Final report Annex 2: Consequence Assessment Methods for Human Health (Task 2)

Development of an assessment methodology under Article 4 of Directive 2012/18/EU on the control of major-accident hazards involving dangerous substances (070307/2013/655473/ENV.C3)

Report for the European Commission (DG Environment)

AMEC Environment & Infrastructure UK Limited

In association with INERIS and EU-VRi

December 2014

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European Commission (DG Environment)

Development of an assessment methodology under Article 4 of Directive 2012/18/EU on the control of major-accident hazards involving dangerous substances

Final report – Annex 2

AMEC Environment & Infrastructure
UK Limited

December 2014

List of abbreviations

ADAM	Accident Damage Assessment Module
ADR	European Agreement Concerning The International Carriage Of Dangerous Goods By Road
ALARP	As Low As Reasonably Practicable
ARIA	Analysis, Research and Information about Accidents
BLEVE	Boiling Liquid Expanding Vapour Explosion
BOD – COD	Biochemical Oxygen Demand – Chemical Oxygen Demand
CE	Critical Event
CFD	Computational Fluid Dynamics
CLP	Classification Labelling Packaging
COMAH	Control Of Major Accident Hazards
DA	Deterministic Approach
ECHA	European Chemicals Agency
e-MARS	Major Accident Reporting System
EU	European Union
EWGLUP	European Working Group on Land Use Planning
F&EI	Fire & Explosion Index
GHS	Globally Harmonised System
JRC	Joint Research Centre
LPG	Liquefied Petroleum Gas
LUP	Land-Use Planning
MAHB	Major Accident Hazard Bureau
MATTE	Major Accident To The Environment
M_F	Material Factor of the Dow’s Fire & Explosion Index
MIMAH	Methodology for Identification of Major Accident Hazards
NFPA	National Fire Protection Agency
NOEC	No Observable Adverse Effects Concentration
PA	Probabilistic Approach
PLG	Pressurised Liquefied Gas

RID	European Agreement Concerning the International Carriage of Dangerous Goods by Rail
RMP	Risk Management Plan
STOT-SE	Specific Target Organ Toxicity (Single Exposure)
USEPA	United States Environmental Protection Agency
UVCE	Unconfined Vapour Cloud Explosion

Physicochemical parameters

BCF	Bioconcentration Factor
EC_{50}	Median Effective Concentration
ΔH_r	Standard enthalpy of reaction
K_{st} / K_g	Maximum rate of explosion pressure rise for dust clouds/gas
LD_{50} / LC_{50}	Median Lethal Dose / Median Lethal Concentration
LFL / LEL	Lower Flammability Limit / Lower Explosion Limit
LOC	Limiting Oxygen Concentration
MIE	Minimum Ignition Energy
MTSR	Maximum Temperature of the Reaction Synthesis
NOEC	No Observed Effect Concentration
P_{max}	Maximum explosion pressure
P_{vap}	Vapour pressure
ΔT_{ad}	Adiabatic temperature rise
T_{eb}	Boiling point
TMR_{ad}	Time to maximum rate in adiabatic condition
UFL / UEL	Upper Flammability Limit / Upper Explosion Limit

Contents

1. Introduction

1.1 Purpose of this report

This report forms part of the outputs of a contract for the European Commission on ‘development of an assessment methodology under Article 4 of Directive 2012/18/EU on the control of major-accident hazards involving dangerous substances’. The work has been undertaken by AMEC, INERIS and EU-VRi.

The present report concerns one of a number of specific tasks under the project. It should not be read in isolation, but in conjunction with the main report and in conjunction with the reports concerning the other project tasks.

1.2 Scope of Task 2

In the context of the assessment methodology under Article 4 of the Seveso III Directive, reference accident scenarios involving the substance in question are to be modelled using a consequence assessment tool[1].

During the course of this project, it became clear that it is important to assess what major accident scenarios are possible involving a dangerous substance, before undertaking any detailed consequence assessment (see the Task 4 report). Whether modelling of consequences should be undertaken will depend on factors such as:

- Whether there are identified major accident scenarios that cannot be ruled out based only on factors such as physicochemical properties.
- Whether modelling will add value to understanding the potential for a major accident. In particular, since exclusion under Article 4 should not take into account site-specific considerations, any modelling will need to take into account the worst-case conditions across the EU in terms of potential for a major accident. This could involve, for example, undertaking many different modelling scenarios.

The remit of this task was to gather detailed information on national/EU/international consequence assessment models with the aim of presenting a selection of reliable and robust models for assessing health and environmental consequences of accidents involving hazardous substances. The report is expected to provide a detailed overview and description of suitable models, including guidance as to how to interpret and compare the results of modelling exercises, and information on their sensitivity.

The objective of this modelling phase is to estimate distances of effects for different thresholds that could determine whether the substance may generate a major accident. It should be highlighted that consequence

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[1] An ad-hoc meeting of experts on 1 February 2013 agreed that: “An initial screening would allow to eliminate those cases for which it is obvious that a major accident could happen. For all other cases, consequence assessment models (national or provided by the Commission) will be used by the Member States when preparing notifications.”

assessment tools only enable calculation or estimation of effects distances of dangerous phenomena (explosion, fire, etc.). They are not substance-specific tools.

The choice of the scenarios to model is further explored in Task 4 and the criteria determining whether the accident generated is to be considered as “major” are set out in Task 6. The objective of the present task is to provide explanations on the different modelling tools that can be used, with the aim of guiding the choice toward the best suited tool for the purpose of the assessment methodology.

The purpose of this document is to identify and analyse suitable consequence assessments tools in the case of accidents involving hazardous substance on an industrial site. This task focuses on the consequences of industrial accidents on human health. Environmental consequences are covered in Task 3. The scope of the task is to provide a detailed overview and description of suitable models, including guidance as to how to interpret and compare the results of modelling exercises, also including information on their sensitive parameters.

It is important to note that all of the material presented in this report is considered only in the context of the Seveso Article 4 assessment method and is not prescriptive. The conclusions drawn do not necessarily apply in any other contexts. The approaches to consequence and risk assessment considered in this report are not the only approaches available, and those persons undertaking an assessment under Article 4 could decide to adopt alternative approaches where they are better suited to the particular case or substance under consideration.

1.3 Structure of this report

This report is structured as follows:

- Section 2 describes the different types of models on which consequence assessment tools rely.
- Section 3 provides detailed explanations on the dangerous phenomena and the physical and mechanical effects that may be generated by major accidents. For each dangerous phenomenon, the following elements are examined:
    - Description of the physical phenomenon and outline of the scenario that can lead to the dangerous consequences;
    - Effects to be considered for each dangerous phenomenon;
    - Modelling methodology: short description of the different stages of the modelling approach and the important parameters. The reference values to adopt in order to estimate the effects distances of the dangerous phenomena are not considered in the present task. They will be addressed in Task 6; and
    - Review of the models available to assess the consequences of these phenomena and reference documents describing these models.
- Section 4 presents the main consequence assessment tools, together with the physical models that form their basis and the dangerous phenomena that may be modelled using this tool. For a selection of tools, a template has been designed to present the following information:

  - A general description of the tool;
  - The physical models which form the basis of the tool;
  - The tool's domain of validity;
  - How to interpret the results of the modelling (i.e. the outputs of the tool); and
  - A short evaluation of the robustness of the model.

- Section 5 includes a synthesis of the existing experimental data. Experimental data campaigns are continuously carried out by the scientific community in order to enhance the knowledge of the hazardous phenomena and the validation of modelling tools. As such they are a valuable source of information.

2. Generalities about Models

2.1 Overview

A wide variety of modelling tools are available in order to represent the possible effects that can be generated by an accident. These tools rely on specific mathematical, physical and chemical models that can be categorised as follows: documented methods, simplified numerical models, and three dimensional methods.

2.2 Documented methods

There are several documented methods or handbooks, such as colour books (e.g. “Yellow Book”- TNO, 1997) or guidelines (e.g. Guidelines from Centre for Chemical Process Safety, CCPS, 2000). These present or gather mathematical models for assessing the physical effects of accidental releases of hazardous materials. Many of them are the result of extensive studies and the review of the existing scientific literature on models for the calculation of physical effects of the release materials.

2.3 Simplified numerical models (or integral models)

This type of model uses parametric or simplified forms of equations for the basic conservation laws (e.g. mass, momentum, energy and species), whose system of equations is simplified in order to make a rapid solution possible. This allows a response within much shorter calculation times (e.g. a few minutes) than 3D models (which can take up to several days in some cases).

Due to their simplicity of use these types of models -which are usually called *integral models*- are those most widely and frequently used. Gaussian models which are used to model atmospheric dispersion belong to this category of simplified numerical models.

2.4 Three dimensional models

This family of models solves the three-dimensional (3D) time-dependent fluid flow equations. The most widely known are the Computational Fluid Dynamics (CFD) models.

CFD models overcome many of the limitations of integral models (i.e. simplified equations for the basic conservation laws, simplified environmental conditions) but they are not suitable for carrying out wide ranging and rapid project screening analysis. CFD codes are based on the solution of mass, momentum and energy conservation equations (Navier-Stokes equations) in order to provide full 3D flow maps for an identified volume.

In recent years, the use of 3D models has increased as it allows the computing of hazardous consequences of toxic/flammable gas dispersion.

Three-dimensional models offer the advantage of filling gaps encountered with simpler models. For instance, 3D atmospheric models allow complex environmental conditions to be taken into account (e.g. the presence of obstacles) on the process of atmospheric dispersion. This is not possible with the traditional models.

On the other hand, 3D models are slow to set up and to run because they require complex implementation (e.g. more numerous and sensitive calculation stages, number of parameters and numeric sub-models can be difficult to pre-calibrate). The calculation times range from several hours to a few days depending on the specificities of the calculation and the computing resources.

Finally, one should keep in mind that:

- 3D models can be initially developed for engineering applications that have nothing to do with dangerous consequences related to an accident scenario;
- The use of 3D models requires a good understanding of the physical mechanisms involved and a sufficient level of expertise in the specific tool; and
- 3D models can potentially be used in the context of a generic assessment of worst-case accident scenarios at EU level, by setting appropriate worst-case parameters, and moreover these can potentially be used in the near-field (i.e. short distance from the source), unlike some other models..

3. Description of Dangerous Phenomena and Modelling Aspects

3.1 Overview

This section provides an overview of the dangerous phenomena that can occur in an industrial accident. They can be grouped into four categories: atmospheric dispersion (e.g. toxic dispersion), explosion, fire and fire balls. In each case, the phenomena and the main consequences models available for these phenomena are described.

3.2 Atmospheric dispersion

3.2.1 Dispersion of a flammable or toxic cloud

Description of the physical phenomenon

Atmospheric dispersion describes the motion and evolution of particles (aerosols, gases and dust) in both space and time following their discharge into the atmosphere. The accidental emission of a product into the atmosphere is due to occasional undesirable release into the atmosphere over time, such as from a leak in a tank or smoke due to a fire.

The conditions of atmospheric dispersion of a product will depend on several parameters, the influence of which depends on the following aspects:

- The release conditions (e.g. nature of the cloud product, mass flow rate);
- The meteorological conditions (e.g. wind field, temperature); and
- The surrounding environment (e.g. presence of obstacles, topography).

Effects to be considered

Health hazards have to be estimated, which depend on the acute toxicity of the chemical.

For each chemical or substance emitted, toxicity thresholds of concentrations for lethal, irreversible, and reversible effects typically have to be taken into account. The calculation of toxic doses is usually used to predict the effect distances (e.g. in France; Penelon, T., 2008).

