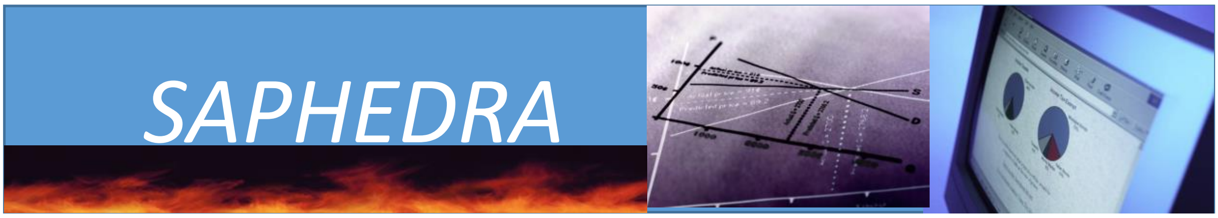
December 2015

S A P H E D R A

SAPHEDRA - Building a European Platform for evaluation of consequence models dedicated to emerging risk

Identification of existing tools for the modelling of hazardous phenomena

SAPHEDRA is a project funded in the framework of the ERA-NET SAF€RA "Coordination of European Research on Industrial Safety towards Smart and Sustainable Growth"



SAPHEDRA - Building a European Platform for evaluation of consequence models dedicated to emerging risks

The research leading to these results has received national funding in the framework of the ERA-NET SAF€RA "Coordination of European Research on Industrial Safety towards Smart and Sustainable Growth" (FP7 / 2007-2013 / GA n° NMP4-SA-2012-319092).

Report D1 "Identification of existing tools for the modelling of hazardous phenomena"

Published by
TNO - Princetonlaan 6
3584 CB Utrecht
P.O. Box 80015
3508 TA Utrecht
The Netherlands

TNO innovation for life

www.tno.nl

Authors:
Hans Boot

Contributors:
SAPHEDRA Consortium

Utrecht, December 10, 2015

Princetonlaan 6
3584 CB Utrecht
P.O. Box 80015
3508 TA Utrecht
The Netherlands

www.tno.nl

T +31 88 866 42 56
F +31 88 866 44 75

TNO report

Identification of existing tools for the modelling of hazardous phenomena

Date	30 Junel 2015
Author(s)	H.Boot
Copy no.	<copy no>
No. of copies	<no.of copies>
Number of pages	487
Number of appendices	<number of appendices>
Customer	<Customer>
Project name	SAPHEDRA WP1
Project number	<Projectnumber>

Contents

1 Introduction

An accidental release of hazardous chemicals will typically result in a number of potential physical effects. Depending on the properties and the storage conditions of the material, several typical phenomena may occur: fire, explosions or toxic exposures. In order to evaluate the potential danger, so-called “consequence assessment” models can be applied to predict the physical behaviour, or the phenomena occurring upon release of a hazardous substance.
Work package 1 of the Saphedra project, “Building a European Platform for evaluation of consequence models”, is aimed at an identification of existing tools for consequence modelling. In order to be able to identify and describe these tools, a classification into various phenomena is proposed.
The following chapter contains a description of typical phenomena, associated with the release of hazardous materials. This classification is then applied to collect and describe various tools in the form of a spreadsheet. This spreadsheet is to be seen as an integral part of the report of WP1.

2 Classification of phenomena incorporated in consequence models

2.1 Families of phenomenon

Typical “consequence models”, predicting the consequences of a release of hazardous materials, provide results that can be divided in different categories of phenomena:

1) Release models: predict a source rate and/or typical conditions (temperature, exit pressure speed, liquid fraction) of the hazardous material in case of an accidental release. Release models are also being referred to as “source” term models.
2) Fire models: predict the shapes and dimensions of flames and the resulting heat radiation or heat load as a function of distance due to fire phenomena.
3) Explosion models: predict the peak overpressure, dynamic pressure and potentially pressure impulse as a result of an physical explosion.
4) Dispersion models: are used to describe the spreading and diluting behaviour of an accidental release of hazardous material in the atmosphere. Dispersion models usually provide results in terms of gas concentrations versus distance and / or time.

Apart from model describing the these physical phenomenon, so-called damage relations are used to translate a physical phenomenon to resulting damage. This can be either in terms of human injury or lethality, or in terms of damage to constructions and installations. Some models first calculate physical results, such as level of heat radiation, overpressure or substance concentration, and then translate these outcomes into physical damage, such as estimated probability of lethality or expected property damage. Straightforward damage relations simply relate physical damage directly to exposure threshold limits being exceeded.

In order to facilitate the description of various models a further distinction in these phenomenon families is proposed.

2.2 Release (source term) models.

Since a release of hazardous material (often referred to as a “Loss of Containment”: LoC) can be a leak or even a catastrophic failure, the Loss of Containment phenomena are often described as “Continuous LoC”, “Instantaneous LoC” or “Semi-Continuous LoC” (time limited continuous release).
Apart from this, release models need to be adapted to the physical state of the product. For specified temperature and pressure, the chemical product studied can be solid, liquid, at boiling conditions (saturated liquid), gaseous, or supercritical. Releases of solids are only studied in specific (exceptional) cases. Releases of mixtures are more complicated, due to the different physical properties of the contributing components (vapour pressure, boiling temperature). Above critical conditions, a distinction in gas or liquid is no longer possible, and these supercritical fluids require a dedicated modelling of substance thermodynamic properties (density influences).
Release models need to consider the type of equipment from which they are released. Typically, different models are used for vessels, short pipes connected to vessels and long pipelines. Models for long pipelines require a description of dynamic pressure waves occurring in long pipelines whereas vessel models include a modelling of vessel dynamics (temperature, pressure, liquid level influencing outflow). For pressurised equipment, a distinction is sometimes made between orifice conditions and conditions following further expansion to atmospheric pressure.
The state of the product can change during expansion to atmospheric pressure. Superheated liquids may evaporate prior to impact with the ground. Evaporation goes very rapidly if the product is gaseous at ambient pressure (flashing). Releases of pressurised gasses on the other hand may cool down during expansion to atmospheric pressure and could partly condensate to liquid or partly turn solid (e.g. CO_2). If liquid (or solid) pools are formed, evaporation from the pool is often relevant for dispersion. Evaporation is usually considered as being part of the source term calculation. Different evaporation models exist for boiling and for non-boiling conditions and for different surface types (e.g. land or water).
Lastly, formation of aerosols during depressurisation can be important as small droplets can be dragged along with the vapour in the cloud for long distances. The occurrence of liquid droplets in the vapour cloud will influence the behaviour during the following dispersion.

The main results of release models are a source rate (amount of material per unit time) and the corresponding conditions (temperature, pressure, density, liquid fraction etc.). For instantaneous releases (gas or pressurised liquefied gas) releases, the initial dimensions of the hemisphere, resulting density and potential rain-out (formation of liquid pool) are the most important results to be obtained.

A proposed distinction in release models would be:
- Gas outflow models
- Liquid outflow models
- Pressurised liquefied outflow models
- Flash and evaporation models

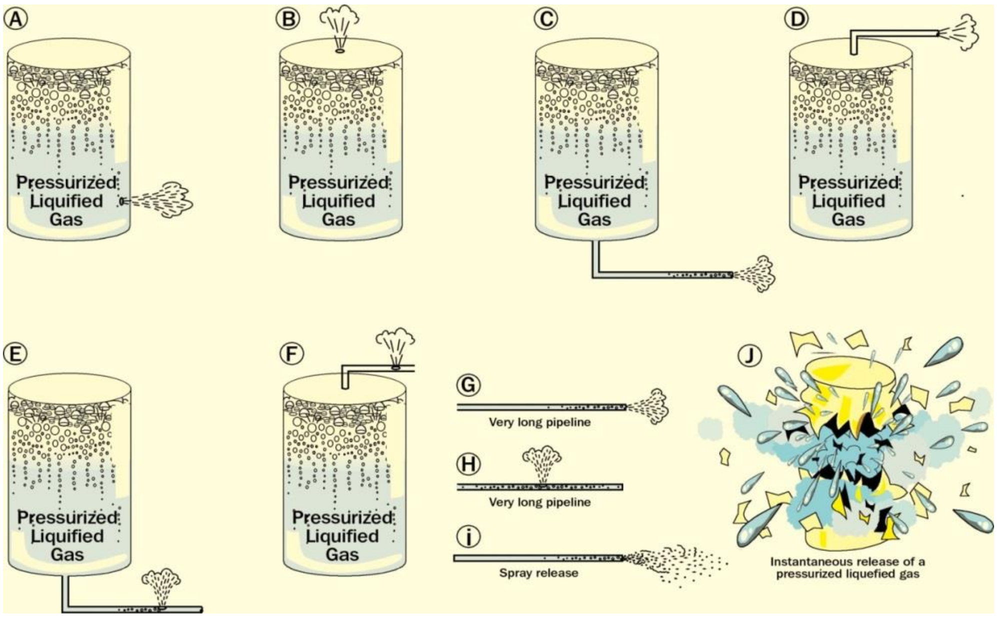


Figure 1 Illustration of various modes of release for a pressurised liquefied gas

