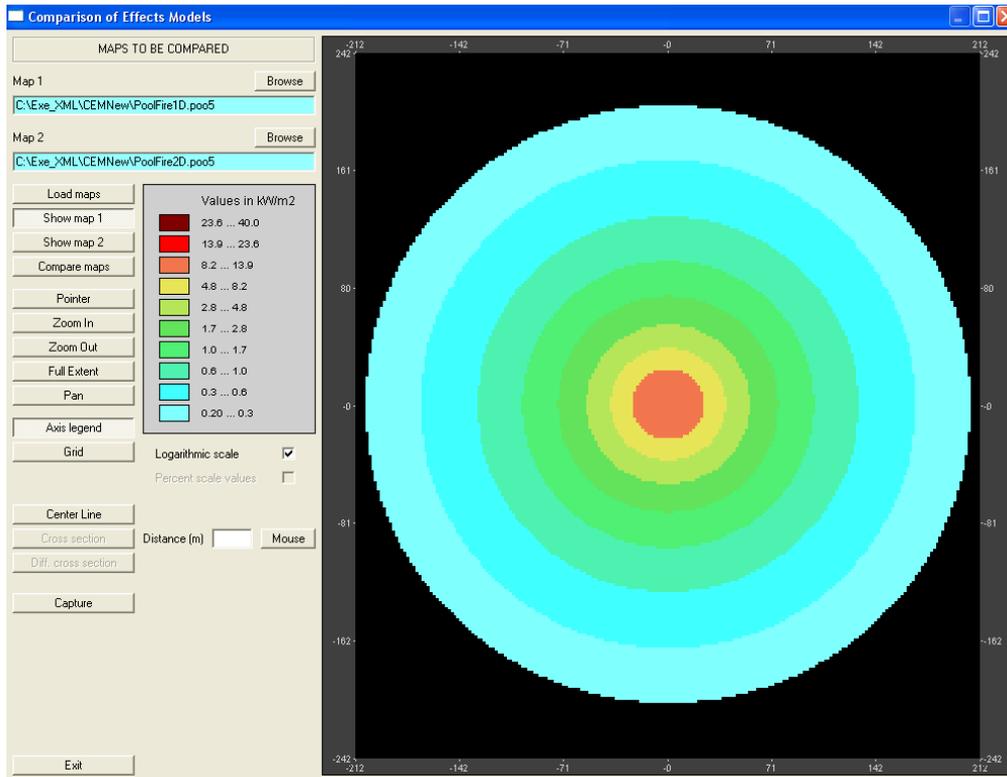
The results of the aforementioned example, the 1D and 2D pool fire models, is shown in Figures 32 and 33, respectively. The comparison is provided in Figure 34 which allows visualising the difference between the two models’ outcome in the different space positions. As it can be noticed by the current example, the difference between these maps is very much negligible with the exception of the central area in proximity of the accident source, which has a diameter of 10m.

When the effect of Map 1 is greater then the effect of Map 2, the difference is represented in red, whilst in the opposite case this difference is in blue.