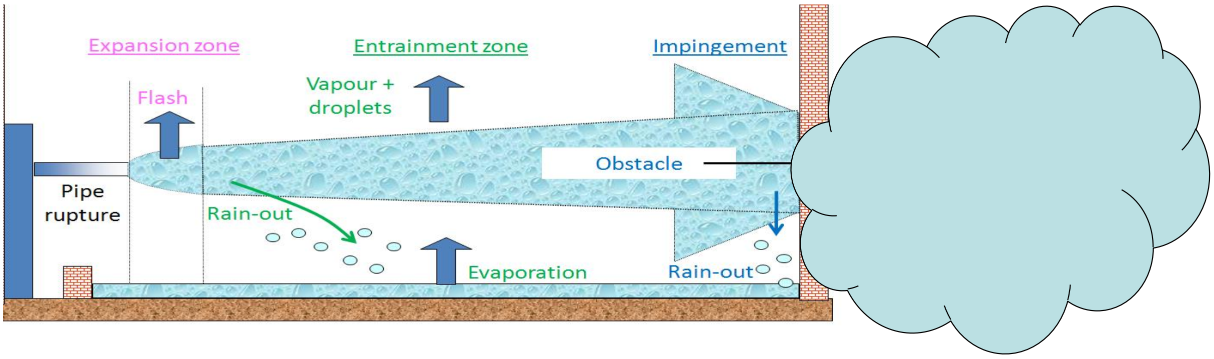
Modelling methodology

Before the atmospheric dispersion of a substance can be modelled, it is necessary to calculate its source term. This preliminary calculation consists of characterising the discharge into the air of the substance in terms of mass flow rate, temperature, physical state, and other relevant criteria.

The figure below (Figure 3.1) presents the different contributions of the source term in the general case of a leak of liquefied gases which is the most complete/ complex case. In this specific example, the source term will consist of the following contributions:

- The thermo-dynamical flash during the evaporation at the breach in the expansion zone (i.e. instantaneous vaporisation of part of the liquid);
- Aerosol and vapour in the entrainment zone;
- Vapour after impact on an obstacle in the impingement zone. When encountering an obstacle, a part of the aerosol evaporates after impinging the obstacle, another part of the aerosol is captured by this barrier and/or contributes to the formation of the pool; and
- Vapour from evaporation of the liquid spilled on the ground.

Figure 3.1 Schematic representation of the different contributions to the source term for an accidental release of liquefied gases



The meteorological conditions (e.g. wind field and temperature) are of primary importance for the toxic/ flammable cloud dispersion. It is therefore very important to set suitable meteorological conditions. These should be set in accordance with several conditions representative of:

- A frequent occurrence: generally a neutral (see below) meteorological condition is chosen; and
- A more specific condition representative of the most severe conditions: generally a stable (see below) meteorological condition is defined.

A well-known tool for the classification of atmospheric stability can be made by using Pasquill atmospheric stability classes [Pasquill, 1974] which vary from A (most unstable atmosphere) to F (most stable). Stability classes may be associated with specific meteorological conditions (see the table below) that take into account conditions such as wind speed, atmospheric turbulence, ambient air conditions, land use and solar radiation. A “roughness length” is also required to characterise the environment of the industrial plants.

Table 3.1 Pasquill atmospheric stability classes

Wind speed at 10 m	**DAY**			**NIGHT**	
	Incident solar radiation			**Nebulosity**	
[m/sec]	**High**	**Medium**	**Low**	**between 4/8 and 7/8**	**<3/8**
<2	A	A-B	B	-	-
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
>6	C	D	D	D	D

Source: Pasquill, 1961

As an example, the French legislation (e.g. Circular of 10th May 2010) requires that a minimal set of atmospheric conditions are defined in accordance with the traditional Pasquill scheme: F3 (very stable) and D5 (neutral), to select the worst configuration.

More complex tools (e.g. 3D tools) allow more complex environment (e.g. presence of obstacles such as building or natural reliefs such as valley or cliff) to be taken into account to understand the process of atmospheric dispersion. However, some efforts of harmonisation on practices and input data are needed in order to achieve homogeneity of the inflow boundary conditions between the different 3D approaches.

The main consequence models

Dispersion models are presented below by order of increasing complexity following the main categories presented in Section 2:

- Gaussian and Integral models; and
- Three-dimensional Models: CFD models and mass consistent model.

The first two (i.e. Gaussian and Integral models) belong to the category of numerical simplified models and use parametric and simplified equations to model atmospheric dispersion.

Gaussian models are based on the Gaussian distribution equation and are widely used to estimate the impact of non-reactive products (those that do not react/ degrade readily in the air). They have a number of limitations, mostly:

- The minimum wind speed for applicability is generally taken as 1 m/s.
- Any vertical component of the wind, which might be generated by up-wash or downwash over buildings, structures and terrain, cannot be included.
- They are only applicable when the release source is sufficiently distant from surrounding buildings for airflow at release height to be undisturbed.

When the discharge is such that it disturbs the atmospheric flow of air, it is inappropriate to use a Gaussian model. Furthermore, some physical mechanisms are not taken into account by Gaussian models. They are:

- The effects of dynamic turbulence, for discharges in the form of a jet with a high emission velocity;
- The effects of gravity for heavy gas discharges; and
- The buoyancy effects for light gas discharges.

The use of integral models allow for these physical mechanisms to be modelled. However, integral models also have some limitations, the main ones are:

- The direction and the wind speed must be constant.
- No effects with the environment (e.g. building) can be taken into account.

The third family of models (3D models) is based directly on the system of Navier-Stokes equations. These models can simulate gas dispersion by taking into account significant phenomena linked to a site such as obstacles or contours. However, it is essential to set the inlet boundary conditions of the 3D model and to correctly simulate a turbulent atmospheric boundary layer above an unobstructed ground or even a flat ground. These are necessary preconditions for the 3D model to be able to estimate the mixing of hazardous cloud due to create turbulence in the atmosphere. Sometimes these requirements are difficult to set accurately (Gorle, 2009). In comparison, simpler Gaussian models include turbulent diffusion parameters, more directly calibrated for the tests. In order to asses this issue, guidelines are continuously being updated in order to set 3D best practices (Franke et al., 2007).

The limitations of all these models have to be kept in mind in the context of Article 4. Calculation of consequences will always be an approximation of what the effects of a major accident could be, if this accident happens to occur.

3.2.2 Dispersion of fire smokes

Description of the physical phenomenon

A fire is a specific emission source of toxic gas because of the mixture of toxic emitted gases, the high temperatures and the general upward movement of smokes due to buoyancy effects. To assess the possible effect distances downwind of a fire emitting toxic smokes, it is necessary to divide the assessment approach in three stages:

- Characterisation of the source of toxic pollutants: the height, the speed and the temperature of the smokes released to the atmosphere as well as the concentrations of toxic gases taking into account the dilution with air entrained by fire combustion;
- Calculation of atmospheric dispersion, and in particular the maximum levels of toxic gases at ground level; and
- Characterisation of the smokes' toxicity by using acute toxicity thresholds.

Effects to be considered

Toxic effects on people have to be assessed according to the pollutants involved in the fire. In case of fire smokes, several toxic gases are likely to be simultaneously released to the atmosphere. The thresholds (often expressed in terms of volume or mass concentration) characterising the toxicity of fumes are not specific to a pure gas but to a mixture of gases, for which a specific equation is used.

Modelling methodology

The source term is the smoke produced by the burning of a liquid pool or by a fire of solid products. It is necessary to determine the composition of the smokes, their speed, their mass release rate and their height of emission. It may also be important to look at the presence of solid particles such as soot and firebrand as they are likely to contribute to the spread of the fire.

It should be reminded that the atmospheric dispersion tool allows the effects of density to be taken into account as smokes behave initially as light gases. In addition, several weather conditions should be considered when the effective release is located above the ground.

The main consequences models

There is no specific method used to determine the source term (e.g. composition and burning rate). However, there is a range of atmospheric dispersion models from the most simple (Gaussian) to the most complex (3D model) that can be used for this task. For the smokes' dispersion calculations, the models described for dispersion of a flammable or toxic cloud can be used. Care will be needed to ensure that the models used are valid for the relevant fields and that they take into account the effects of buoyancy.

3.3 Explosion

The term explosion covers two distinct situations:

- Chemical explosion which usually results from an exothermic reaction of an explosive substance with a combustive (the most common is oxygen from air). This type of explosion produces thermal and pressure effects resulting from the spread of a combustion wave. The main phenomena rising from a chemical explosion are:
    - Decomposition reactions such as solid explosives, unstable substances (see Section 3.3.1),
    - Combustion: ignition and propagation of flame such as Unconfined Vapour Cloud Explosion (UVCE), Gas Cloud Explosion (VCE), explosion of dust in a silo, etc. (see Section 3.3.2).
- Physical explosion resulting from the sudden release of a quantity of product stored at a pressure greater than atmospheric pressure. This type of explosion always produces pressure effects and sometimes thermal effects if the product is flammable. The main phenomena to take into account for physical explosion are:
    - Change of physical state such as explosion of a boiler or BLEVE(see Section 3.3.3),
    - Violent gas depressurisation due to the burst of a gas tank for example (see Section 3.3.4).

These situations could generate emissions of projectiles which is a phenomenon described in Section 3.3.5.

3.3.1 Solid explosives

Description of the physical phenomenon

Solid explosives consist of especially fast and violent chemical reactions that can lead to detonation. Detonation is a violent explosion mode during which the reaction front is propagated by compression, pushed by burnt gases. The other explosion mode is deflagration. In a case of deflagration, the pressure increase is slower and the maximum pressure is lower.

The accident that occurred in Enschede in 2000 constitutes an example of such an explosion.

Figure 3.2 Picture of a solid explosive accident that occurred in Enschede, Netherlands, 13 May 2000 (Source: ARIA)

Effects to be considered

The effects of pressure and temperature on the people and structures surrounding the explosion are to be considered.

Modelling methodology

For these phenomena, the most well-known method is the TNT (trinitrotoluene) equivalent method which has been the subject of numerous publications. This model is generally considered to be robust. The main difficulty of this model arises from the ability of the modeller to estimate the reactivity of the product involved and to "translate" it into a TNT equivalent.

This method was the first used to predict the consequences of any type of accidental explosion. It is based on the assumption that it is possible to reproduce the pressure field generated by a given explosion (e.g. gas or condensed explosive) by detonating the explosive TNT. Thus, the TNT equivalent of a gas mixture is defined as the mass of TNT which, when exploded, generate the same overpressure field as the one generated by the explosion of 1 kg of this explosive gas mixture.

This TNT-Equivalency approach is calculated using the following relationship.

$$M_{TNT} = \frac{a \cdot M_{product} \cdot E_{product}}{E_{TNT}}$$

Where:

- Mproduct represents the mass of product,
- $E_{product}$ represents the energy released by the explosion of 1 kg of product,
- E_{TNT} represents the energy released by the explosion of 1 kg of TNT which is approximatively 4,690 kJ (Brasie and Simpson, 1968), and

- "a" represents the energy efficiency of the reaction, which has different meanings depending on what exactly represents the mass $M_{product}$. Indeed, $M_{product}$ could represent all of the mass of explosive product present in the considered storage, or the mass of explosive product that will actually participate in the explosion:
    - In the first case, "a" is to be considered as global.
    - In the second case, "a" represents the performance of the explosion.

To predict the propagation of the wave, an abacus is used which gives overpressure versus reduced distance (reduced by TNT explosive mass) from the centre of the explosion.

The main consequence models

TNT-equivalent models are used to assess these consequences.