Typical source rate models are aimed at predicting a release rate and resulting release conditions. Apart from results like mass flowrate, exit temperature and exit velocity, the resulting density and potential liquid fraction will have a major influence on following dispersion process.
Typical inputs: Release conditions (pressure, temperature, substance definition, hole dimensions, coefficient of discharge
Typical output: Release rate, release conditions (temperature, liquid fraction, speed, expanded diameter)

2.3 Fire phenomenon models

Several types of fire can be distinguished, depending on the state/phase of the product involved:

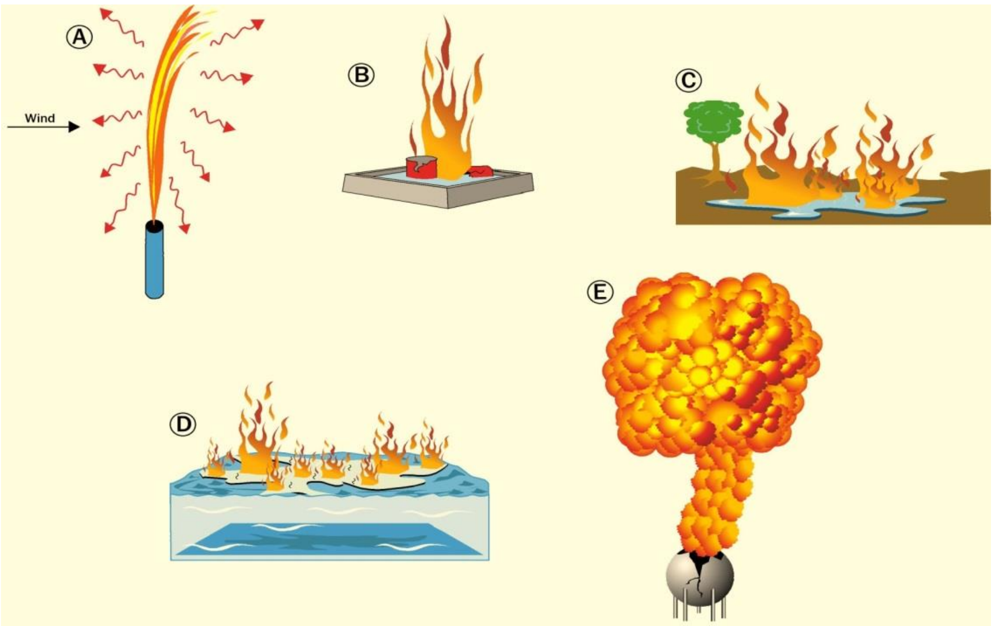


Figure 2 Typical fire phenomena: jet fire, pool fire (in tank pit, freely spreading, on water) and a BLEVE fireball

2.3.1 *Jet fire phenomenon*

A jet fire model describes the fire phenomenon of a gaseous or two phase (e.g. Propane at saturated conditions) continuous release. A jet fire model (sometimes referred to as “torch fire”) generally describes the size and shape of a cone or cylindrical shaped fire surface, and provides information about the heat radiation emitted from this surface. These data can be combined in order to obtain heat radiation intensity at various locations surrounding the jet fire. Lift-off describes the effect that a flame is not combustible near the orifice. The lift-off distance depends on the release velocity among others. The flame direction depends on the release direction, the buoyancy of the flame and the wind. A jet fire is typically straight near the orifice and becomes curved as wind and buoyancy effects take over, Many models use cones, frustum of cones or even cylinders as simplifications for this complex (banana) shape.
Two-phase and liquid releases can only burn as a jet fire if the product is sufficiently volatile.

Jet fire consequence models

The main effects to be considered for jet fires are heat radiation and direct flame contact on people and structures. Typical jet fire consequence models can be dedicated to outflow phases (gaseous / 2 phase or even liquids) or limited to specific outflow directions (vertical or horizontal).
In case the jet flame model incorporates damage relations, typical results will also include heat dose or even lethality and 1st and 2nd degree burns.

Typical inputs: released product (including physical and chemical properties), release conditions (temperature, pressure, orifice size), release direction and meteorological parameters (wind speed, wind direction vs. release direction, humidity), Typical outputs: flame shape, flame surface heat intensity or temperature, heat radiation contours and heat radiation intensity at specific location.

2.3.2 *Pool fire phenomenon*

A pool fire describes a flame surface above a burning liquid pool. Typically, it is assumed that the pool is circular, in which case the pool fire has a cylindrical shaped flame geometry, which is tilted by the wind.

Pool fire consequence models

The main effects to be considered for pool fires are heat radiation and direct flame contact to people and structures.
Typical results of a pool fire model contain flame shape and orientation, heat radiation intensity of the flame, and heat radiation levels at various distances from the pool.

For pool fires, it is usually required to:

- Define the characteristics of the liquid fuel involved (i.e. heat of combustion, burning rate and density); These are empirical values listed in publications or based on Burgess formulation.
- Identify the expected size of the liquid pool: maximum surface, dimensions, height of liquid. The liquid height parameter is used to estimate the maximum duration of the fire;
- Determine the characteristics of the flames: height and radiation emittance values;
- Estimate the heat flux received by the target taking into account the atmospheric transmissivity. Depending on the size of the pool and the flame dimensions, there are mainly two approaches to calculate the heat flux: a model based on "solid flame" or a model based on a "source point".

Common modelling approaches are described in Yellow Book (2005), HSE (2002) and CCPS (2010) publications.
Dedicated models might deal with non-cylindrical pool shapes, which can be applied when the liquid spreading is limited by bunds or other local geometric obstacles. The presence of thermal screens or obstacles, that block radiation should be taken into account, but are usually only incorporated in 3D fire models.

Typical inputs: released product (including physical and chemical properties), shape and size of the pool, meteorological parameters (wind speed, humidity),
Typical outputs: flame shape, flame surface heat intensity or temperature, heat radiation contours and heat radiation intensity at specific location.

2.3.3 *Fire ball phenomenon*

A fireball describes a typical “sphere shaped” fire phenomenon, which itself can be the result of various thermodynamic effects: an instantaneous pressurised gas release, a pressurised liquefied gas **BLEVE**, an atmospheric liquid tank **Boil-over** or a (atmospheric tank) **fixed roof pressurisation**.

2.3.3.1 *Fireball due to an instantaneous release of pressurised gasses(flashfire)*

An instantaneous release of pressurised flammable gasses can cause a sort of fireball phenomenon upon ignition. The pressurised gasses expand after rupture of

the tank. Ignition initially creates a hemispheric fire that further expands as air and combustion gasses get entrained. As a result of expansion and combustion (temperature increase) and resulting buoyancy effects the fire will rise up, creating a more spherical or mushroom shaped flashfire.
If pressurised gasses are released from transportation pipelines, ignition may give a phenomenon that initially looks like a fireball but subsequently transforms into a jet fire.

Figure 3 Leak, ignition and resulting fireball and jet fire for a propane release

Typical inputs: released product (including physical and chemical properties), release conditions (temperature, pressure, volume) Typical outputs: fireball diameter, elevation, flame surface heat intensity or temperature, heat radiation contours and heat radiation intensity at specific location.

2.3.3.2 *Fireball due to an instantaneous release of pressurised liquefied flammable substances (BLEVE)*

An instantaneous release of a pressurised liquefied flammable substance can cause a typical fireball phenomenon upon ignition. The pressure decrease associated with the rupture of the tank causes flash evaporation of the superheated liquid and subsequent expansion. Ignition creates a fireball that further expands and rises as air and combustion gasses get entrained and burning evolves. The combined effect looks like a mushroom.

More advanced models describe the dynamic behaviour of the fireball, less advanced models use a static fireball radius and fixed elevation.

Typical inputs: released product (including physical and chemical properties), release conditions (temperature, pressure, volume) and environmental conditions (humidity), Typical outputs: fireball diameter, elevation, flame surface heat intensity (SEP=surface emissive power) or temperature, heat radiation contours and heat radiation intensity at specific location.