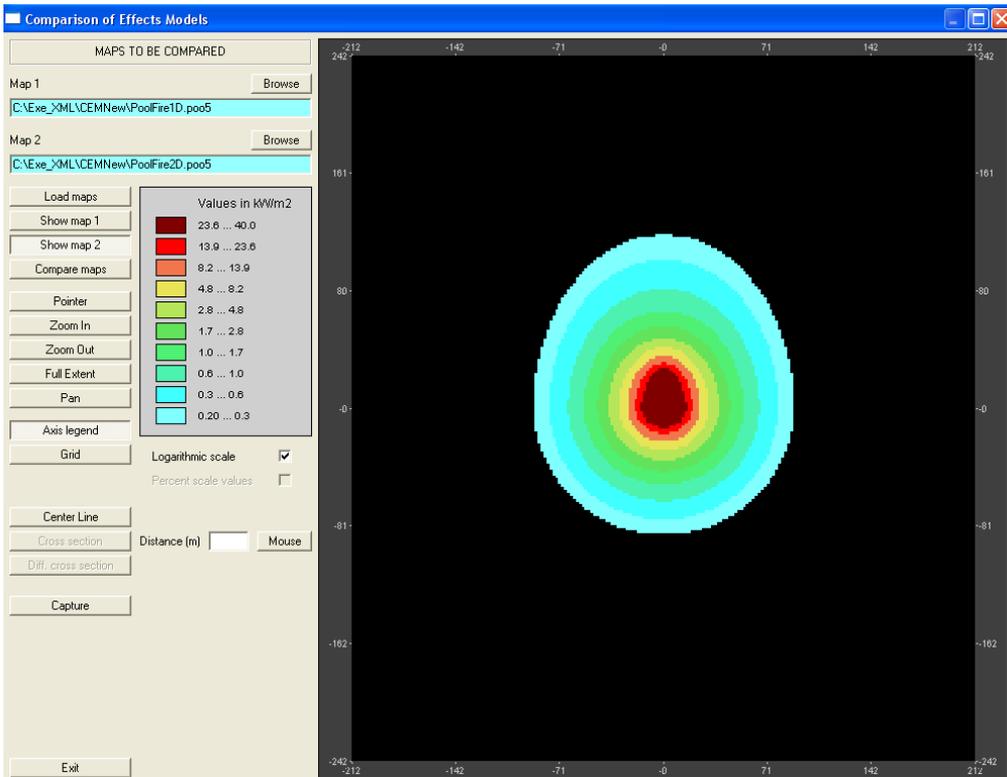
Another possible way to better understand these differences is to look at the map cross sections given in Figure 35 and Figure 36. The first represents the two curves at the centreline (downwind effect). The maximum value of Map2 ( $40.1\text{Kw/m}^2$ ) is three times greater than that of Map1 ( $13.6\text{Kw/m}^2$ ). However, the effect of Map1 is distributed over a larger surface.

Figure 37 shows the difference between the two cross sections at 25m from the fire.

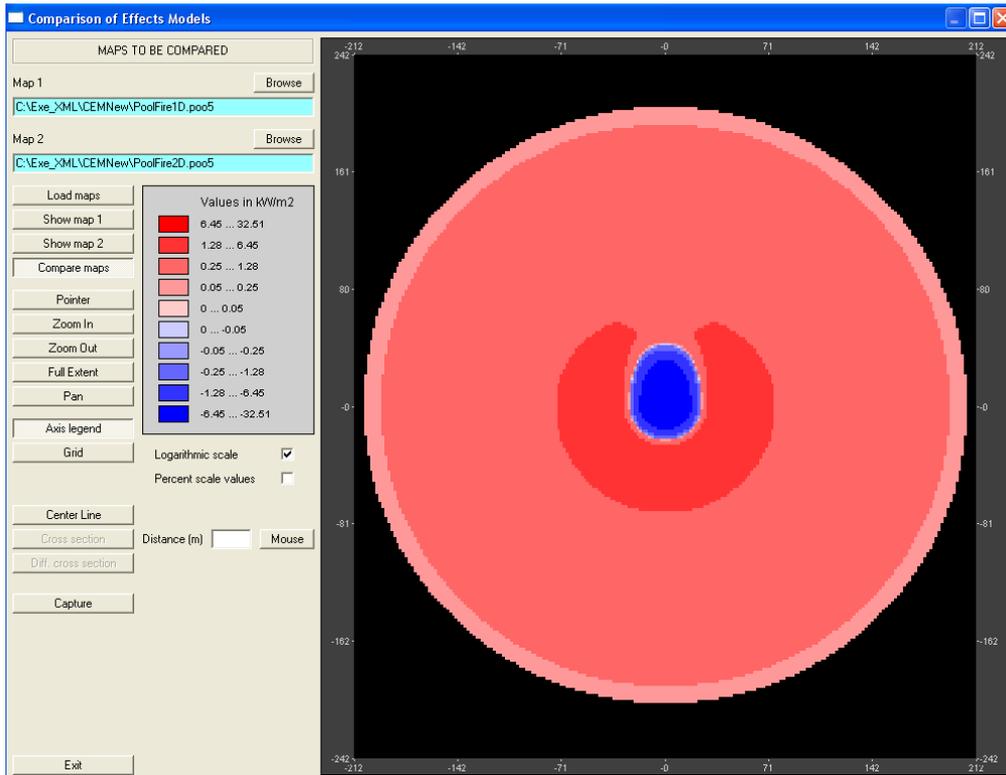
Another alternative way is to compare the two maps determining the differences between two contours, starting from the innermost and representing the results on a histogram. More precisely, each bar of the histogram would represent the mean value of the total difference of the effects between the two considered contours. This feature will be probably included in the CEM program in the future.