3.3.2 VCE (vapour cloud explosion)

Description of the physical phenomenon

The accidental explosions of gas venting, or VCE ("Vapour Cloud Explosion"), are one of the most feared events when considering the safety of activities associated with flammable gases. This type of accident usually includes the succession of the following events:

- Release into the atmosphere of a combustible material, which is in gas or liquid phase; released liquid fuels can remain in suspension (aerosol formation) or disperse to the ground to form a pool whose evaporation leads to a diffuse discharge of gases.
- Mixture with oxygen from the air to form a flammable volume, in conjunction with the dispersion of the gas cloud.
- Inflammation of this volume.
- Propagation of a flame front through the flammable cloud parts; this flame front works like a piston on the surrounding gas and can be at the origin of the formation of a pressure wave if its propagation speed is sufficient or if the gases are confined. In any case, the flame spreading is accompanied by an expansion of the gases passing through temperatures of hundreds of degrees and up to around 2000°C.

Effects to be considered

Thermal and pressure effects on people and structures are to be considered.

Modelling methodology

The main stages of the effects produced by VCE modelling are as follows:

- Determination of source term: this step is identical to that described for the dispersion of toxic or flammable products.

- Calculation of the dispersion of the flammable cloud: this step is also identical to that described for the dispersion of toxic or flammable products. The objective is to determine the flammable cloud mass and whether the cloud concentration is greater than or equal to the Lower Explosive Limit (LEL).

- Assessment of the pressure effects resulting from the ignition of the flammable cloud and the flame propagation that generates a pressure wave. The flame propagation in the flammable cloud will depend on several parameters:

    - The amount of energy provided by the source of ignition (at a given time);

    - The concentration of the cloud and the propagation speed depend on the richness of the gaseous mixture: the closer to the stoichiometric amount, the faster it will propagate;

    - The turbulence of the jet which speeds up the flame;

    - The confinement of the cloud that speeds up the propagation of the flame; and

    - The presence of obstacles generates turbulence and therefore speeds up the flame.

- Assessment of thermal effects: it is commonly accepted that the distance to lethal and irreversible effects is of the order of magnitude of the distance to the LEL.

The main consequence models

The “multi-energy model” is one of the most well-known methods which represent the underlying process in the propagation of a flame front.

3.3.3 BLEVE (Boiling Liquid Expanding Vapour Explosion)

Description of the physical phenomenon

A BLEVE (Boiling Liquid Expanding Vapour Explosion) is a type of explosion occurring on tanks containing pressurised liquids which are attacked by a fire. The pressure inside the tank is greater than the rupture pressure and generates a catastrophic rupture of the tank. The rapid depressurisation causes a violent boiling (i.e. an explosive boiling) resulting in the instantaneous vaporisation of the liquid. The liberation of energy generates the propulsion of fragments and a wave of overpressure. In the case of flammable vapours, the instantaneous ignition of the mixture with air can also generate a fireball.

Effects to be considered

Heat radiation, overpressure effects and fragments projection on people and structures are expected.

Modelling methodology

Modelling the fireball can be divided in three main steps:

- Inflammation of the cloud and development of the fireball up to its maximum diameter (i.e. the expansion phase).
- Combustion of the fireball: the lifetime of the ball of fire is considered equal to the burning time of the droplets formed during the release of the product to the atmosphere.
- Shut-down phase: the extinction of the fireball is assumed to be complete when the last drops are consumed.

The main consequence models

Related to the thermal effects, the Thornton Research Centre (i.e. Shell research centre) has developed a phenomenological approach entitled the TRC Model or Shield model. The Roberts Method and the Yellow Book are also widely used.

Related to the effects of pressure, most of the available models encountered in the literature are based on a TNT equivalent method (Prugh 1991, Birk 1997, Planas-Cuchi 2004) calculated from the energy provided by the whole amount of released material which is formed by a biphasic mixture of gas and droplets. CCPS has also developed a model to assess these consequences.

3.3.4 Vessel burst

Description of the physical phenomenon

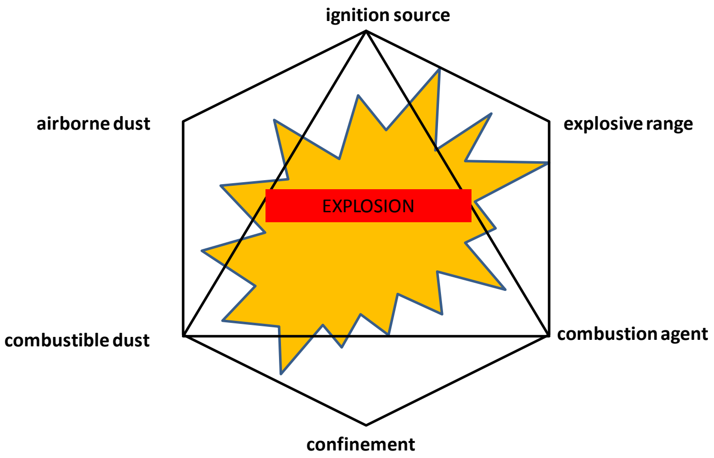
When the pressure in a tank is increasing, the most fragile wall breaks when the rupture pressure is reached. The rupture of the containment allows the release of contained pressure which results in the external propagation of an air pressure wave (i.e. the motion of an overpressure in air).

The catastrophic rupture of a tank may be the result of the following:

- The characteristics of the tank envelope: the mechanical fatigue of the envelope, an excessive corrosion; and/ or
- Involving the contents of the tank: an internal explosion or a slower and accidental pressure increase under the effect of a heating or overfilling.

The typical case of dust explosions requires more specific conditions which can be expressed in the form of the hexagon as presented in the figure below.

Figure 3.3 Specific conditions which generate dust explosion



The consequences of the collapse of a tank are firstly the emission of a pressure wave and secondly the projection of fragments. The pressure wave is the result of the rapid expansion of the gas stored in the tank, or steam if the tank contains a superheated liquid.

Effects to be considered

Effects of overpressure and projectiles on people and structures are to be considered.

Modelling methodology

Several models are available for the calculation of the effects of overpressure due to a tank explosion. They are based mostly on the theory of near-field shock tubes and multi-energy decay curves for the far field.

The main consequence models

Many of the models available to predict overpressure effects are phenomenological models (e.g. Baker's model and Shock Tube-TNT 's model). These models present the advantage of being easy to run in principle. However, in the specific field of the catastrophic rupture of tanks, they do not take into account the progressive failure of the tank, or the geometrical details which can reinforce or, on the contrary, attenuate the field of pressure.

Baker's method (see Section 3.3.5) is one of the most well known models used to predict the projection of fragments.

3.3.5 Emission of projectiles

Description of the physical phenomenon

The term "projectile" means all or part of the equipment that is likely to cause mechanical shocks on a target. The types of projectiles identified are as follows:

- Fragments of a vessel following an explosion (e.g. air gas storage tanks or tank truck).
- Detached parts from a turning piece of equipment after a mechanical failure (e.g. a wind turbine blade).

Effects to be considered

Perforation or the rupture of mechanical structures are expected.

Modelling methodology

The production and emission of fragments are phenomena affected with randomness which depends on various factors such as the energy implementation, the mass and the shape of fragments, and the projection direction as well as the presence of potential obstacles.

Concerning the projection of fragments induced by vessel burst, a plausible projection distance, in line with current knowledge, is in the order of a few hundred metres.

The analysis of past accidents has shown that, for the BLEVE of horizontal cylindrical tanks (e.g. trucks or cars) the majority of the fragments were emitted with a 30° angle around the axis of the tank, because of the rocket effect arising from the ends of the tank. However, the projection of fragments in other directions could not be excluded.

The main consequences models

Models related to the emission of fragments are available, for example the BAKER's model or MOORE's model, developed by the C.C.P.S (Centre for Chemical Process Safety), or INERIS's model Projex.

These models rely on an estimation of the speed of the fragments from an assessment of the energy available to move them.

These pure energetic approaches, assume either the projection of a single fragment whose mass is equal to the mass of the vessel, or the projection of several fragments of identical masses and whose total mass is equal to the vessel. In addition, the trajectory of these fragments cannot be calculated in a simple way. As long as the internal surface of the projectile is subjected to a driving pressure, the projectile gains speed. The fragment impacts the ground at a distance which depends on the combination of momentum, friction of air and gravity. It is not possible to make elaborate assumptions regarding the fragmentation mode of the vessel because of the variability of relevant criteria (e.g. geometric shapes, mass and directions of projection).

3.4 Fire

3.4.1 Description of physical phenomena

One of the most important hazards in an industrial plant is fire. Different types of fire can occur; the main categories are flash fire, jet fire, solid fire, and pool fire.

3.4.2 Flash fire

Description of the physical phenomenon

The flash fire could be defined (in agreement with the "Yellow Book" definition) as the combustion of a flammable vapour and air mixture in which flame passes through that mixture at less than sonic velocity, such that negligible damaging overpressure is generated. The flammable area is bounded by the Lower Explosive Limit (LEL) and the Upper Explosive Limit (UEL).

Effects to be considered

Thermal effects are expected.

Modelling methodology

The main modelling methodology consists of estimating the flammable area bounded by the LEL, which is usually determined by the source term model or dispersion model.

The main consequences models

Most of the models estimate thermal effect distance by considering it as proportional to LEL distance (i.e. predicted by source model or any atmospheric dispersion model). One of the most widely used and cited source is the model of Raj & Emmons (1975, 2007) which is based on the following assumptions (Mudan and Croce, 1988): the geometry of the fuel vapour cloud is two dimensional, the combustion is controlled by natural convection, and the flame propagation velocity with respect to the unburned gases is constant.

3.4.3 Jet fire

Description of the physical phenomenon

A jet fire takes place when a liquid or gas jet is released from an accidental leak and ignites through an ignition source (e.g. a hot surface).

The fuel jet is either released from a pipeline or a hole and happens as described below:

- The fuel jet mixes with air and, by means of an ignition source, begins to burn when fuel and air concentrations are included in the flammability range; or
- After ignition of the jet, the jet fire sets up. From it results a diffusion flame whose appearance depends on the nature of fuel and on the velocity of the fuel jet.

Effects to be considered

Thermal effects are expected.

Modelling methodology

The calculation of the consequences of a jet fire is performed following two main steps.

The first step is related to the source term and more specifically to the mass flow rate. It is calculated with the same tools and models as those used in atmospheric dispersion. The model best suited to use mainly depend on the characteristics of the chemical and on the scenario (i.e. vessel leak or line rupture, pressure and temperature of storage and phase of the compound). It should be highlighted that the phenomenon of combustion does not change the calculation of the source term.

The second step is related to the development of the jet fire itself. The calculation takes into account the following characteristics: the geometric dimensions (i.e. length, diameter and height) and the characteristics related to combustion (e.g. flame emittance). This calculation depends mainly on the characteristics of the product released (i.e. mass flow rate determined in the previous step and heat of combustion). On the basis of the characteristics of the flame, it is then possible to determine the possible impact on people and structures with the assumption of a solid flame.

It should be noticed that the geometry and the position of the flame (particularly its slope) are influenced by the wind.

The main consequences models

The most well-known models are the API RP 521 (American Petroleum Institute, 1973) and the models of Chamberlain (Chamberlain, 1987), Cook (Cook, 1987) and Johnson (Johnson, 1994).

3.4.4 Solid fire

Description of the physical phenomenon

The risk of fire should be considered when a combustible material is likely to encounter a source of ignition of sufficient energy in the presence of oxygen (see the earlier "fire triangle").