To describe this behaviour, specific fireball models have been developed which are sometimes called BLEVE models. Although the abbreviation BLEVE itself refers to an explosion phenomenon (Boiling Liquid Evaporation Vapour Explosion), the potential rupture of a propane vessel BLEVE is most feared for its fireball.

Apart from a heat radiation effect, the BLEVE itself will also create overpressure damage and damage due to fragmentation. These overpressure phenomenon can be modelled with dedicated “explosion models”.

2.3.3.3 *Fireball due to a boil-over.*

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 at the bottom of a tank that could rapidly transform into steam (i.e. temperature near or above atmospheric boiling point);
- 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, cannot easily escape 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.

The boil-over phenomenon can also be limited to a so-called “thin layer boil-over”. A thin-layer boil has been observed at small scale and only for domestic heating oil, diesel and kerosene. It occurs without the creation of a heat wave. Therefore the steam crosses a thinner layer of hydrocarbons compared to a classic boil over.

Boil-over fireball models

INERIS has developed two specific models for both the full-scale and thin-layer boil-over. One of the most important outcomes is the time needed before a boil-over occurs. It uses a fixed diameter/height ratio and typical SEP value of 150 kW/m2.

2.3.3.4 *Fireball due to fixed roof pressurisation*

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.

Fixed roof fireball models
There are only a few existing models that can quantify the fireball 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 (UFIP, 2003). INERIS has developed a model in order to describe the pre-rupture phenomena (Fouillen and Duplantier, 2011).

2.3.4 Flash Fire phenomenon

A flammable cloud, created by a release of flammable products, can create a so-called flash-fire. The name illustrates the speed of this phenomenon, the flammable cloud will burn rapidly, because the chemical is pre-mixed with air. The requirements for this phenomenon are a mixture of a flammable gas with air (or oxygen), at concentrations between LFL (Lower Flammability Limit) and UFL (Upper Flammability Limits). Ignition of this mixture generates a fire with a flame front that typically moves with speeds between 1 and 10 m/s.
Because the duration of the flash fire is short, the integrated heat load outside the cloud will be low, so the phenomenon is mainly relevant for objects within the flammable cloud. The shape, size and location of a flammable cloud is typically a function of time, and is generally calculated with the use of **dispersion models**. If a flammable cloud drifts into a confined or congested area, ignition of the flammable cloud might also lead to a vapour cloud explosion (overpressure) phenomenon. This vapour cloud explosion is modelled using dedicated explosion models.

Flash fire models
The main modelling methodology consists of estimating the flammable area bounded by the LFL, which is usually determined by the source term model or dispersion model. Apart from the direct flame contact, heat radiation itself may be considered. Most of the models estimate thermal effect distance by considering it as proportional to LFL distance (i.e. predicted by source model or any atmospheric dispersion model). Some users use 50% LFL as a boundary, to take into account turbulent effects associated with fires.

Typical inputs: Source rate, meteorological conditions
Typical outputs: flash fire footprint.

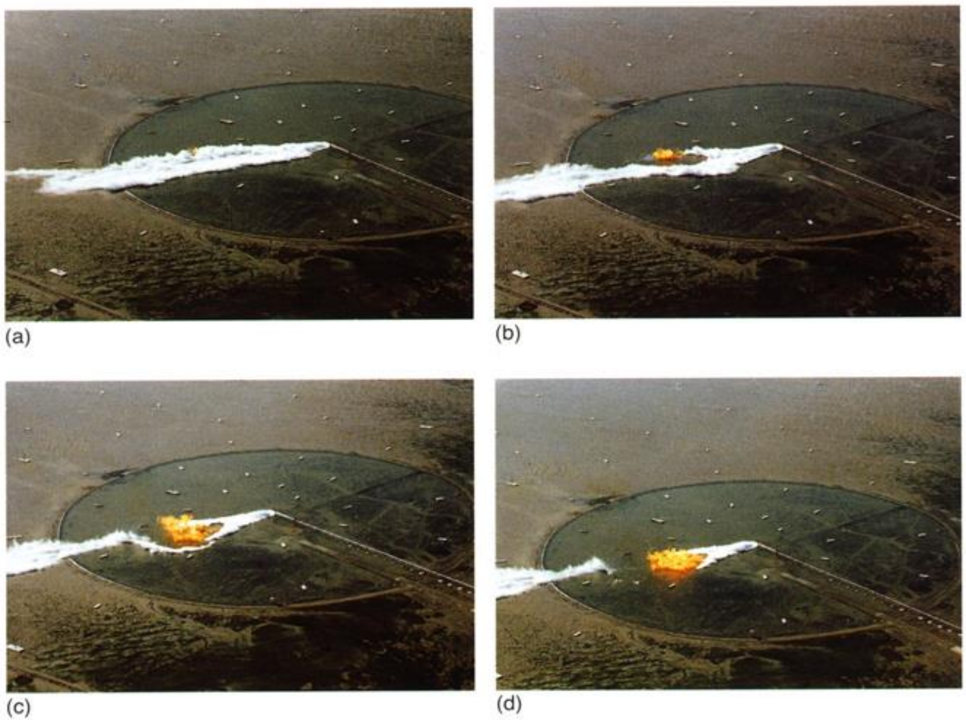


Figure 4 Flash fire upon ignition of a flammable cloud, the flame potentially travels back to the source creating a jet fire (Maplin sands trails, reproduced by permission of Shell research)

2.3.5 *Warehouse Fire phenomenon*

Two different types of phenomena can be considered for warehouse fires:

1. Warehouse fires emit heat radiation from the burning surfaces of the warehouse (doors, window panes, walls and roofs);
2. Combustion products created in a warehouse fires can be toxic and toxic powders that are stored in a warehouse can be released in a fire without combustion.

The risk of warehouse fires should be considered when a packaged combustible material is likely to encounter a source of ignition of sufficient energy in the presence of oxygen.
Because storage warehouses may contain large quantities of flammable materials, packaged inside plastic or paper board enclosures, small warehouse fires can easy escalate into large warehouse fires. The storage locations for IBC's (Intermediate Bulk Containers, plastic containers with a volume of 1 m^3) filled with various flammable substances are also very sensitive to these escalating events. These stacked containers will easily fail upon exposure to flames/heat and the released flammable liquid will quickly spread the fire. Apart from the direct flame and heat radiation effects, the formation of toxic combustion products or dispersion of toxic powders may need to be evaluated as well.

Warehouse fire modelling

For warehouse fire (or fires involving packaged 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).
Warehouse fire models can also be dedicated to establishing the “external risk” due to the toxic combustion products. These potential toxic consequences are however highly dependent of the occurrence of plume-rise effects and smoke composition, requiring detailed knowledge of fire evolution in time and stored products.

2.4 Explosion phenomenon models

The term explosion covers two distinct situations:

- Chemical explosion which usually results from an exothermic reaction 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
  - Combustion: ignition and propagation of flame such as Unconfined Vapour Cloud Explosion (UVCE), Gas Cloud Explosion (VCE) or Dust explosion in a confined space.
- 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
  - Violent gas depressurization due to the burst of a pressurized gas containment.

An explosion model typically describes peak-pressures, dynamic pressure, pressure impulse and duration of an explosion overpressure wave. Explosions could also generate emissions of projectiles

2.4.1 Pressure vessel burst

This describes a physical explosion due to a full (catastrophic) rupture of a pressure vessel. This can be any process vessel or reactor (runaway reaction) but also the BLEVE (Boiling Liquid Expanding vapour Explosion) itself is typical pressure vessel burst overpressure phenomenon.
When the pressure in a tank is increasing, the most fragile part of the tank will break 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). Rupture of a tank also leads to the projection of missiles.
The catastrophic rupture of a tank can be caused by:

- Weakening of the tank envelope (tank wall), e.g due to mechanical fatigue of the envelope, excessive corrosion or external heating;

- Internal pressure build-up, e.g. due to overfilling, internal overheating or exothermic reactions and internal explosions (ignition of combustible fumes within the tank).

Pressure vessel burst models
For vessel burst, effects of overpressure and projectiles on people and structures are to be considered.

Models describing the vessel burst usually report overpressure as a function of distance (having a circular footprint) and throwing range of vessel fragments (projectiles).
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 have 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 is one of the most applied models used to predict the projection of fragments. 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. These projectile 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).