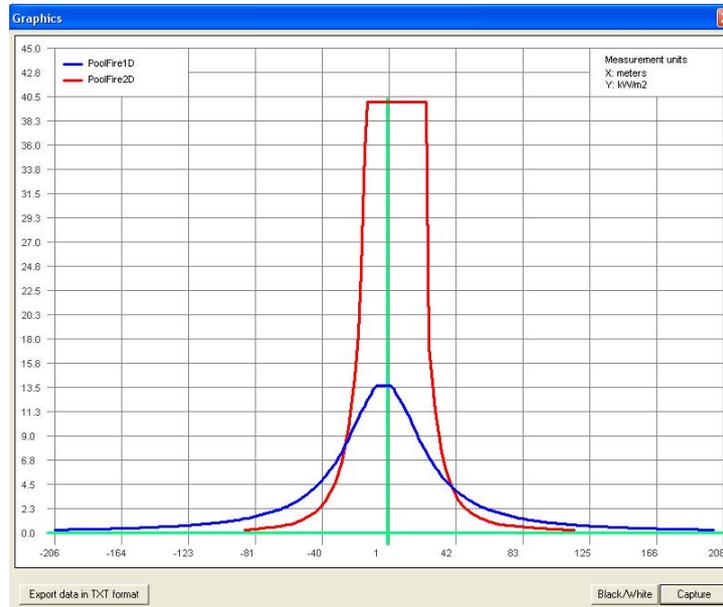
**Figure 32: Map1 resulting from the interpolation of the radiation values for the 1D-model**



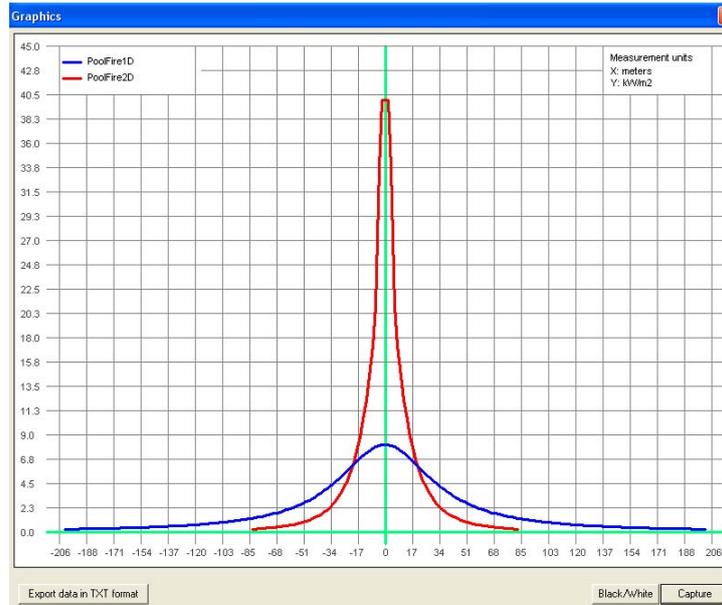
**Figure 33: Map2 resulting from the interpolation of radiation values for the 2D-model**



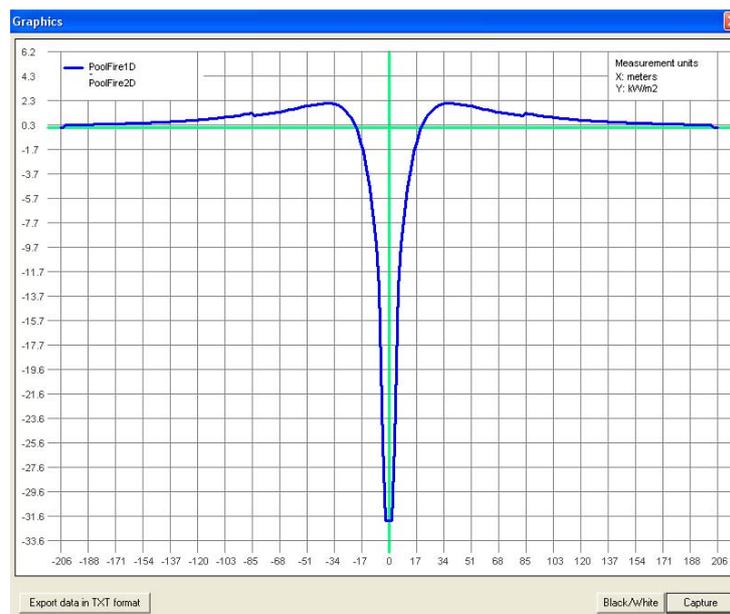
**Figure 34: Result of the difference between the 1D model and the 2D model.**