A solid fire can occur in warehouse, where the combustion is due to the vapours arising from pyrolysis. In short, fuel emits a specific amount of vapours for a given temperature. This emission of vapours leads to the formation of a fuel-rich zone. As the fuel vapours are rising, the cold ambient air is heated. Once the air-fuel mixture is in the flammability area and in presence of an ignition source, the mixture ignites.

Effects to be considered

Thermal effects on people and structures are to be encountered. For some products, it is also necessary to look at the toxic effects of smoke.

Modelling methodology

For solid fire and particularly warehouse fire (or fires involving products stored outside), one of the most suitable models developed is the FLUMilog model. This model allows the kinetics of the combustion propagation within the storage to be taken into account. This constitutes one of the main differences with pool fires where fire propagates almost instantaneously across the pool. The FLUMilog model allows the calculation of the effects on targets by a similar approach to that described for liquid fires (i.e. a solid flame surrounded by walls whose capacity to play the role of heat shield may evolve over time).

The main consequence models

The FLUMilog model was specifically developed to model the effects of solid fires and more specifically of warehouse fires. It is relied on by some Member States, for example, the FLUMilog model is referenced in the national legislation on warehouses issued by the French Ministry of Sustainable Development.

3.4.5 Pool fire

Description of the physical phenomenon

The description of this physical phenomenon is similar to solid fires. A pool fire occurs, for example, when a flammable liquid spills onto the ground and is ignited.

Effects to be considered

Thermal effects on people and structures are to be calculated.

Modelling methodology

For pool fires, it is necessary to:

- Define the characteristics of the liquid fuel involved (i.e. heat of combustion, burning rate and density);

- Identify the expected size of the liquid pool: surface, dimensions, height of liquid. The height parameter is used to estimate the maximum duration of the fire;

- Determine the characteristics of the flames by using these values and empirical correlations: height (Heskestad, 1984; Hofmann, 1982; Thomas, 1963; Moorhouse, 1982) and emittance values (Mudan and Croce, 1995);

- Estimate the heat flux received by the target taking into account the atmospheric transmissivity (Bagster and Pitalbo, 1989). Depending on the size of the pool and the flames, there are mainly two approaches to calculate the heat flux: a model based on "solid flame" or a model based on a "source point". The presence of thermal screens, that enable all or part of the flame to be hidden, should be taken into account.

The main consequence models

Most existing models use the modelling methodology presented previously but the relevancy of correlations or parameter values should be checked given the characteristics of the burning substance (e.g. hydrocarbon, solvent) and the size of the pool.

3.5 Fire balls

In addition to BLEVE (thermal effects), others types of fire balls can occur:

- Classic boil-over;

- Thin-layer boil-over; and

- Pressurisation of fixed roof storage.

3.5.1 Classic boil-over

Description of the physical phenomenon

A boil over is a brutal foaming phenomenon, involving a tank under atmospheric pressure, impacted by a fire, and resulting from the transformation of liquid water contained in the tank (free water or emulsion) into steam. This phenomenon generates violent fuel projections, extension of flames and formation of a fireball. A boil-over occurs when the following three conditions are met:

- The presence of water that could transform into steam;

- The creation of a heat wave (i.e. a hot zone) that comes into contact with the water at the tank bottom located under the mass of hydrocarbons; and

- A hydrocarbon sufficiently viscous so that the steam, produced by contact between the hot area and the water at the tank bottom, could not easily cross the hydrocarbon from the bottom of the tank.

These conditions mean that the occurrence of the phenomenon is limited to some rather heavy hydrocarbons and with a wide range of boiling temperature (this property is necessary but not sufficient to observe the formation of a wave of heat made with the heaviest compounds of the hydrocarbon) such as fuel oil and crude oil.

Effects to be considered

Thermal effects on people and structures are to be considered. Missile effects are also relevant for consideration.

Modelling methodology

The main stages of the modelling are as follows:

- Determination of the amount of hydrocarbon that participates in the formation of the fireball;
- Estimation of the characteristics of the fireball (i.e. height, diameter and emittance); and
- Characterization of the effects of thermal radiation from the fireball on impacted person and on the environment.

The main consequence models

Some of the oldest models are Broeckmann's model (Broeckmann et al. 1995) and the model jointly developed (Michaelis et al., 1995) by several companies (TOTAL, EDF and INERIS).

An extensive description of the existing models is available in the INERIS's report (Duplantier, 2010).

3.5.2 Thin-layer boil over

Description of the physical phenomenon

The description of this physical phenomenon is similar to the previous one (i.e. classic boil over) and has been observed at small scale and only for domestic heating oil, diesel and kerosene. A thin-layer boil over occurs without the creation of a heat wave. Therefore the steam crosses a thinner layer of hydrocarbons compared to a classic boil over.

Effects to be considered

Thermal effects on people and structures are to be considered. Missile effects are also of relevance.

Modelling methodology

The main stages of the modelling are as follows:

- Determination of the amount of hydrocarbon that participates in the formation of the fireball and its discharge velocity;
- Estimation of the characteristics of the fireball (e.g. height, diameter, emittance); and
- Thermal radiation on the target.

The main consequences Models

The only model available to assess the consequences of this phenomenon was developed by INERIS and mentioned by the French circular of 10 May 2010 defining methodologies for regulatory hazard studies. The model is free of charge on http://www.ineris.fr/aida/consultation_document/files/aida/file/text4593_05.xls.

3.5.3 Pressurisation of fixed roof storage tank

Description of the physical phenomenon

When a fixed roof storage tank catches fire, the pressure of the vapour phase will gradually rise if there is no device to evacuate the excess pressure produced by the evaporation of the liquid. In the absence of devices such as a pressure relief valve, the pressure can reach the rupture pressure of the fixed roof storage tank and thus lead to the release into the atmosphere of superheated liquid. The released superheated liquid would vaporise brutally and may entrain a fraction of the liquid present within the tank. Because of the presence of flames around the fixed roof storage tank, inflammation of the mixture of liquid and gas will lead to the formation of a fireball whose extent will depend on the characteristics of the liquid but also of the rupture pressure of the tank.

Effects to be considered

Thermal effects on people and structures are to be considered. Missile effects are also of relevance.

Modelling methodology

The main stages of the modelling are as follows:

- Determination of the rupture pressure of the fixed roof storage tank. This influences the quantity of products likely to be in suspension;
- Determination of the amount of hydrocarbon that participates to the formation of the fireball;
- Estimation of the characteristics of the fireball (e.g. diameter, height and emittance); and
- Characterization of the effects of thermal radiation from the fireball on an impacted person and on the environment.

The main consequence models

There are only a few existing models that can quantify the fire ball and its effects after the rupture. One model has been described in the French Instruction Technique of 1989 (IT 89). It has a rather conservative approach and was developed by the UFIP (i.e. "Guide méthodologique pour la réalisation des études de dangers en raffineries, stockages et dépôts de produits liquides et liquéfiés" Guide Bleu de l'UFIP – 2003). INERIS has developed a model in order to describe the pre-rupture phenomena (Fouillen and Duplantier, 2011).

3.6 Synthesis

The tables below (see Table 3.2 and Table 3.4) synthesises the elements detailed in the previous sections. The objective of this section is to provide a general overview of the effects that may need to be modelled and the different types of models that can be used for each specific phenomenon. It should be highlighted that these tables do not aim at being exhaustive. However, they present the elements commonly considered when a dangerous phenomenon is to be modelled.

Table 3.2 Dangerous phenomena and types of effects generated

Dangerous Phenomenon	Thermal Effect	Overpressure Effect	Toxic Effect	Missile Effect
Flammable (gas, bi-phase) cloud dispersion	X	X		
Toxic cloud (gas, bi-phase) dispersion			X	
Solid explosives	X	X		
Vapour Cloud Explosion	X	X		
BLEVE	X	X		X
Vessel burst		X		X
Flash-fire	X			
Jet fire	X			
Solid Fire	X		X	
Pool Fire	X			
Boil over	X			X
Thin –layer Boil over	X			X
Pressurisation of Fixed-Roof Storage Tank	X			X

Table 3.3 Dangerous phenomena and models used to assess their consequences

Dangerous Phenomenon	Models
Flammable (gas, bi-phase) cloud dispersion	Gaussian Model Integral Model 3D models
Toxic cloud (gas, bi-phase) dispersion	Gaussian Model Integral Model 3D models
Solid explosives	TNT-Equivalent
UVCE	Multi-energy method
BLEVE (thermal effect)	TRC model Roberts Method Model from TNO ("Yellow Book")
BLEVE (overpressure)	Model from CCPS TNT-Equivalent (Prugh 1991, Birk 1997, Planas-Cuchi 2004)
Vessel burst	Baker’s model (CCPS)
Emission of projectiles	Baker ‘s model Moore’s model (CCPS) Projex model (INERIS)
Flash-fire	Raj & Emmons (1975, 2007) model All atmospheric dispersion models
Jet fire	Chamberlain, Cook, Johnson API RP 521
Solid Fires	Warehouse fire : FLUMILOG model
Pool Fire	Heskestad, 1984; Hofmann, 1982; Thomas, 1963; Moorhouse, 1982 Mudan and Croce, 1995 Bagster and Pitalbo, 1989 Model based on " source point" Model based on "solid flame"
Classic Boil over	Broeckmann's model Total/EDF/Ineris model
Thin –layer Boil over	INERIS model
Pressurization of Fixed Roof Storage	French IT 89 UFIP model INERIS model

4. Main tools available for consequence calculations

4.1 Main available tools and description

A list of the most used tools in European countries to estimate consequences of hazardous phenomena is presented in the table below (Table 4.1). A tool usually consists of software using one or several mathematical models such as these presented in section 3 in order to estimate the effects of a dangerous phenomenon.

This list builds on the results of the survey that has been conducted within the framework of this project. The results were received during autumn 2013. The list does not aim at being exhaustive but does highlight the main tools used within the European Union. The models (presented in section 2) used within the tools are mentioned and general comments regarding the availability of the tools are provided.

As indicated in the introduction to this report, the approaches to consequence and risk assessment considered here are not the only approaches available, and those persons undertaking an assessment under Article 4 could decide to adopt alternative approaches where they are better suited to the particular case or substance under consideration.

Table 4.1 List of Tools for Consequences Calculation of Hazardous Phenomena (non exhaustive)

Name of the tool	Type of model used by the tool	Developer
ADAM (Accident Damage Assessment Module)	Integral model	Major Accident Hazards Bureau (MAHB) Joint Research Centre (Ispra, Italy)
ALOHA	Integral model	National Oceanic and Atmospheric Administration (NOAA) and the U.S. Environmental Protection Agency (EPA).
ARIA RISK	3D model	Aria Technologies
COLOUR BOOKS ("Yellow Book") -	Documented method	TNO
Database on explosives safety distances	Documented method	http://www.reglugerd.is/interpro/dkm/WebGuard.nsf/5ed2a07393fec5fa002569b300397c5a/fda13fad19c734a200256a62004cf40a/$FILE/684-1999.doc
DEGADIS	Integral model	US EPA/ US Coast Guard
EFFECTS	Integral model	TNO
FDS	3D model	National Institute of Standards and Technology (USA)
FLACS	3D Model	GEXCON
FLUENT	3D Model	ANSYS
Fluidyn-PANACHE	3D Model	Fluidyn-Transoft
FLUMILOG	Integral model	INERIS - www.ineris.fr/flumilog
FRED	Integral model	SHELL
Guidelines for Evaluating the Characteristics of Vapor Cloud Explosions, Flash Fires, and BLEVEs	Documented method	Center for Chemical Process Safety (2000).
HGSYSTEM	Integral model	Developed by Shell Research Ltd with the support and sponsorship of industry groups (http://www.hgsystem.com/)
MERCURE_SATURNE	3D Model	EDF
ORDER/FROST	Integral model	GL Noble Denton (UK) . Utilisation limited to developer and industrial partners under a specific contract
PHAST	Integral model	DNV
ProNuSs	Integral model	http://www.pronuss.de/
Similinks	Integral model	http://www.simlinks.es/
SLAB	Integral model	Lawrence Livermore National Laboratory
S.T.A.R. - Safety Techniques for Assessment of Risk	Integral model	ARTES S.r.l. Analisi Rischi e Tecnologie di Ecologia e Sicurezza; http://pc-ambiente.como.polimi.it/model../schede/STAR.htm
TRACE	Integral model	Safer System

Some of the tools, such as PHAST and EFFECTS, consist of several models intended to simulate physical or chemical phenomena involved within hazardous phenomena. As a result, they allow several or all types of dangerous phenomena and their effects to be estimated. Others (e.g. ALOHA and FLUMILOG) focus only on one or two hazardous phenomena. This link between the dangerous phenomena to be modelled and the relevant tools listed in Table 4.1 is highlighted in Table 4.2 below.