BLEVE overpressure models
Most of the available BLEVE overpressure 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. Also Baker, CCPS and van den Berg have developed a model to assess these consequences.

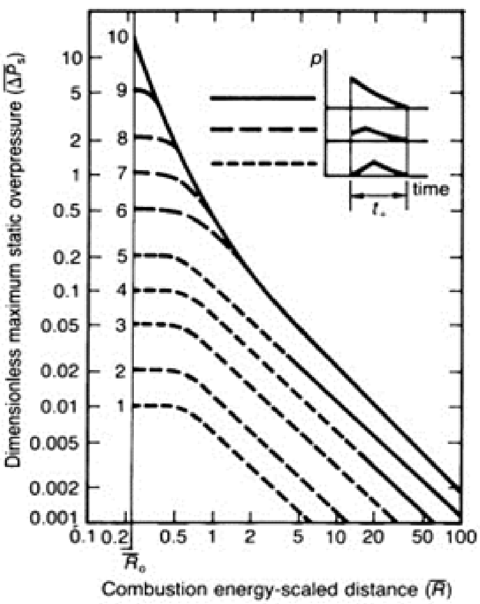
2.4.2 Vapour Cloud Explosion
This explosion is caused by a (partly) congested or confined flammable cloud which is ignited. Because this congestion (e.g. pipes, installation parts, trees or parked cars) or confinement (e.g. solid walls) will block the free expansion of combusting products and/or increase the flame surface area due to turbulence, this will lead to flame acceleration where a deflagration (subsonic combustion propagation) may eventually turn into a detonation (supersonic flame front).

Vapour cloud explosion models

Several methods have been developed to predict the blast strength of the resulting overpressure wave. Difficult parameters to assess are the area or volume that contribute to the explosion and the maximum explosion strength (overpressure) that is generated. Simple models correlate the explosion strength to a TNT equivalent, more dedicated models such as BST (Baker Strehlow Tang) or ME (Multi Energy) use a blast strength classification which can be based on congestion/confinement and (chemical) laminar burning speed considerations.

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 fuel concentration is greater than or equal to the Lower Flammability Limit (LFL).
- Assessment of the part of the flammable cloud that is involved in the explosion (potential explosive mass of congested or confined volume)
- 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 parameters describing ignition strength, obstacles generating congestion, confinement (walls, ceilings) and mixture flame speed.



$$\overline{\Delta P_s} = \frac{P_{static} - P_o}{P_o}$$

P_o = ambient pressure

P_{static} = static total blast pressure

$\overline{R} = R[P_o / E]^{1/3}$

R = distance from the center of explosion

E = total available combustion energy

Figure 5 Multi Energy curves illustrating dimensionless overpressure versus dimensionless distance for 10 blast classes

For offshore applications, the risk of VCE's is highly relevant, leading to application of detailed CFD based methods to evaluate local 3D geometry influences on concentration distribution and overpressure calculations. These CFD methods will be described in dispersion models.

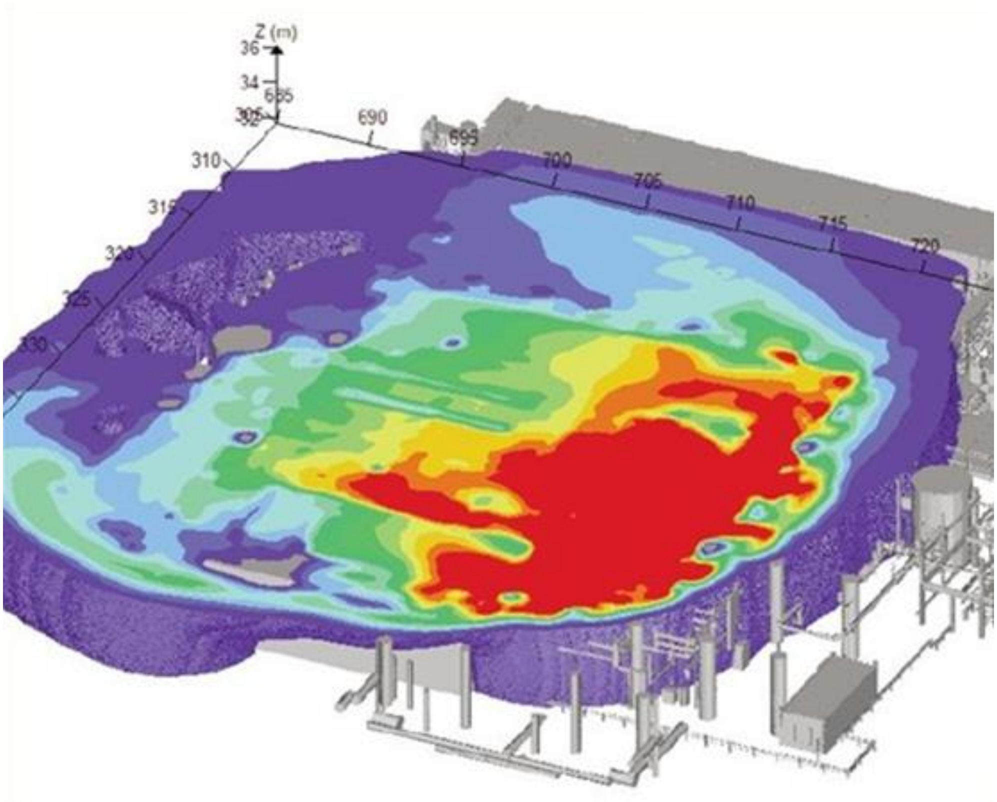


Figure 6 Typical result of a CFD based flammable cloud and VCE overpressure calculation

2.4.3 *Solid explosions*

Typical solid explosive substances are capable of providing detonation phenomena without the need of any congestion or confinement. Solid explosion models originated from the military and mining application, but because of to the explosive properties of chemical compounds such as Ammonium Nitrate (a material used in fertiliser production) these models are used in chemical industry as well.

Solid explosion models

For this phenomena, the most used method is the TNT (trinitrotoluene) equivalent method, which has been the subject of numerous publications. This model is generally considered to be very robust. However, the main difficulty of this model arises from necessity for the user to estimate the reactivity of the product involved and to "translate" it into a TNT equivalent. Fortunately, these TNT equivalence factors have been investigated and published for several commonly used potential explosive substances (e.g. Ammonium Nitrate in various grades),

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.

Figure 7 Toulouse 1974, A crater of 50 m wide and 10 m deep resulting from an explosion of Ammonium Nitrate

Combustible dust explosions need to be separated from solid explosions because these combustible materials will only provide overpressure when mixed with air and when confined in an enclosing construction. The overpressure created is highly dependent of the construction strength of the enclosing walls. Dust explosions are generally not regarded as hazardous material phenomenon, because even “harmless” substances like milk powder, sawdust or corn starch can provide dust explosions. For this reason, dust explosion model are not evaluated in the phenomena model overview table.

2.5 Atmospheric dispersion phenomenon models

Hazardous material that is being released into the atmosphere will be transported and diluted with the wind. Since the resulting gas concentrations will determine the potential (toxic or flammable) danger, so-called atmospheric dispersion models are used to predict the occurring gas concentrations as a function of time and location.

Atmospheric dispersion models describe the motion and evolution of particles (aerosols, gases and dust) in space and time following their discharge into the atmosphere. The models are used to predict the (time and location dependent) concentrations occurring due to the accidental emission of a hazardous product into the atmosphere, such as 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).

The dispersion process is highly influenced by meteorological conditions such as wind speed and wind stability (amount of turbulence) but also by local circumstances such as surface roughness and topography of the surroundings. To be able to describe different atmospheric stability situations, a classification method can be used (Pasquill Gifford or Monin-Obukhov). These stability classes may be associated with specific meteorological conditions that take into account conditions such as wind speed, atmospheric turbulence, ambient air conditions, land use and solar radiation. A “roughness length” classification can be used to characterise the environment of the industrial plants.

The dispersion modelling of chemical substances following accidental releases is usually limited to spreading in the atmospheric mixed layer (or ‘mixing layer’), implying that downwind distances should be less than 10 km (otherwise, reliability of outcomes may fail). Spreading of material above the mixing layer (volcanic dust or ashes, spreading of radioactive material) requires models that incorporate interactions between the mixing layer and higher atmospheric layers.

Dispersion models can first be distinguished to the behaviour they describe: neutral dispersion, dense gas dispersion, or buoyant dispersion (plume rise and light gas dispersion).
However, dispersion models can also be classified based on the calculation method applied: Integral (or empirical) models, Gaussian models, Eulerian models, Lagrangian models, Computational Fluid Dynamic (CFD) models or even Bayesian network based models have been published.
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.