**Figure 35: Centreline cross section of Map 1 and Map2**



**Figure 36: Cross sections at 25 meters from the centre of the pool.**



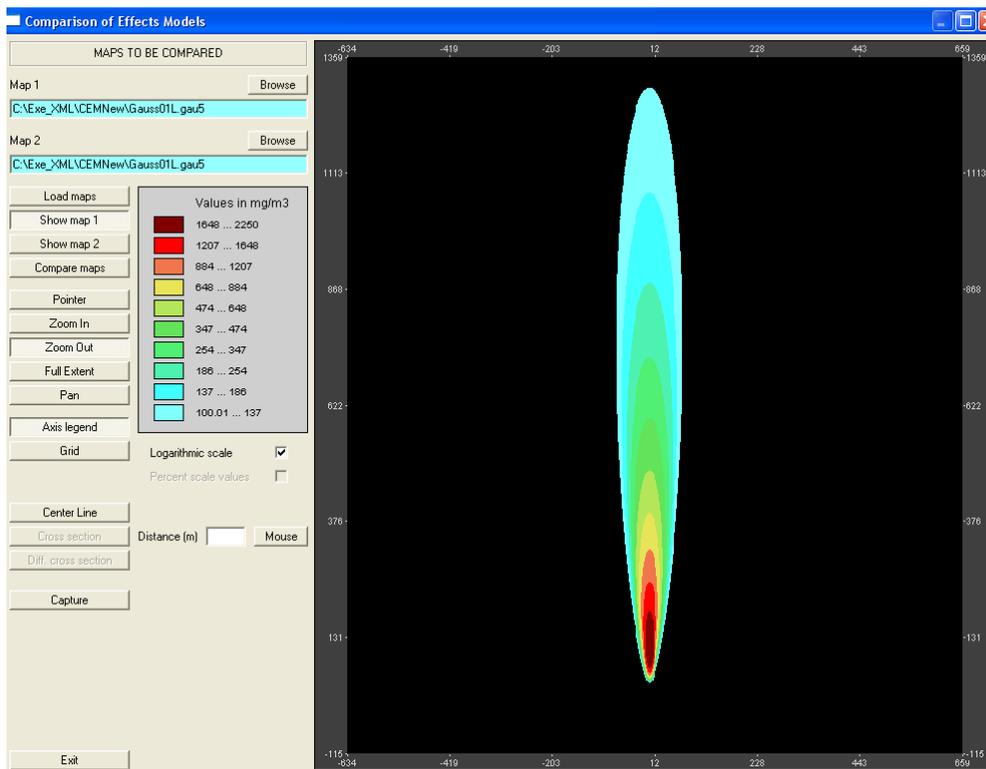
**Figure 37: Cross section at 25 meters of Map1 – Map2**

### 5.2.2 Comparison of different interpolation models

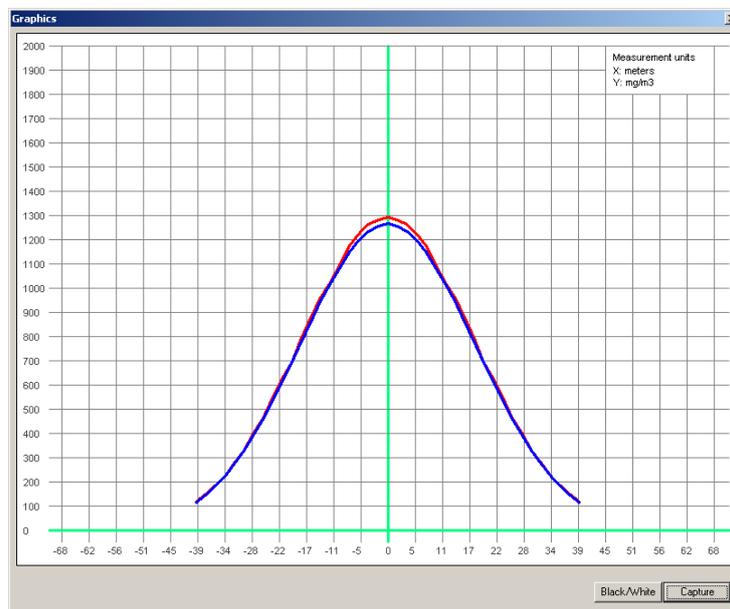
The *CEM* program may also be used to compare the results of the same model interpolated using two different methods, e.g. linear and spline. This allows exploring what is the influence of different interpolation methods on the consequence effect data under investigation.