Table 4.2 also puts forward (for information) different experimental campaigns that have been conducted for different types of dangerous phenomena. They are conducted to set and validate the mathematical models chosen to be used in the tool. A detailed description of these campaigns is given in section 5. Note that not all of the modelling tools have been validated based on *all* of the experimental campaigns, but all of the tools have been based on at least one of the campaigns.

Table 4.2 Link between the Dangerous Phenomena and the Modelling Tools

Dangerous Phenomena	Main experimental campaign (See Section 5)	Modelling Tools
Flammable/toxic (gas, bi-phase) cloud dispersion	Burro Coyote Thorney Island Prairie Grass Desert Tortoise FLADIS Kit Fox field experiment The mock urban setting test field experiment : MUST	ADAM (Accident Damage Assessment Module) ALOHA ARIA RISK DEGADIS EFFECTS FDS FLACS FLUENT Fluidyn-PANACHE FRED Guidelines for Evaluating the Characteristics of Vapor Cloud Explosions, Flash Fires, and BLEVEs HGSYSTEM MERCURE_SATURNE PHAST ProNuSs Similinks SLAB S.T.A.R TRACE Yellow Book
Solid explosives	Brasie and Simpson, 1968	Guidelines for Evaluating the Characteristics of Vapor Cloud Explosions, Flash Fires, and BLEVEs Yellow Book

Table 4.3 (Continued) Link between the Dangerous Phenomena and the Modelling Tools

Dangerous Phenomena	Main experimental campaign (See Section 5)	Modelling Tools
UVCE	CEC-S DISCOE Harrison and Eyre experimental program. Hjertager MERGE MTH- BA Lathen (Field experiments) RIGOS research programme	ADAM (Accident Damage Assessment Module) EFFECTS FLACS FLUENT FRED Guidelines for Evaluating the Characteristics of Vapor Cloud Explosions, Flash Fires, and BLEVEs HGSYSTEM PHAST ProNuSs Similinks S.T.A.R Yellow Book
BLEVE (thermal effect)	BRITISH GAS tests Birk's tests Tests of the JIVE project Tests of NFPA Test of BAM Stawczyk's tests	ADAM (Accident Damage Assessment Module) Yellow Book EFFECTS FRED Guidelines for Evaluating the Characteristics of Vapor Cloud Explosions, Flash Fires, and BLEVEs HGSYSTEM PHAST ProNuSs Similinks S.T.A.R
BLEVE (overpressure)	BRITISH GAS tests Birk's tests Tests of the JIVE project Tests of NFPA Test of BAM Stawczyk's tests	ADAM (Accident Damage Assessment Module) EFFECTS FRED Guidelines for Evaluating the Characteristics of Vapor Cloud Explosions, Flash Fires, and BLEVEs HGSYSTEM PHAST ProNuSs Similinks S.T.A.R Yellow Book

Table 4.4 (Continued) Link between the Dangerous Phenomena and the Modelling Tools

Dangerous Phenomena	Main experimental campaign (See Section 5)	Modelling Tools
Vessel burst	Tests of Baum	Baker's method Projex (INERIS's method) Shock Tube-TNT 'smodel
Flash-fire	Tests of Raj P.K.	ADAM (Accident Damage Assessment Module) EFFECTS FLACS FRED Guidelines for Evaluating the Characteristics of Vapor Cloud Explosions, Flash Fires, and BLEVEs Database on explosives safety distances HGSYSTEM MERCURE_SATURNE PHAST ProNuSs Similinks SLAB S.T.A.R TRACE Yellow Book
Solid Fires	Wood Crib Fires Experimental Fires in Enclosures	Flumilog FDS
Jet fire	Cook 1987 Bennett 1991	ADAM (Accident Damage Assessment Module) EFFECTS FRED Guidelines for Evaluating the Characteristics of Vapor Cloud Explosions, Flash Fires, and BLEVEs PHAST ProNuSs Similinks S.T.A.R Yellow Book
Pool Fire	Large liquid pool fires (Koseki, 1988) Wood Crib Fires Mudan and Croce's tests	ADAM (Accident Damage Assessment Module) Yellow Book EFFECTS FRED PHAST S.T.A.R.

Table 4.5 (Continued) Link between the Dangerous Phenomena and the Modelling Tools

Dangerous Phenomena	Main experimental campaign (See Section 5)	Modelling Tools
Boil over	Broeckmann's test	Broeckmann 's model INERIS model
Thin –layer Boil over	INERIS test	INERIS model relative to thin-layer boil over
Pressurisation of Fixed Roof Storage	INERIS test	INERIS model relative to pressurisation of fixed roof storage

4.2 Guidance on how to choose a suitable model to assess health consequences

4.2.1 General validity and uncertainties

Modelling tools have been calibrated and validated for a certain set of conditions and distance range. For instance, for toxic or flammable atmospheric dispersion a wide set of conditions that have been tested such as meteorological conditions, topography, types of substances. The validity of the output data is important and extensive literature exists regarding the analysis of models/tools that provide reliable results within a certain distance range. The Yellow Book considers that the diffusion coefficients of Gaussian models are valid between 100 m and 10 km. However, integral models like jet models are considered valid in the near-field, provided there is no significant local effect. 3D models presented in section 2.4are expected to provide reliable results in the near-field and could be used in the context of Article 4 by setting generic worst-case conditions. In any case it is the user’s responsibility to ensure that the modelling results fall into the validity domain of the tool (see section 4.2.2).

It should also be borne in mind that effects constituting a major accident could potentially occur at distances less than those of the validity of these models.

Moreover, it is a well-established fact that all modelling of physical phenomena is imperfect. As described in the report “Consequence modelling” from OGP:

“Any use of software must be within the limitations set out for the software, and even then the analyst must carry out a reality check on the results. For example: a jet fire model applied to a large, high pressure gas release will predict a jet flame several hundreds of metres long; the analyst must consider whether this is credible, or whether the flame will impinge on an obstruction within this distance [...]”.

In addition, from the same source:

“All modelling suffers from uncertainties. For a given set of input (initial) conditions, it is unlikely to match exactly the physical outcome that would result in reality from the same initial conditions. Indeed, numerous physical realisations of the same release would give different results, whereas consequence modelling software gives the same result each time.

Sources of uncertainty in consequence modelling include the following:

[...]

- *Ambient conditions (wind speed, wind direction) do not stay constant over the duration of a release as is modelled,*
- *Box models for dispersion, and models of equivalent complexity for other phenomena, cannot deal with solid or porous barriers (buildings, process units, bund walls, etc.).”*

These elements have to be taken into account when modelling the consequences of a dangerous phenomenon.

4.2.2 Applicability in the context of the assessment methodology of Article 4 - guidance

Selection of the best suited tool

The selection should be justified related to its suitability, taking into account the dangerous phenomena of relevance, the limitations set out for the tool chosen and its validity domain (regarding both input and output data).

To illustrate this first important step, template summaries have been developed for four of the most established modelling tools in Europe: PHAST (DNV), EFFECTS (TNO), ALOHA (NOAA-EPA) and FLUMILOG (INERIS). Their specificities in terms of phenomena or validity domain are presented through a template. A general description of the tool and the physical models which form its basis, but also the tool domain of validity, its outputs (see Section 4.2.2.2) and a short evaluation of its robustness are presented. This information aims at providing elements to assess the relevance of the tool in the context of the assessment methodology under Article 4 of the Seveso III Directive. The templates are provided in Appendix A.

However, due to emergence of new materials, new technologies (e.g. nanomaterials) or new contexts (e.g. large amount of LNG, H_2 in confined spaces, releases of aerosols which might contain bio-active compounds) in which old technologies are used, new scenarios will be generated where the relevance of current models and tools is not obvious because they have not always been validated for these materials, technologies or circumstances. The validation of these tools for the modelling of new scenarios is one of the main challenges today in the field of numerical calculation of consequences. As an example, the European EPHEDRA project forms an initiative that aims to openly and transparently communicate strategies to select the optimal model when different models have different levels of complexity and provide information to get access to the relevant models and tools available.

ADAM tool

JRC/ MAHB is developing a novel software package named ADAM (Accident Damage Assessment Module), as a specific calculation module of the novel JRC tool for area risk assessment. The intended users are Competent Authorities in charge of environment protection and control of Seveso establishments.

The first test session has already started. This consists mainly of benchmarking results obtained on a series of reference scenarios with the outcome of similar software packages (i.e. DNV PHAST and TNO EFFECTS). In addition, a comparison with the results of experimental tests taken from the literature will be carried out. After the testing campaign a beta-version will be available for the Competent Authorities in EU Member States. The policy for a possible distribution of the software for other organisations has still to be established.

ADAM consists of two main modules: Source Terms calculation and Physical Effect Assessment. A vulnerability module is also present. The following dangerous phenomena are covered:

- Toxic dispersion: ADAM uses an improved version of SLAB, which was suitably modified to account of the existing drawbacks for catastrophic releases;
- Explosion (UVCE): ADAM uses TNT Equivalent, multi-energy, and Backer-Strehlow-Tang methods;
- BLEVE;
- Boil Over;
- Jet Fire;
- Pool Fire.

The use of this tool could be a way for authorities to check the relevance of calculation results made by another tool in the context of Article 4.

How to interpret the results of modelling

The estimation of effects distances on human health is the result of analysis and interpretation of modelling tool output data combined with the use of vulnerability data for human beings (i.e. human health thresholds: toxic thresholds, thermal thresholds).

Some tools include vulnerability data for human beings, while others do not. Where they do not, it is necessary to post-process the modelling tool output and to report the post-processing procedure. For instance, atmospheric dispersion tools allow the calculation of the decrease of toxic concentration with distance from the accidental source. The role of the user is to find out the maximum distance at which the concentration exceeds toxic thresholds. Since vulnerability data for human beings will vary hugely across circumstances across the EU, a sensitivity analysis of the results is likely to be appropriate, when conducting an assessment that needs to have EU-wide applicability, such as under Article 4.

Once the validity of the chosen theoretical model is assessed, relative to the dangerous phenomena and the substance involved in the calculation, the objective is to demonstrate the consistency between calculated results and the data reported by the validation documents. For example, when some of the substance characteristics are not well assessed, a sensitivity analysis on these parameters may be required to see the influence on the results and to take into account the uncertainties relative to these characteristics. Also, as highlighted in section 4.2.1, it is the user’s role to ensure that the modelling results fall into the validity domain of the tool as some models/tools provide reliable results within a certain distance range.