A first distinction to **behaviour** would be:

2.5.1 Neutral buoyancy or passive (Gaussian) gas dispersion

Neutral gas or passive dispersion describes the spreading of material without the influence of buoyancy, thus neglecting density differences. This means that the highest concentrations will always occur at the height of the release (leak height).

Because the concentration is described using an analytical concentration profile which is a Gaussian distribution around the plume axis (in height and width), the models are also referred to as Gaussian models. The Gaussian function describing the concentration as a function of time and location (x,y,z) involves typical “sigma” dispersion coefficients. The main differences between different Gaussian models relate to the formulations for those Sigma y, Sigma z and Sigma parameters. The neutral/passive/Gaussian dispersion model is a typical empirical model where sigma descriptions have been fitted to match with experiments under various weather conditions. The Gaussian model can be used for both instantaneous and continuous release, which are often referred to as “Puff” and “Plume” mode inside the dispersion model.

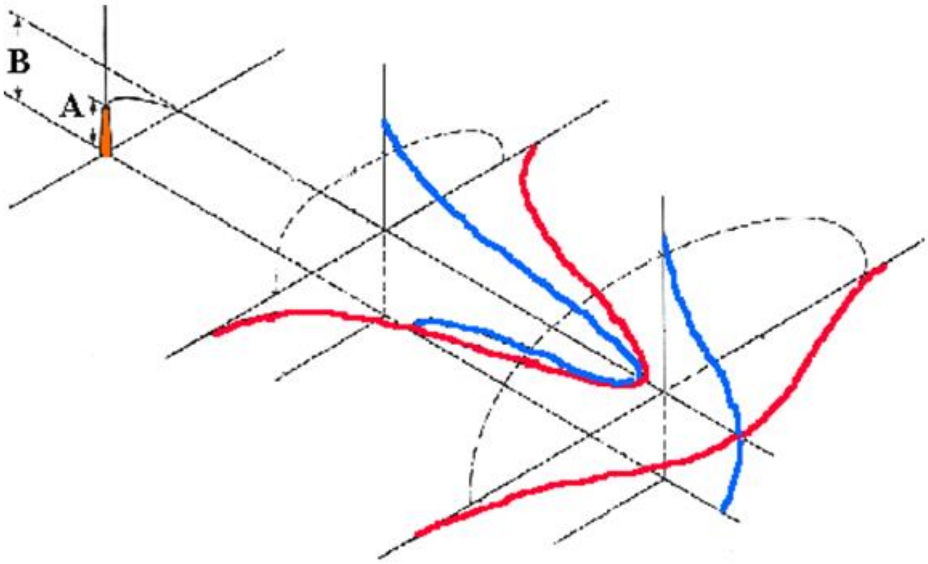


Figure 8 Gaussian concentration distributions for plume mode

2.5.2 *Negative buoyancy/ Heavy (dense) gas dispersion*

This family of models is dedicated to predicting the behaviour of ”heavier than air” gas concentrations. These models tend to be rather important in consequence modelling, because many hazardous releases will have a high density. This can be either a result of low temperatures (flash cooling during outflow or cryogenic releases), the existence of liquid droplets (aerosols) or because the release involves heavy molecules in high concentrations (e.g Chlorine).

The important difference with neutral or passive dispersion is the effect of gravitational forces, pulling the cloud downwards, thus creating wider clouds. For instantaneous releases, there is also upwind spreading of the cloud due to these density effects. Because the heavy gas release might include liquid droplets in the cloud, these models should also include a thermodynamic model for the droplet evaporation in the cloud. A heavy/dense gas dispersion model is typically an empirical model, fitted to experimental data provided by various field tests.

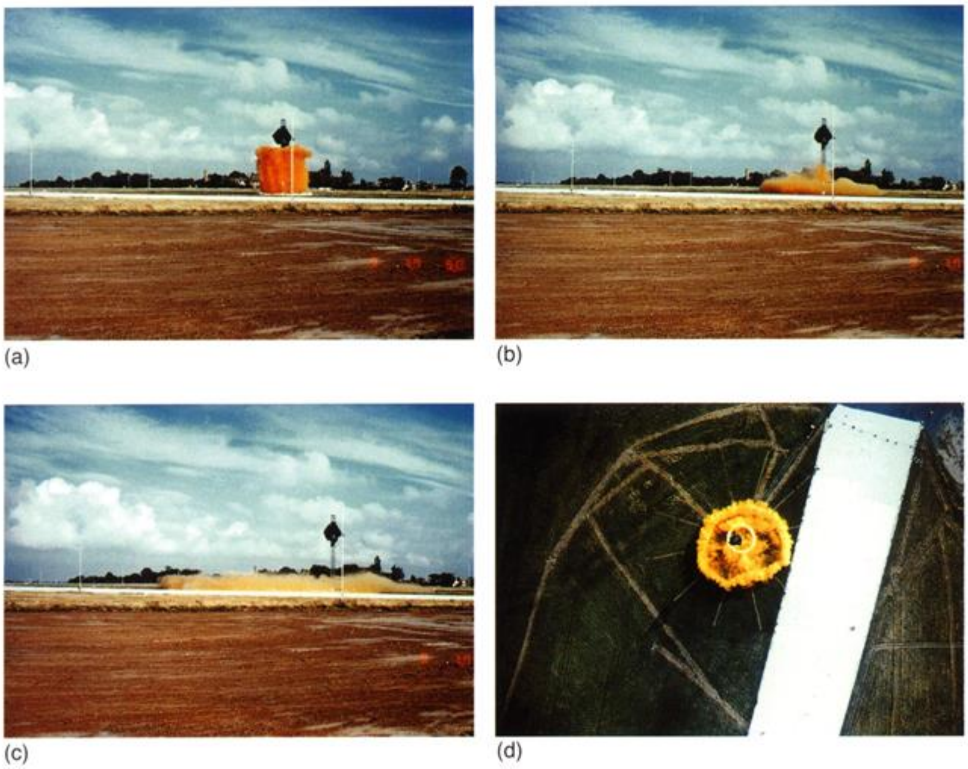


Figure 9 Example of Thorney Island trials for instantaneous heavy gas dispersion using orange coloured gas: (a-c =successive times, d=aerial view, pictures by HSE)

2.5.3 *Positive buoyancy dispersion*

Materials having a very low molecular weight (such as hydrogen), or hot materials may have a positive buoyancy, causing them to be drifted upwards following release. Because this rising effect of a gas cloud also means that the gas disappears form the built environment, positive buoyancy materials usually do not expose hazard risks, unless a roof or ceiling blocks this upward flow. Captured gas under a roof or ceiling would also mean that the gas gets confined, creating explosion risks. To be able to predict this capturing process, a definition of 3D geometries would be required in the dispersion model, which is typically the domain of CFD models.

Usually, the heavy gas models mentioned above, are designed to deal with density differences and are thus also capable of modelling “lighter than air” behaviour. Unfortunately “heavy gas” models are rarely designed or even validated for this ‘lighter than air” gas dispersion.

2.5.4 *Complex terrain / short distance / 3D dispersion modelling*

An important disadvantage of these empirical and Gaussian models is the fact that they are not capable of dealing with a non-uniform flow patterns, atmospheric flows that are being obstructed by larger geometries or influenced by local topography.

It is difficult to accurately calculate a concentration directly behind a building or large process installation. In empirical models, this effect of obstacles is basically averaged out by using an “increased surface roughness” which will lead to more turbulence and thus lower average concentrations. Because geometric obstacles can have a big influence on local concentrations, which can be very relevant from the point of view of emergency response, a lot of effort has been put on “short distance” or “complex terrain” modelling, or 3D modelling which includes a non-uniform flow pattern. Several methods have been used for this advanced flow modelling:

2.5.4.1 *Gaussian Fixed Flow field:*

A potential improvement of the standard Gaussian or integral approach would be to force a flow and turbulence field on top of a standard Gaussian approach. Such a flow and turbulence field can be calculated by complex terrain models, or be provided by large scale meteorological models (with potential feedback from meteorological stations or remote sensing). This flow field is a typical required external input for these Gaussian Fixed Flow field models.