The steps of the procedure to follow are as before. It is necessary to run the Maps-Generation and Interpolation module (step *ii*) by using the same file for accident consequences but selecting two different interpolation methods. The difference between the corresponding maps can be displayed, as shown in Figure 38, which represent the case of a toxic release following the Gaussian model interpolated by both the linear and constrained cubic spline methods. Also for this case cross sections

can be produced to better identify the extent of the differences. An example is given in Figure 39, which depicts the profiles of two interpolation methods at 213m from the source.



**Figure 38: The CEM interface displaying the results of the different maps on the same input model, which were generated using different interpolation methods**



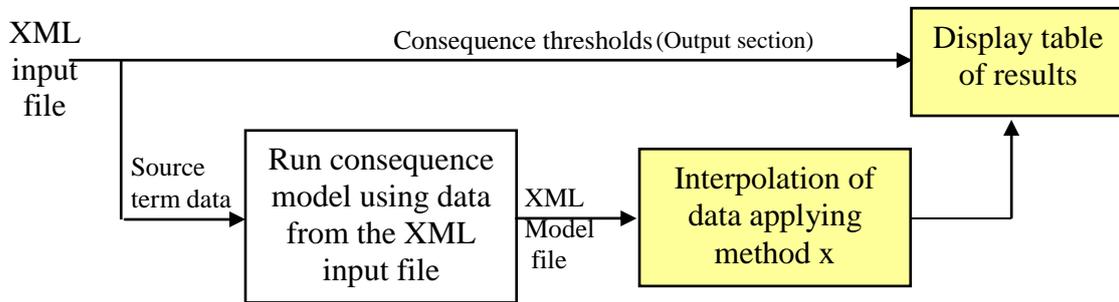
**Figure 39: Cross section of the two interpolated maps at 213m from the source**

### 5.3 The CET program

Let's consider now the particular case in which one of the XML files contains the results of a 1D model but with a number of data, which is too small to generate a proper interpolation data set on the grid. This is a typical situation, when only two effect-values at the centreline are available i.e. for instance distances at LC50 and IDLH; 12 Kw/m<sup>2</sup>, and 4 Kw/m<sup>2</sup>; and other similar situations. In this case a possible way forward is to run another model, whose output should fit with these data and which can produce a reasonable grid for risk assessment purposes.

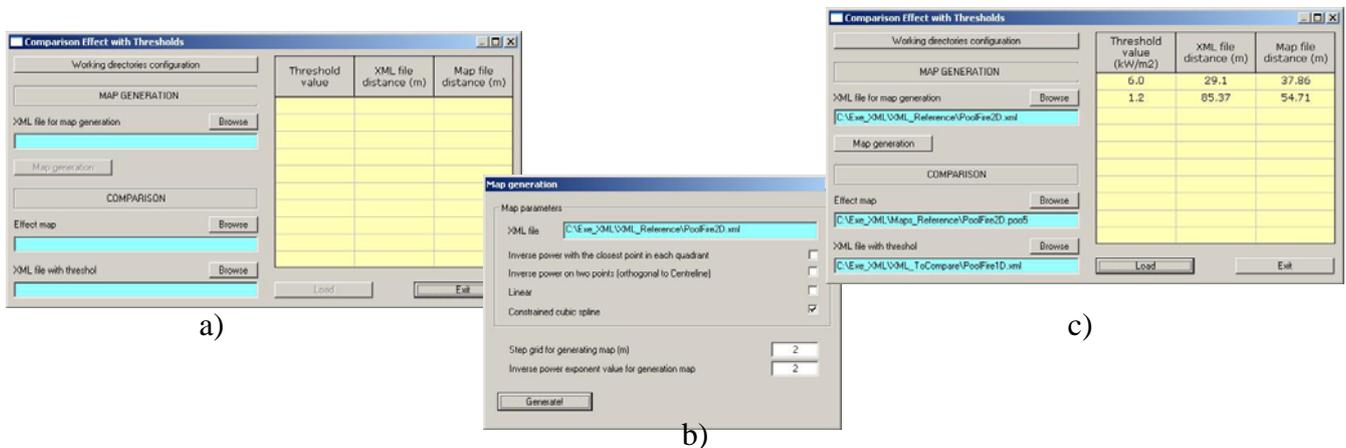
If the XML input file contains sufficient information about the source terms, then it is possible to run an external model to implement correctly the interpolation. After this process, the results of the model can be compared with the consequence thresholds and displayed in tabular form.