The expertise of the user always plays a key role in both the interpretation of the results of modelling and the combination with human health thresholds. Thus, it is not infrequent that several users may obtain very different results in terms of effects distances even if the same modelling tool was used and the same vulnerability data were taken into account. It is very important to remember that a calculation will always be an approximation. Therefore, it is important to underline the need for a third party review of the calculation of effects distances as well as a review of the validity of the results.

5. Synthesis of reference experimental data

In section 4, Table 4.2 puts forward different experimental campaigns associated with different types of dangerous phenomena. These campaigns are usually used to set and validate numerical models.

A list of these experimental campaigns is presented in the table below. This list cannot be exhaustive but many of these campaigns allowed experimental data bases to be set up, on which numerical models have been built and/ or validated. The list is divided into several sections depending on the dangerous phenomena studied. Each of these experimental campaigns is briefly described, with references where more information can be found.

Table 5.1 Synthesis of the reference experimental results available

Experimental campaign name	**Description**	**References / Availability**
Atmospheric Dispersion		
Burro (LNG)	This experiment investigated the downwind dispersion that resulted from a spill of LNG onto a pool of water, 58 m in diameter and 1 m in depth. Concentrations were measured from an array of concentration sensors located on an arc at downwind distances of 57, 140, 400 and 800m.	Koopman, R., and Coauthors, 1982: Burro series data report LLNL/NWC—1980 LNG Spill Tests. Lawrence Livermore National Laboratory report UCID-19075, Vol. 1, 286 pp.
Coyote (LNG)	The Coyote series of liquefied natural gas spill experiments was performed at the naval Weapons Center (NWC), China Lake, California (1971). These tests were a (joint effort of Lawrence Livermore National Laboratory, Livermore, and NWC). There were ten Coyote experiments, five primarily for the study of vapour dispersion and burning vapour clouds, and five for investigating the occurrence of rapid-phase-transition (RPT) explosions.	Goldwire et al., LNG Spill Tests: dispersion, vapor burn, and rapid phase transition, UCID - 199953, Lawrence Livermore National Laboratory, Livermore, California (1983)
Desert Tortoise (ammonia)	In this experiment ammonia was released approximately 1m above the ground to form a two-phase aerosol. Concentration measurements were made from an array of sensors located on an arc at downwind distances of 100 and 800m.	Goldwire, H. C., T. G. McRae, G. W. Johnson, D. L. Hipple, R. P. Koopman, J. W. McClure, L. K. Morris, and R. T. Cederwall, 1985: Desert Tortoise series data report—1983 pressurized ammonia spills. Lawrence Livermore National Laboratory.
FLADIS (ammonia)	The experiment was designed to investigate the downwind dispersion of an ammonia aerosol. Liquefied ammonia was released under pressure through a nozzle situated at a height of 1.5m. These experiments differed from the Desert Tortoise experiments because the release rates were much lower, allowing for the investigation of far field passive effects. In addition, no liquid pool was observed as in the case of the Desert Tortoise experiments	Morten Nielsen, Sören Ott. Field experiments with dispersion of pressure liquified ammonia: Fladis Field Experiments. Risø–R–898(EN). July 1996.

Experimental campaign name	Description	References / Availability
Kit Fox field experiment (SO_2)	The Kit Fox field experiment took place at the Nevada Test Site, where two types of flat ‘‘billboard shaped’’ obstacle arrays were used—the larger ERP array (with height 2.4 m) and the smaller URA array (with height 0.2 m)	Hanna, S.R., Chang, J.C., 2001. Use of the Kit Fox field data to analyze dense gas modelling issues. Atmos. Environ. 35, 2231–2242.
Prairie Grass (passive)	Project Prairie Grass included 68 10-minute samples at 1.5 m along five arcs, 50 to 800 m, downwind from a point source release of sulphur dioxide 46 cm above ground. The 20-minute releases were conducted during July and August of 1956, with an equal number of cases occurring during the daytime and night-time. The sampling was for the 10-minute period in the middle of the 20-minute release. Site roughness was 0.6 to 0.9 cm	Barad, M.L., 1958: Project Prairie Grass, a field program in diffusion. Geophys. Res. Pap. 59. Air Force Cambridge Centre.
The mock urban setting test field experiment : MUST	The MUST field experiment consisted of 37 releases of propylene tracer gas in an array of 120 obstacles at the Dugway Proving Ground desert site. The obstacles were shipping containers, which are about the size of the trailer in a tractor-trailer rig (12.2m long by 2.42m wide by 2.54m high)	Biltoft, C.A., 2001. Customer Report for Mock Urban Setting Test (MUST). DPG Doc. No. WDTC-FR-01-121, West Desert Test Center, U.S. Army Dugway Proving Ground, Dugway, UT 84022-5000.
Thorney Island	Approximately 2000m^3 of an unpressurised mixture of Freon and Nitrogen was released at ground level. Concentrations were measured up to 600m from the release point.	McQuaid, J., and Roebuck, B. (1985) and DG Wilde. Large-scale field trials on dense vapour dispersion. Safety Engineering Laboratory - Health and Safety Executive.
UVCE		
CEC-S	Experimental parameter study into flame propagation in a diverging channel was carried out and to mimic a full expansion process, experiments were performed in a wedge-shaped channel of 2 m length, 0.25 height and a 45 degrees top angle.	J.G. Visser and P.C.J. de Bruijn. Experimental parameter study into flame propagation in diverging and non-diverging flows.TNO Prins Maurits Laboratory report no. PML 1991-C93.
DISCOE	An extended experimental study on flame propagation in 0.08 m diameter vertical obstacle arrays and partially confined between parallel planes.	C.J.M. van Wingerden. Experimental investigation into the strength of blast waves
Harrison and Eyre experimental program.	An experimental rig was designed to represent a pie-shaped segment of a large pancake shaped cloud by using two walls each 30 m long and 10 m high to constrain 4000 m^3 fuel-air-mixture.	A.J. Harrison and J.A. Eyre. The effect of obstacle arrays on the combustion of large premixed gas/air clouds. Comb. Science and Techn. Vol. 52, (1987), pp. 121-137.
Hjertager	An experimental study on gas explosions developing in a 3D corner of 3 * 3 *3 m^3 was carried out. The corner was filled with configuration of cylindrical obstructions. Methane-air and propane-air were used as test mixtures.	B.H. Hjertager. Explosion in obstructed vessels. Course on Explosion Prediction and Mitigation. University of Leeds, UK, 28-30 June, 1993.
MERGE	Gas explosion (H_2, CH_4) developing in various flammable mixtures obstructed by regularly spaced grids were studied on three different scales.	MERGE. W.P.M. Mercx. Modelling and experimental research into gas explosions. Overall final report of the MERGE project CEC contract STEP-CT-011 (SSMA).

Experimental campaign name	**Description**	**References / Availability**
MTH- BA Lathen (Field experiments)	The LATHEN campaign was carried out by Riso. and TüV Nord Deutschland to study the behaviour and the dispersion of continuous liquefied propane gas release under obstacle patchiness	A collection of data from Riso-R-845(EN) dense gas experiments. Morten Nielsen and S. Ott.
RIGOS research programme	A series of small-scale explosion experiments have been performed with vapour clouds containing a donor and an acceptor configuration of obstacles separated by some distance.	A.C. Van den Berg N.H.A. Versloot. The multi-energy critical separation distance.
Pool Evaporation		
Okamoto et al. 2010	Evaporation of several mixtures of organic solvents (including n-pentane, n-hexane, n-heptane, toluene and p-xylene), with no wind and a pool surface of 0,1 m²	Okamoto K. et al. (2010): Evaporation characteristics of multi-component liquid, Journal of Loss Prevention in the Process Industries 23, 89-97, 2010 Okamoto K. et al. (2012): Evaporation and diffusion behavior of fuel mixtures of gasoline and kerosene, Fire Safety Journal, Volume 49, Pages 47-61.
Fingas (1997, 1998)	Large number of evaporation tests with hydrocarbon mixtures like AVGAS, gasoline, diesel fuel, heptane-octane, heptane-octane-nonane, etc. Evaporation from Petri dishes (of diameter 139 mm – 0,015 m²) was observed during several tens of hours, up to four days, with and without wind.	Fingas F. (1997): Studies on the evaporation of crude oil and petroleum products : I. the relationship between evaporation rate and time, Journal of Hazardous Material, Journal of Hazardous Material, 56, 227-236, Fingas F. (1998): Studies on the evaporation of crude oil and petroleum products: II. Boundary layer regulation, Journal of Hazardous Material, *Journal of Hazardous Material, 57, 41-58.*
Mackay & Matsugu (1973)	Evaporation of water, cumene and gasoline from pans of 1,5 m² and 3 m² in outdoor conditions.	Mackay D. & R.S. Matsugu (1973): Evaporation Rates of Liquid Hydrocarbon Spills on Land and Water, Canadian Journal of Chemical Engineering vol 51, August 1973
Esso (1972)	LNG spills (boiling pool) over water (volume 0.73–10.2 m3), pool radius 7–14 m.	G.F. Feldbauer, J.J. Heigl, W. McQueen, R.H. Whipp, W.G. May, Spills of LNG on water—vaporization and downwind drift of combustible mixtures, API Report EE61E-72, 1972
Maplin Sands (1982)	LNG and Propane spills (boiling pool)over water – Volumes of 5–20 m3 spilled in a dyked area. Pool radius ~ 10 m. Twenty-four continuous and ten instantaneous spills were performed in average wind speeds of 3.8–8.1 m/s	J.S. Puttock, D.R. Blackmore, G.W. Colenbrander, Field experiments on dense gas dispersion, J. Hazard. Mater. 6 (1982) 13–41. D.R. Blackmore, J.A. Eyre, G.G. Summers, Dispersion and combustion behavior of gas clouds resulting from large spillages of LNG and LPG on to the sea, Trans. I. Mar. E. (TM) 94, paper 29, 1982. D. Blackmore, et al., An updated view of LNG safety, in: American Gas Association Transmission Conference, Operation Section Proceedings, 1982, pp. T226–T232. G.W. Colenbrander, J.S. Puttock, in: Fourth Int. Sym. on Loss Prev. and Safety, vol. 90, Dense gas dispersion behavior experimental observations and model developments (1983), pp. F66–F76.