2.5.4.2 *Lagrangian complex terrain dispersion models*

A Lagrangian model will describe the path of particles in turbulent flows by means of series of 3D vectors. By evaluating many particles in different potential realisations of the flow paths, it is possible to derive a probability of a particle occurring at a location, which can be related to a concentration. This method can be extended with a complex terrain definition, providing specific boundary conditions (e.g. flow pattern limitations) to specific 3D regions. Lagrangian models are also used within air quality modelling (although not by definition as complex terrain model) but also in predicting large distance effects from plumes of volcanic ashes or nuclear accidents.

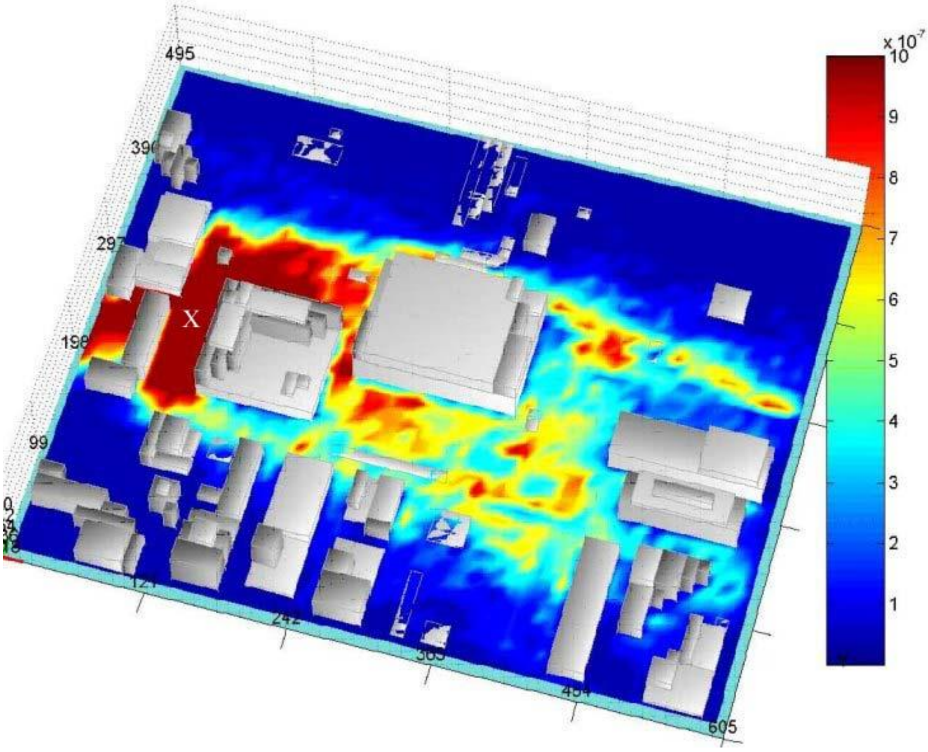


Figure 10 Example of Lagrangian dispersion approach as used in Quic-Plume

2.5.4.3 *Eulerian complex terrain dispersion models;*

Eulerian dispersion models are based on differential equations describing the continuous change of concentration in time and space. These equations can be solved for a complete 3D grid (mesh) of cells which, for a complex terrain modelling, are fitted around a geometric model of the surroundings/obstacles. Boundary conditions which are forced at the edges of the cells determine starting conditions, and a brute force calculation procedure will calculate concentrations and concentrations variations at all cells of the mesh at various time steps. Computational Fluid Dynamic (CFD) models are typical examples of Eulerian complex terrain models, where these CFD models can be divided into LES-based (Large-Eddy Simulations) and RANS (Reynolds Averaged Navier Stokes equations) based approaches.

These CFD models simulate gas dispersion by taking into account significant geometries linked to a site definition, including obstacles or topographic contours. However, it is essential to set the inlet boundary conditions of the CFD model and to correctly simulate a turbulent atmospheric boundary layer above an unobstructed ground or even a flat ground. These boundary conditions 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. 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).

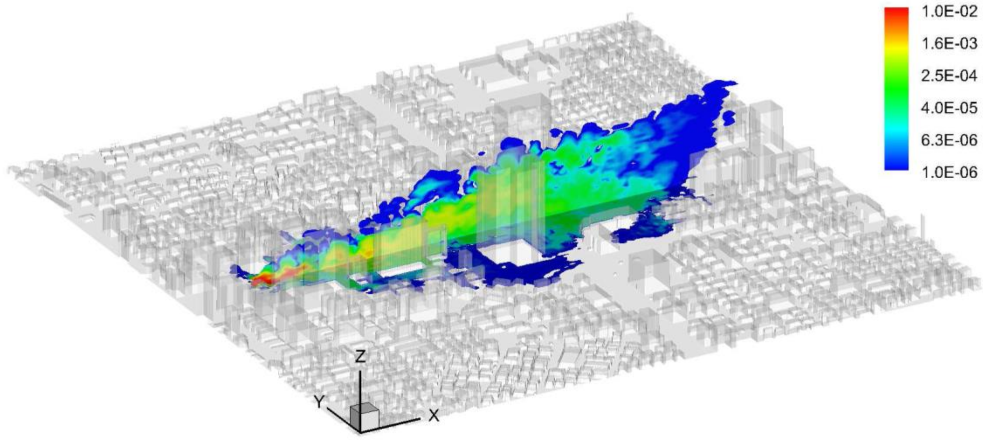


Figure 11 Example of Eulerian CFD dispersion calculation

Note that the evaluation of CFD and other complex terrain dispersion tools is the explicit task of the EU COST Action ES1006: "*Evaluation, improvement and guidance for the use of local scale emergency prediction and response tools for airborne hazards in the built environment*". The results of this project are very useful inside the SAPHEDRA project, and some main conclusions of the COST action project are listed in chapter 4 .

2.5.5 *Phenomenon potentially included in Dispersion models*

2.5.5.1 *Turbulent Free jet (High Pressure gas expansion)*

A continuous release of a compressed (high pressure) gas will result in a high velocity expansion area, where mixing with air is intensified in the turbulence zone between expanding gas and surrounding air. This expansion region, sometimes referred to as "turbulent mixing" or "turbulent free jet" zone, requires dedicated procedures to be able to describe the average concentration and expanded jet width at the end of the expanded jet. At lower storage pressures, a methane jet can already be diluted below lower flammability limits at the end of this expansion zone, implying that no further dispersion model is required to evaluate flammable hazards.

2.5.5.2 *Plume rise phenomenon*
High temperature releases from a stack or smoke plumes from fires might also involve a plume rise effects, due to thermal draft, which is also a typical buoyancy effect. Dispersion models can be equipped with dedicated plume rise algorithms.

2.5.5.3 *Deposition of solids*
In specific occasions (e.g. warehouse fires) a gas release can be loaded with solid particles which can create hazards upon deposition. Examples are asbestos fibres, carbon particles with absorbed unburned chemicals or radioactive fallout material. Dispersion models might contain modules to be able to calculate deposition, potentially even divided in dry and wet deposition (with rain)

2.5.5.4 *Toxicity / dose calculations*
In order to be able to derive a toxic load (exposure to people) of a chemical release, the concentration profile needs to be integrated over time. This dose, the integral of concentration over time: $\int C(t)\, dt$ can even be corrected with an exponential vale n: Dose $=\int C^n(t)\, dt$. Dispersion models for toxic exposure should also report this dose where exponent n and so-called probit values should be dependent on the chemical substance. Unfortunately there is no international nor European consensus on toxic dose properties of chemicals, which requires the toxic properties to be adjustable. Toxicity calculations can be based on integrated toxic dose, using probits, SLOD or SLOT doses or be using AEGL, ERPG, IDLH concentration threshold based thresholds which relate to a specific exposure duration. For instantaneous and semi-continuous releases, the concentration profile is highly time dependent, which means that there is no fixed relation between maximum concentration and dose.

2.5.5.5 *Explosive mass calculations*
In case of atmospheric dispersion of a flammable cloud, the potential explosion (overpressure) damage is highly dependent on the amount of mass in the cloud. Apart from that, the footprint of the flammable cloud is also relevant for damage due to the flash fire. Both results: the footprint of the flammable cloud, and the total incorporated mass within flammability limits, need to be calculated by the dispersion model to be able to perform a vapour cloud explosion calculation. Dispersion models for explosive mass need to integrate the mass inside the flammable cloud over the cloud volume (volume limited by LFL or 50% LFL concentrations)

3 Identification of phenomena models in consequence modelling tools

3.1 Consequence model template

To be able to identify available phenomena models on the European market, a template has been provided, which lists the most relevant properties of the models. The template has separate tables for phenomena families: RELEASE models, FIRE models, EXPLOSION models and DISPERSION models. Each phenomena group has been be subdivided into different types of phenomena, e.g. Pool fire , Jet fire and Fire ball phenomenon models.
The template summarises the following properties:

- Model name: The name by which the phenomenon model is usually referred by. Very often the name of the original publisher.
- Model description: a brief description of the purpose and main targets of the model
- Field of application: a description of the typical application region, potentially providing boundaries for which regions the model is applicable.
- Limits in application: some phenomena models have typical limits, implying that they may have specific drawbacks or problems with reliability in specific situations.
- References: The original literature references fully describing the phenomenon model
- Software tools: The software application that is using this phenomenon model.
- Validation in: available validation reports, describing the experiments that the model was validated against, with the results of this comparison.