This procedure is schematically reported in Figure 40 and it is complementary to the previous one. A specific software: *CET* (Comparison Effects with Thresholds), has been developed to implement it.



**Figure 40: Functional diagram of the CET module to compare the results of an accident consequence model with given thresholds**

The user interface of CET is presented in Figure 41. Part a) shows the first window that allows the user to insert the name of the XML input file. The input data are used to feed the consequence model, whose results are exported in XML format. Part b) shows the window for running the Grid generation and interpolation programme after having selected the interpolation method and the grid cell dimension. Part c) shows the results of the comparison i.e. the threshold values together with the corresponding distances given as input data and the distances extracted from the grid (i.e. the consequence model).



**Figure 41: The CET user interface**

## 6. CONCLUSIONS

The feasibility study presented in this report was intended to demonstrate the possibility to define a Common Data Exchange Format (CDEF) to facilitate data exchange amongst different software for consequence assessment. The final goal was the possibility for competent authorities (who have the task of reviewing the safety reports) to import both input data and results of accident consequences provided by the operators in their safety reports. A CDEF is also useful to other stakeholders, e.g. risk analysts, software developers, model developers.

The present study consisted of defining a first prototype of CDEF, which was developed in XML. Few application examples were executed on a selected number of accident scenarios (i.e. fires, explosions and toxic releases) using proprietary software. These tests demonstrated the full interoperability of the software used and allowed to address the problems resulting from the use of common data format e.g. the model's parameters to consider, the different measurement units, the use of "extra data", multi-model software vs. single model software.

The first test concerned the interoperability between two different pool fire models. The availability of the source codes allowed us to perform a complete test, i.e. a two-way data exchange by implementing the import-export modules in XML. Some other tests have been carried out using PHAST, EFFECTS and ALOHA, which are well known tools for consequence analysis. Unfortunately, due to the unavailability of the source codes for these tools, it was not possible to carry out two-way tests. For this reason it was decided to perform a one-way transfer of data from the output of these tools (i.e., consequence profiles) to ARIPAR, an area risk assessment tool which makes use of such data.

As a conclusion on this part of the study it can be said that the interoperability is a reachable goal, which requires the contribution of all stakeholders (i.e. European Committee for Standardization, EU safety authorities, industry representatives, software and model developers, etc).

Another objective of the project was the development of a specific tool for comparing results of different accident consequence models, described by means of the CDEF. To this regard an important phase was the transposition of their results in a common spatial grid. A series of trials on a toxic dispersion case was conducted in order to assess the errors introduced by the interpolation process. These trials consisted of interpolating the effect contours of a Gaussian dispersion model using six different interpolation methods. The influence of the number of contours and the density of points in each contour were also investigated. The outcome of this analysis showed that, although several interpolation methods produce acceptable results, the Constrained Cubic Spline (CCS) method is by far the best for this type of applications, provided that the number of available contours is greater than 5-6, preferably equally spaced on the logarithmic scale within the range between the maximum and the minimum concentration values. The Linear interpolation method was also considered as acceptable even though in certain situations it could produce too conservative results. The CCS method was tested also on fire scenarios and on instantaneous heavy gas dispersions, which were simulated by using PHAST.

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**Abstract**

The present report describes the outcome of a feasibility study to explore the possibility to make consequence assessment software tools interoperable through the definition of a suitable Common Data Exchange Format (CDEF). In this way the input data used by the operators of Seveso type establishments for consequence assessment can be easily exported in a format compatible with the corresponding tools in use by the competent authority. As an outcome of this feasibility study, a first prototype of CDEF was developed in XML and applied for data exchange amongst different commercially available consequence-related tools. The software CEM to rapidly compare the results of two software packages for accident consequence assessment has been implemented to prove the usefulness of the CDEF. Another test consisted in importing into ARIPAR, a GIS-based tool for area risk analysis, the results of accident consequences obtained using well known accident assessment software packages: PHAST, EFFECTS, and ALHOA.



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