Experimental campaign name	Description	References / Availability
BLEVE		
BRITISH GAS tests,	5 experimental BLEVEs of LPG (propane or butane) horizontal vessels(5.659 and 10.796 m^3), with thermal insulation, were carried out : Heating by internal electric resistances Rupture of vessels performed by an explosive charge set up at the top and at the middle of the vessel Inflammation of the released LPG set up by three lances	Johnson, Pritchard, 1990, Large-scale experimental study of boiling liquid expanding vapour explosions (BLEVE), Commission of the European Communities Report EV4T.0014.UK (H). Data were used for the development of TRC Model (Shield model)
Birk's tests	11 experimental BLEVEs of propane horizontal vessels (300 and 375 liters), with a design pressure of 17 or 21.5 bars and a wall thickness of 5 or 6mm, were carried out : Heat flux from combinations of jet fire and pool fire	Birk, Cunningham, Kielec, Maillette, Miller, Ye, Ostic, 1997, First Tests of Propane Tanks to study BLEVEs and other Thermal Ruptures : Detailed Analysis of Medium Scale Test Results, Report for Transport Canada, Dpt of Mechanical Engineering, Queen's University, Kingston, Ontario
Tests of the JIVE project	Aims of the tests : study of rupture pressure and temperature, failure mode and properties of fire ball Propane vessels were exposed to heat flux from liquid propane jet fire (around 1.5 kg/s) Properties of vessels : horizontal, 4,546 litres, design pressure of 18.7bar, test hydraulic pressure of 23.4bar, with a safety relief valve set on 17.2bar, several liquid levels were tested	Terry, Roberts, 1995, Fire protection of tanks, Safe handling of pressure liquefied gases, Londres, Nov 1995.
Tests of NFPA	6 experimental trials of propane BLEVE with horizontal vessels of 1.9m^3 exposed to pool fire or propane (liquid or gaseous) jet fire, several filling liquid levels were carried out	Melhem, Croce, Abraham, 1993, Data summary of the National Fire Proctection Association's BLEVE tests, Process Safety Progress, vol. 12, n° 2, April 1993.
Test of BAM	An experimental BLEVE of a propane road tank of 45m^3 (fill liquid level 22 %) was performed by exposure to a fuel fire : Thermocouples for internal temperature (in gaseous and liquid parts), wall temperature and external temperature Pressure sensors for internal pressure and overpressure Radiation sensors for heat flux produced by the fireball	Ludwig, Balke, 1999, Untersuchung der Versagensgrenzen eines mit Flüssiggas gefüllen Eisenbahnkesselwagens bei Unterfeuerung, Rapport B.A.M. 3215, Berlin, Septembre 1999
Stawczyk's tests	Bleve of LPG vessels (5 and 11 kg) were carried out by heating the bottom (liquid phase) of the vessel Measurements: internal temperature (gaseous and liquid phase), outside wall temperature, internal pressure, overpressure Several liquid levels and container positions (vertically, horizontally) were tested	Stawczyk, 2003, experimental evaluation of LPG tank explosion hazards, Journal of Hazardous Material B96 pp.189-200

Experimental campaign name	Description	References / Availability
Vessel Burst		
BAUM'test		BAUM, 1999, Failure of a horizontal pressure vessel containing a high temperature liquid: the velocity of end-cap and rocket missiles, Elsevier, Journal of Loss Prevention in the Process Industries 12, pp.137-145. BAUM, 2001, The velocity of large missiles resulting from axial rupture of gas pressurized cylindrical vessels, Elsevier, Journal of Loss Prevention in the Process Industries 14, pp. 199-203.
Jet Fire		
Cook 1987	Data obtained from fifty seven field scale experiments is described. The flares employed were of natural gas, with both subsonic and sonic releases having been considered. Experimental data on the size, shape and radiative characteristics of the flares has been obtained, in addition to measurements of thermal radiation incident about the flares.	Cook, D, K, Chem Eng Res Des, 1987, 65(4): 310-317
Bennett 1991 (Spadeadam test site, cumbria)	Large scale experiments (up to ~50m flame length): LPG and natural gas, up to ~55kg mass flow rate Incident radiation flux at different locations and flame SEP were measured.	Bennett, J.F, Cowley, L T., Davenport, J. N. And Rowson, J. J., 1991, Large-scale natural gas and LPG jet fire final report to the CEC, CEC research programme: Major Technological Hazards, CEC contract (Shell Research Ltd)
FIRE (flash-fire, solid fire, pool fire)		
Wood Crib Fires	Experimental correlations relating flame height and mass flow rate have been derived for wood crib fires. The amount of wood and design of the crib have been varied to gain access to a range of mass rates of burning. The effect of wind was also studied in the experiment.	“The size of Flames from Natural Fires”, P.H. Thomas, Symposium (International) on Combustion, Vol.9, Issue 1, 1963, Pages 844-859
Experimental Fires in Enclosures	Experiments involving cellulosic products first, then ethyl alcohol and paraffin oil were conducted in box-type enclosures. The smaller enclosure was 48 cm wide, 101 cm long and 53 cm high. The larger enclosure was 105 cm wide, 203 cm long and 98 cm high (only for cellulosic products). Dual, full-width windows were symmetrically placed at the centre of opposite walls. Fire behaviour was studied with respect to 4 parameters: ventilation parameter, burning rate, gaseous product composition and temperature. For the tested products, 4 distinct regions appeared as the ventilation parameter was varied. An empirical correlation was derived to characterise critical region transition corresponding to extreme danger.	“Some Observations on Experimental Fires in Enclosures. Part 1 : Cellulosic Materials”, A. Tewarson, Combustion and Flame, Vol. 19, 1972, Pages 101-111 “Some Observations on Experimental Fires in Enclosures. Part 2 : Ethyl Alcohol and Paraffin Oil”, A. Tewarson, Combustion and Flame, Vol. 19, 1972, Pages 363-371

Experimental campaign name	Description	References / Availability
The Flumilog Project	Experimental tests aiming at feeding a new calculation method and involving 9 medium-scale set-ups (12 x 8 m² cell of 3.5 m height) and one large scale set-up (36 x 24 m² and 12 m) were carried out. The main parameters investigated were the type and layout of combustible material, type of the boundary walls, type of roof covering and scale effect. Temperature and radiative heat flux measurements were taken for each test. The final full-scale test was undertaken in a warehouse-like building manly composed of a steel structure and containing wooden pallets. Wall collapse, flame height and smoke plume were also observed and filmed.	"Flumilog – A computational method for radiative heat flux emitted by warehouse fire - Part 1: Experimental results" under internal review process. "Description de la méthode de calcul des effets thermiques produits par un feu d'entrepôt "" http://www.ineris.fr/flumilog/node/1
Large liquid pool fires	A compilation of large liquid pool fire tests is summarised. The products were mainly gasoline, kerosene and heptane. Pool diameters range from 0.5m to 20m. Burning rate, flame temperature, radiative heat flux and radiative fraction were reported as functions of pool diameter for the tested products.	"Combustion properties of Large Liquid Pool Fires", H. Koseki, Fire Technology, 1989, Vol. 25, Issue 3, Pages 241-255
Heavy goods vehicle fires in tunnels	Four large-scale fire tests involving Heavy-Goods Vehicles were carried out in the Runehamar tunnel in Norway, which is 6m high, 9m wide and 1600 m long. Different mixtures of cellulose and plastic materials, furniture and fixtures were set on fire. Heat release rate of the tested fires ranged from 66 to 202 MW, and the maximum measured temperatures at the ceiling were from 1281°C to 1365°C. The gas temperature development was represented by a combination of classical fire curves, and a mathematical expression was derived to best fit the fire development.	"Gas Temperatures in Heavy Goods Vehicle Fires in Tunnels", A. Lönnermark, H. Ingason, Fire Safety Journal, Vol.40, 2005, Pages 506-527
Mudan and Croce's tests.	Experimental correlations regarding flames have been derived from trial tests with pool diameter ranges from 1m to 80m with different hydrocarbons (diesel, kerosene).	Mudan, K.S. and Croce, P.A. Fire hazard calculations for large open hydrocarbon pool fires", - SFPE Handbook of fire protection engineering, second edition, National Fire Protection association, Quincy, MA, 1995
Boil over		
INERIS' test	Experimental observations were performed from trial tests with bund diameter up to 60 cm and different hydrocarbons (domestic fuel hydrocarbon, kerosene).	Duplantier. Boil-over classique et boil-over couche mince. INERIS-Omega 13

Some of these experimental data bases are available free of charge. For example, some relevant experimental databases related to atmospheric dispersion are listed below:

- The ASTM standard guide for Statistical Evaluation of Atmospheric Dispersion Models (http://www.harmo.org/astm);
- The Atmospheric Transport and Diffusion Archive (http://www.jsirwin.com/Tracer_Data.html);

- The DAM, dataset for atmospheric modelling (http://rem.jrc.ec.europa.eu/cgi-bin/dam/query2.cgi?R&0&Acronym); and

- REDIPHEM, a collection of data from dense gas dispersion experiments in the field and laboratory (http://cordis.europa.eu/result/report/rcn/18212_fr.html).

However, there is a gap in the availability of experimental data according to all the dangerous phenomena. The reason for this gap may be due to the numerous criteria that need to be taken into account when designing and implementing an experimental campaign such as (inter alia) the technical criteria, the safety criteria and the costs.

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Appendix A: Modelling Tools Templates

Summary

1. ALOHA

ALOHA - Areal Locations of Hazardous Atmospheres	
ALOHA is initially a tool that allows the user to estimate the downwind dispersion and hazardous threats of a chemical cloud based on the toxicological/physical characteristics of the released chemical, atmospheric conditions, and specific circumstances of the release. An enhanced version of ALOHA includes consequence calculations for additional dangerous phenomena such as fires and explosions.	
General information	
Developer Name and contact information	Developed jointly by the National Oceanic and Atmospheric Administration (NOAA) and the U.S. Environmental Protection Agency (EPA). To access ALOHA: http://www2.epa.gov/cameo/cameo-downloading-installing-and-running-aloha contact information : orr.cameo@noaa.gov
Name, version number and release date of the version described here	ALOHA 5.4.4 – July 2013 ALOHA Development History : http://response.restoration.noaa.gov/oil-and-chemical-spills/chemical-spills/response-tools/aloha-development-history.html
Distribution/availability	Freeware

Minimum computer resources required	standard laptop / computer
Some reference documents related to ALOHA	• USER'S MANUAL/February 2007. EPA and NOAA • ALOHA (Areal Locations of Hazardous Atmospheres) 5.0 .THEORETICAL DESCRIPTION (DRAFT Document). R. Michael Reynolds. Seattle, Washington 98115. August 1992
Chemical Database Name	DIPPR chemical data. More than 700 pure chemicals are included.
Level of knowledge/training needed to operate software	ALOHA is designed for easy use and interpretations.

Health Hazard - Dangerous Phenomena

Health Hazard	Toxic effects	Overpressure effects	Thermal effects			
Dangerous Phenomena	Dispersion	UVCE	Flash fire	BLEVE	Jet fire	Pool Fire
Is vulnerability data for human beings included?	Vulnerability data from AEGLs, ERPGs, and TEELs are included.	Vulnerability data from American Institute of Chemical Engineers (1994), Federal Emergency Management Agency et al. (1988), and Lees (2001) are included.				
Short description of model	• Gaussian Model • Heavy gas dispersion calculations model (based on DEGADIS Model, Spicer and Havens 1989)	• Baker-Strehlow – tang method • Explosion is considered to be unconfined with varying levels of congestion	• Flash fire hazard footprint corresponds to 0.6 Lower Explosive Limit (LEL)	• Standard formulas for fireball diameter and burn duration (TNO - 1979	• Chamberlain (1987) empirical formulas are used to describe the geometry of the flame	• Flame is represented by solid tilted cylinder which length is determined from pool diameter using Thomas equation • Average emissive power estimated

				Yellow Book) - Liftoff of fireball is neglected		from the heat of combustion and burn regression rate (constant)
Short description of domain of validity or limitations	Unreliable results with obstructed terrain, low wind speed, very stable conditions, concentration patchiness particularly near the source	ALOHA does not model confined vapor clouds	Assumptions taken for flash fire consequence calculation are considered conservative	Overpressure hazard and missiles are not calculated	- Gas releases from pipe or tank, Two-phase flow from tank - Burning gas is assumed to behave similar to a hydrocarbon (methane, propane and ethylene). - Visible flame described by a frustum of a cone	- Pool is assumed to be circular, uniformly thick, and at the surface level - Pure chemicals burn clean - Flames are optically thick

Main input data	• Release flow rate (term source module : gas/liquid/two-phase leak, pool evaporation,...) or given by user • Meteorological conditions	• vapour cloud concentrations (taken from other ALOHA modules) • level of congestion • ignition time (optional) • choice of hard or soft ignition	• Vapour cloud concentrations (taken from other ALOHA modules)	• Amount and type of chemical • Tank failure pressure or temperature	• Release flow rate (term source module : gas/liquid/two-phase leak, pool evaporation,...) or given by user • Meteorological conditions	• Pool area initial pool thickness • Wind speed
Main output data	• Graphic contour and effect distances: threat zones for toxic, thermal and overpressure effects; distances of the LEL zone within a flammable cloud. Levels of concern can be defined by the user.					
Available documents related to comparisons with experimental data	• ALOHA has been verified by comparisons with DEGADIS • DEGADIS results have been verified by comparisons to field experiments (Havens, 1990) • Technical documentation and software quality assurance for project Eagle-ALOHA (NOAA-EPA, 2006) • Quality Assurance of ALOHA (NOAA) (M. Evans, 1994).					