The resulting spreadsheets, which includes additions of various members of the SAPHEDRA consortium,, has to be seen as an integral part of this report. The resulting tables have been added to appendix but may be difficult to comprehend in this printed table form. Furthermore, the spreadsheet may be subjected to additions and modifications while the project evolves.

3.2 Consequence modelling software tools

A list of the most used tools in European countries to estimate consequences of hazardous phenomena is presented in the table below. The list does not aim at being exhaustive but does highlight the main tools used within the European Union. The models used within the tools are mentioned and general commentary regarding the availability of the tools is provided.

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 consequences to be estimated. Others (e.g. ALOHA, 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 below.
This table 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 numerical models.

Dangerous Phenomena	**Main experimental campaign**	**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 HGSYSTEM MERCURE_SATURNE PHAST ProNuSs Similinks SLAB S.T.A.R TRACE
Solid explosives	Brasie and Simpson, 1968	EFFECTS PHAST FRED
Vapour Cloud Explosion	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 HGSYSTEM PHAST ProNuSs Similinks S.T.A.R

Dangerous Phenomena	Main experimental campaign	Modelling Tools
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 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 HGSYSTEM PHAST ProNuSs Similinks S.T.A.R
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 HGSYSTEM MERCURE_SATURNE PHAST ProNuSs Similinks SLAB S.T.A.R TRACE Yellow Book

Dangerous Phenomena	Main experimental campaign	Modelling Tools
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.

4 Applicability and limits of identified consequence models

4.1 Introduction

Although the provided spreadsheet gives a comprehensive list of all relevant properties of identified models, some additional information is added to be able to determine whether listed models are actually “fit for purpose”. This chapter aims at providing additional insight in model applicability for the selected model groups and extends some of the remarks made in the column “Limits in application” as listed in the spreadsheet..

4.2 Release models

Release models, usually divided into models for liquids, two-phase flow or pure gasses can be applied straightforward.
However, in some special situations, models may not be reliable or require special attention:

- **Mixtures outflow**: A two phase outflow is highly influenced by the occurrence of potential vapour bubbles in the flow, occurring as soon as the pressure reaches saturation pressure due to friction losses. If a two phase material is a component mixture (e.g. Propane/Butane) the vapour pressures of the substances will differ resulting in the evaporation of the most volatile component, leading to a change of composition of the remaining liquid. This change of composition of vapour/liquid is not taken into account.
- **Mixtures evaporation**: The same composition shift situation for mixtures also occurs during (spray) flashing and pool evaporation situations. Because it is very complicated to take into account a time dependent composition of a release in following dispersion models, this composition change is usually neglected,
- **Supercritical condition**: High pressure gasses may already be in supercritical conditions: above its critical pressure. Due to important density influences in this supercritical region, the application of outflow models require dedicated “Equation Of State” relations, which are not always available or reliable for the chemicals/mixtures released.
- **Long pipelines rate**: An outflow from a “long pipeline” is often modelled as if the pipeline itself is blocked system, and expansion from the pipeline section is the driving force. In reality this “in line” expansion takes place within seconds/minutes, whereas closing the main valves may take hours. These “long pipeline models” predict a huge outflow during very short time, whereas the real outflow after this initial expansion is determined by the system and control strategy in front of the rupture.
- **Evaporation from water secondary effects**: During pool evaporation from water, various secondary effects may occur: the liquid may dissolve or react with water, the liquid may sink, or cryogenic liquid (LNG) may even create an ice layer. All these effects will influence evaporation and are usually not taken into account.

- **Cascading "splashing" liquids**: The Buncefield accident was caused by very rapid evaporation in a cascading liquid, falling down from the top of a tank and splashing against a wind shield and the ground. Together with the very low wind speed, this created fine droplets and resulted in highly concentrated vapour slowly spreading out at ground level. This kind of enhanced evaporated is often not taken into account, but can now be modelled with a HSE vapour cloud formation model. Note that the Buncefield "no wind" situation is actually a specific difficulty for dispersion models, since the spreading of the (flammable) cloud is mainly driven by local topology. This would require very detailed 3D modelling of the surroundings, because even low height obstacles (cars, fences, bushes) appear to influence the end shape of the flammable cloud and also introduce confinement and congestion, leading to overpressure (explosion) phenomena..

4.3 Fire models

For jet fire models, there are e few limitations and remarks have to be made with respect to applicability of listed models:

- **Flame bending effect:** Within the category of jet fire models, the "Chamberlain" approach, which is predicting the cone (frustum) shape of a radiating flame body, is very often applied. Is was originally developed for vertical flares, but is also being used for tilted flames. If the direction becomes more "horizontal" the effects of thermal draft, will be bending the flame upwards at the end part. These kind of effects are not taken into account by the "standard" Chamberlain approach but require dedicated flame path modelling (available in Barker model)
- **Lift off correction:** One of the results of the jet fire models is the lift off height, representing the starting (bottom) part of the flame surface. In case of buried gas pipelines, it is expected that the flame will be forced upwards, as a result of a impingement to the crater and/or two sided collapsing outflow. Due to this impingement, the impulse has decreased considerably, and the flame lift off height will reduced as compared to the original height corresponding to the outflow rate. This phenomenon is only taken into account by dedicated models (Dome fire model HSE)

The pool fire models mainly describe the pool fire as a tilted cylindrical flame shape. The main uncertainty with applying these models is the fact that the user has to enter a specific "fraction of heat radiated" (as compared to the combustion energy) and a "soot fraction", which will both have a big impact on the resulting SEP (Surface Emissive Power) of the flame. The "two zone" model (Rew & Hulbert HSE publication) approach will overcome this uncertainty by providing substance dependent values for the clear and sooty part of the flame.

For fire ball models, describing a fireball as a result of a BLEVE of a flammable substance, some differences in the modelling occur due to: the description of the height of the fireball (either the radius or twice the radius) and the potential "dynamic" (rising and growing sphere) description of the fireball. All models use the same empirical approach of estimating the BLEVE mass based on "3 times adiabatic flash".

Flash fire models are not often used to describe consequences because the most pragmatic approach would be to assume 100% damage within the flame and no damage outside the flame footprint. Because the flash fire has a very short duration, the heat load is typically not generating damage. To be able to describe the flash fire shape (LFL footprint and potential mass in the LFL cloud) the flash fire requires a dispersion model to predict cloud dimensions.

4.4 Explosion models

The **TNT equivalence method** is still used often to predict overpressures of VCE (Vapour Cloud explosions). When applying the TNT method, the explosive energy of a vapour cloud is translated into an equivalent charge weight of TNT, using an equivalence factor and heat of combustion of the substance. This “TNT equivalency” factor needs to be derived from statistical analysis of the damage observed in a limited number of vapour cloud explosions incidents. Unfortunately, the TNT equivalency model is a poor model for prediction of VCE blast strength. While a TNT charge produces a shock wave of high amplitude and a short duration, a real VCE produces a blast of lower amplitude and longer duration. Apart from this, practical values for the TNT equivalence factors are averages, based on the wide statistical distribution found in practice. As a consequence, a predictive estimation with TNT-equivalency on the basis of an average has very little statistical reliability.

For **solid explosions**, the TNT model is an appropriate model to use, but still requires the equivalence factor (as compared to TNT) for the substance to be defined. For common modelled substances like AN (Ammonium Nitrate) these values are available but also depend on the specific grade of the material.

A more deterministic estimate of VCE blast effects is possible if a parameter could be found that correlates with the process of blast generation in vapour cloud explosions. Such a parameter is introduced within **VCE blast curve methods**, where the ME (Multi-Energy) and BST (Baker-Strehlow-Tang) method are the most widely used models. One of the difficulties when applying these methods however is the determination of the appropriate blast strength class, which requires substantial experience. The so-called GAME correlations (Guidance on the Application of Multi-Energy) were developed to provide a more quantitative method to correlate blast strength with parameters characterizing the congestion and confinement of the environment in which the vapour cloud is drifting. For BST a similar congestion assessments evaluation is required to determine blast strength.