2. EFFECTS

EFFECTS

EFFECTS performs calculations to predict the physical effects (gas concentrations, heat radiation levels, peak overpressure etc), of the escape of hazardous materials. Models in EFFECTS are based upon the Yellow Book, third edition 1997.

General information

Developer Name and contact information	Developed by TNO Safety software. Contact information : https://www.tno.nl
Name, version number and release date of the version described here	EFFECTS 9
Distribution/availability	Commercial licence
Minimum computer resources required	standard laptop / computer
Some reference documents related to EFFECTS	TNO Safety software EFFECTS Version 9 User and reference manual Yellow Book, Methods for the calculation of Physical Effects Due to releases of hazardous materials (liquids and gases) - Third edition Second revised print 2005 •
Chemical Database Name	Toxic, flammable and thermodynamic properties of over 2000 chemicals.
Level of knowledge/training needed to operate software	Knowledge on whole set of dangerous phenomena.

Health Hazard - Dangerous Phenomena

Health Hazard	Toxic effects	Overpressure effects		Thermal effects		
Dangerous Phenomena	Dispersion	UVCE	BLEVE	BLEVE	Jet Fire	Pool Fire
Is vulnerability data for human beings included?	Vulnerability from users'input					
Short description of model	• passive dispersion, jets, plume rise, dense gas dispersion	• Multi-Energy concept • TNT Equivalent model	• Method derived from Bakers 'method • consequences of construction fragments Green Book 1st edition 1992;	• Dynamic method based on (Martinsen and J.D. Marx, 1999) • Static method (see Yellow Book, third edition 1997	• Chamberlain relations have been extended with the theory of Cook to make this approach applicable for releases of pressurised liquefied gasses (two phase e.g.	• correlation of Burguess and Hertzberg is used to estimate the burning rate • Thomas correlation is used to set the flame height • Flame tilt calculated by means several methods : Moorhouse (1982)
Short description of domain of validity or limitations	• No obstacles	• A special procedure is needed to divide an area into obstructed and unobstructed region. A high level of expertise is required	• There is a relatively small number of experimental validation data	• There is a relatively small number of experimental validation data	• There is a relatively small number of experimental validation data	• method were mainly validated on fuel experimental data

Main input data	• Release flow rate taken from term source module of Effect (gas/liquid/two-phase leak, pool evaporation,...) or given by user • Meteorological conditions	• vapour cloud concentrations calculated from EFFECTS dispersion module	• Amount and type of chemical • Tank failure pressure or temperature	• Amount and type of chemical • Tank failure pressure or temperature	• Release flow rate taken from term source module of Effect (gas/liquid/two-phase leak, pool evaporation,...) or given by user • Meteorological conditions	• Pool area • Release flow rate • Initial pool thickness • Wind speed
Main output data	• Graphic contour and effect distances: threat zones for toxic, thermal and overpressure effects, damage effects (fragments) on structure. Levels of concern can be defined by the user.					
Health Hazard - Dangerous Phenomena						
Available documents related to comparisons with experimental data	• Yellow Book. Third edition Second revised print 2005. • Yellow Book. Methods for the calculation of Physical Effects Due to releases of hazardous materials (liquids and gases).					

3. FLUMILOG

<table>
<tr><td colspan="2">FLUMILOG (FLUx éMIs par un incendie d’entrepôt LOGistique) – A reference method to compute radiative heat flux associated with warehouse fire</td></tr>
<tr><td colspan="2">Based upon classical correlations and real-scale experiments, Flumilog is a software that computes radiation heat fluxes stemming from warehouse fires of practical interest. Various warehouse geometries, combustion products and storage configurations can be taken into account in calculations.</td></tr>
<tr><td colspan="2">General information</td></tr>
<tr><td>Developer Name and contact information</td><td>Developed by INERIS and CTICM
Technical Consortium : INERIS, CTICM, CNPP, IRSN, Efectis
http://www.ineris.fr/flumilog/</td></tr>
<tr><td>Name, version number and release date of the version described here</td><td>Flumilog V3.03 released on 12/09/2012,
Interface V2.13.3 released on 05/06/2013</td></tr>
<tr><td>Distribution/availability</td><td>Freeware</td></tr>
<tr><td>Minimum computer resources required</td><td>General server freely available for all users</td></tr>
<tr><td>Some reference documents related to ALOHA</td><td>Technical document “Description de la methode de calcul des effets thermiques produits par un feu d’entrepôt » available on http://www.ineris.fr/flumilog/flumilog_process</td></tr>
<tr><td>Chemical Database Name</td><td>The software includes its own database for classical warehouse products</td></tr>
<tr><td>Level of knowledge/training needed to operate software</td><td>General knowledge on solid fuel fire and heat radiation. Trainings provided by INERIS, CTICM and CNPP to operate the software</td></tr>
<tr><td colspan="2">Health Hazard - Dangerous Phenomena</td></tr>
<tr><td>Health Hazard</td><td>Thermal effects</td></tr>
<tr><td>Dangerous Phenomena</td><td>Fire</td></tr>
<tr><td>Is vulnerability data for human beings included?</td><td>No</td></tr>
<tr><td>Short description of model</td><td>Classical correlations and mathematical relations are used to compute radiation heat flux including view factor, flame height and radiation emission fraction. An innovative method is used to compute heat release rate associated with the combustion of classical warehouse products. Walls collapsing with time are also taken into account.</td></tr>
<tr><td>Short description of domain of validity or limitations</td><td>Computations are limited to classical warehouse products (palets made of plastic, glass, wood, water, steel, aluminium …) and classical warehouse configurations. Close-field effects (anywhere closer than 10 m from building) are unreliable as convective heat transfer is not taken into account. Warehouse height is limited to 23 m. Up to three buildings can be simultaneously taken into account.</td></tr>
<tr><td>Main input data</td><td>• Building geometry
• Structural materials (steel, concrete …) of walls and roof, including their fire resistance
• Storage configuration : rack storage or bulk storage
• Products details among available list and dimensions of palets</td></tr>
<tr><td>Main output data</td><td>• Maximal mapping in time of radiative heat flux around building for 5 threshold values : 3 kW/m^2, 5 kW/m^2, 8 kW/m^2, 16 kW/m^2 and 20 kW/m^2
• Flame height, fire power, flame emissive power as functions of time
• Calculation note summarizing all the input parameters and radiative heat flux mapping aroung buildings</td></tr>
<tr><td>Available documents related to comparisons with experimental data</td><td>A technical document entitled “Description de la methode de calcul des effets thermiques produits par un feu d’entrepôt » is available on http://www.ineris.fr/flumilog/flumilog_process showing comparisons with radiation heat flux data obtained from real-scale fire experiments (ground surface of burning buildings spanning from 100 m^2 to 800 m^2) performed within the framework of the Flumilog project</td></tr>
</table>

4. PHAST

PHAST	
DNV's Phast software, is a tool used to analyse situations which present hazards to life, property and the environment, and to quantify their severity	
General information	
Developer Name and contact information	Developed by DNV. Contact information : http://www.dnv.com/services/software/products/phast_safeti/index.asp
Name, version number and release date of the version described here	PHAST 6.53
Distribution/availability	Commercial licence
Minimum computer resources required	standard laptop / computer
Some reference documents related to PHAST	See available documents related to comparisons with experimental data
Chemical Database Name	DIPPR chemical data. User can introduce specific substances.
Level of knowledge/training needed to operate software	Knowledge on whole set of dangerous phenomena. Training provided by DNV.

Health Hazard - Dangerous Phenomena

Health Hazard	Toxic effects	Overpressure effects		Thermal effects			
Dangerous Phenomena	Dispersion	UVCE	BLEVE	Flash fire	BLEVE	Jet Fire	Pool Fire
Is vulnerability data for human beings included?	Vulnerability data from users' input						
Short description of model	• near-field jet dispersion • non-equilibrium droplet evaporation and rainout, touchdown • pool spread and vaporisation • heavy gas dispersion • far field passive dispersion	• Three methods : TNT, Baker-Strehlow method, TNO Multi-energy	• Overpressure effects : Method largely based on CCPS Guidelines	• The envelope is given to the LFL and to half the LFL.	• Radiation Effects from the fireball : DNV Method • Roberts - HSE Method, Yellow Book Method	• Single and two-phase Jet Fire • Shape of the flame Shell model and the API RP521 model • Three methods to calculate radiations based on :Jonhson method (1987), Cook model (1990), Chamberlain model (1987) •	• The burn rate and surface-emissive power formulations are modified for a general –not specifically hydrocarbon) compound • Thomas correlation is used to set the flame height • Excess air entrainment into the poll fire is calculated based on a procedure developed by Delichatsios

Short description of domain of validity or limitations	• Low wind speeds cannot be treated. Effect of topography or buildings and obstacles on flow and dispersion cannot be modelled. • for the momentum jet release the direction of the jet must be in a vertical plane in the wind passing through the source	• A special procedure is needed to divide an area into obstructed and unobstructed region. A high level of expertise is required	• See BLBL (Bleve Blast) document	• Assumptions taken for flash fire consequence calculation are considered conservative	• See BLEV (Fire Ball) document	• See JFSH (Jet Fire) document	• A cylindrical shape of the pool fire is presumed
Health Hazard - Dangerous Phenomena							
Main input data	• Release flow rate (term source module : gas/liquid/two-phase leak, pool evaporation,...) or given by user • Meteorological conditions	• vapour cloud concentrations calculated from Phast dispersion module	• Amount and type of chemical • Tank failure pressure or temperature	• Vapour cloud concentrations calculated by dispersion model	• Amount and type of chemical • Tank failure pressure or temperature	• Release flow rate (term source module : gas/liquid/two-phase leak, pool evaporation,...) or given by user • Meteorological conditions	• User-specified burn rates and fire diameters • Pool area • Release flow rate • Initial pool thickness • Wind speed
Main output data	• Graphic contour and effect distances: threat zones for toxic, thermal and overpressure effects; distances of the LEL zone within a flammable cloud. Levels of concern can be defined by the user.						
Available documents related to comparisons with experimental data	• SMEDIS. "Model Evaluation Protocol". Cambridge Environmental Research Consultants Ltd. Ref. No. SMEDIS/96/8/D Version 2.0 7 December 2000 • A. HOLT, H.W.M WITLOX. "Validation of the unified dispersion model". Consequence modelling documentation, DNV software. March 2000 • Overpressure effects : Method largely based on CCPS Guidelines • BLBL (Bleve Blast) Theory Document. Oct 2005 • BLEV (Fireball) Theory Document. Oct 2005. • JFSH (Jet Fire) Theory Document. Oct 2005 • POLF (Pool Fire) Theory Document. Oct 2005.						