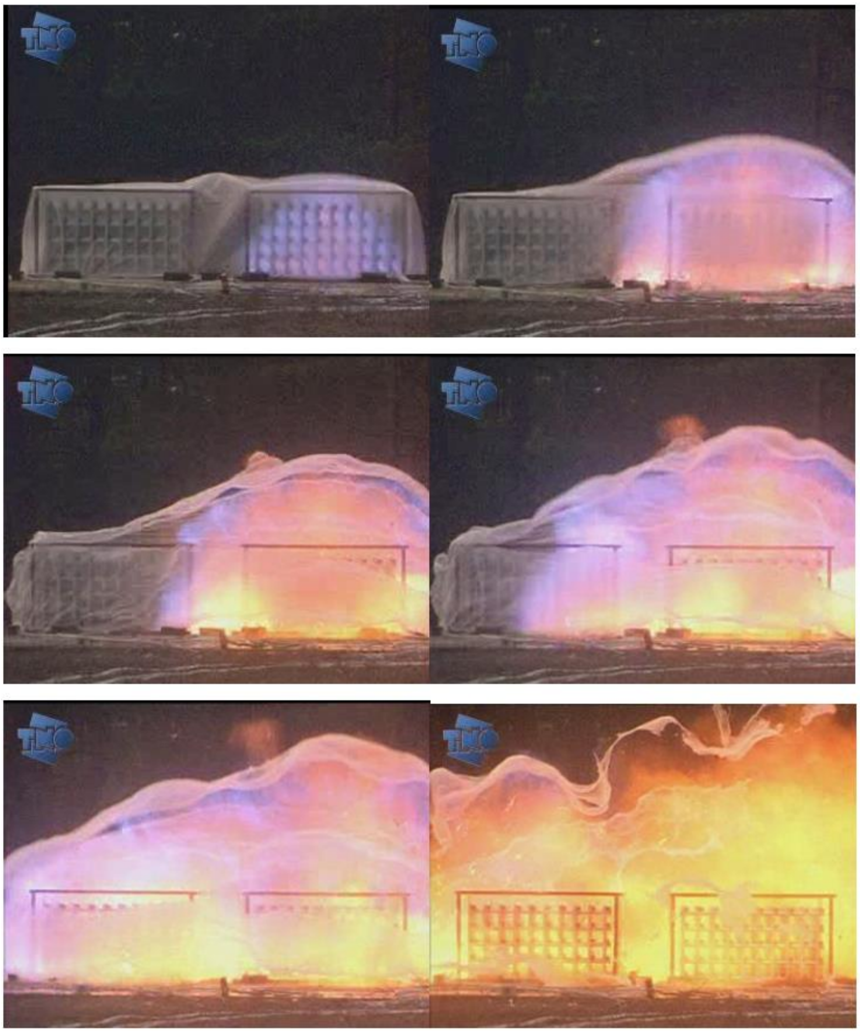


Figure 12 Vapour cloud explosion test performed at TNO with typical congestion structures

Another difficulty in applying these blast curve models is the fact that they require an estimation of the fraction of the flammable cloud which is actually confined or congested. Such an explosive mass estimation should involve the overlap of congestion zones with potential locations and shape of the LFL cloud, requiring a dispersion model as well.

Because concentrations on short distances may be highly influenced by local geometries and obstacles (whereas obstructions also play a role in the congestion assessment) dedicated CFD models are now also used for VCE evaluation. These models require a detailed 3D geometry description and are nowadays used for offshore platform risk assessments, combining a CFD dispersion calculation with detailed flame acceleration and overpressure calculations.

So-called "**pressure vessel burst**" explosions can also be modelled with specific models (Baker model). A commonly used model describes overpressure due to a BLEVE, but similar models can also be used to model pressure vessel ruptures due to runaway reactions, ideal/non-ideal gas expansion and other causes. To be able to determine potential "throwing range" of vessel fragments from the rupture, an estimation has to be made about the "fraction of liberated energy going into kinetic energy", which involves substantial uncertainty.

4.5 Dispersion models

Gaussian models are based on the Gaussian distribution equation and are widely used to estimate the impact of non-reactive pollutants. 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 ('jet air entrainment');
- the effects of gravity (heavy gas dispersion)
- the buoyancy effects (light gas dispersion).

The physical mechanisms above can be accounted for when integral models are used. However, integral models also have some limitations, the main ones are:

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

More complex tools (e.g. CFD tools) allow more complex environment (e.g. presence of obstacles such as building or natural reliefs such as valleys) to be taken into account to describe 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.

One particular important issue is the traceability and reproducibility of results produced with CFD models: it should be reported explicitly which turbulence models have been used, which mesh coarseness has been used, and which boundary definitions and settings were used to obtain the results. It has been observed that even when using the same CFD tool, different (experienced) users still may come up with different results due to the large number of choices and decisions to make during CFD modelling.

In the framework of the COST action ES 1006, several ADM's (Atmospheric Dispersion Models) used for emergency prediction and response were evaluated. The main conclusions, that were drawn for the application in built environments (an environment with obvious obstacles and geometries influencing the flow pattern), were:

- Gaussian models are still the most used models, both for risk assessment and in case of emergency. However, this model type does not provide a realistic view on the dispersion pattern (thus on release consequences) in industrial and urban built environments. Moreover, contrary to a common opinion among stakeholders, these models do not systematically provide conservative results.
- Gaussian models might be advisable only on condition that they take account of buildings in some simplified way and are applied in configurations for which they have been established.
- Lagrangian models taking account of the buildings may give accurate results in the order of 10-30 minutes, with moderate computational resources. Input turbulent flow data may be issued: either on line by diagnostic flow models or off-line by pre-computed and tabulated CFD approach.
- Eulerian models with the same input turbulent flow data as for Lagrangian models may be used when they are able to meet the time constrains of the event phase which is targeted (thus the pre- or post-event evaluation, not likely in the emergency phase).

And another obvious but still highly relevant conclusion on models in software tools in general:

- ADMs in Emergency Response Tools should be developed not only respecting scientific criteria (like verification and validation), but also meet practical criteria (about response time, interface, output etc.)

Within the framework of this COST ES 1006 action, the dispersion models were divided into 3 groups: Type 1 = Gaussian (including integral models), Type 2 = Lagrangian (Puffs or fluid particles trajectories) and type 3 = Eulerian (Full transport equation, LES or RANS models). The reported guideline provides a very useful decision scheme on the selection of these 3 types of models:

START						
Location clearly defined?	No	Source can be defined and toxicological data available?	No	No solution		
Yes		Yes				
Source can be defined and toxicological data available?		Type 1				
Yes						
Short duration/small scale?	No	Access to global NWP?	No	ERG/Template		
Yes		Yes				
Urban/ industrial location?	No	Access to detailed meteorological data/NWP?	No	Access to land-use and terrain data?	No	ERG/Type 1
Yes		Yes		Yes		
		Type 2/3		Type 1/2		
Access to urban /building geometric data?	No	Type 1				
Yes						
Access to detailed meteorological data?	No	Type 1/2				
Yes						
Detailed concentrations required close to source?	No	Type 1				
Yes						
Type 2/3						

Figure 13 COST ES 1006: Decision scheme for the selection of dispersion model type

5 References

CCPS (2010). Guidelines for Vapor Cloud Explosion, Pressure Vessel Burst, BLEVE and Flash Fire Hazards. New York: Wiley.

Chamberlain, G. A., "Developments in design methods for predicting thermal radiation from flares"; Chem. Eng. Res. Des., Vol. 65,pp 299-309, (July 1987).

Cook, D, K, (1987) Chem Eng Res Des, 65(4): 310-317.

J. Cook, .Z. Bahrami and R.J. Whitehouse (1990) A comprehensive program for calcultion of flame radiation levels. J. Loss Prev. Process Ind., 3:150-155. G.T Kalghatgi, (1983) Combustion and Flame 52:91-106.

COST action ES 1006 (2015), “Evaluation, improvement and guidance for the use of local-scale emergency prediction and response tools for airborne hazards in built environments” , Best practice guidelines.

Eggen, J.B.M.M (1998) , GAME: development of guidance for the application of the multi-energy method, HSE contract research report 202..

Fouillen F., Duplanter S. Pressurization of Fixed Roof Storage Tanks Due to External Fires. Process Safety Progress, 2011, vol. 30, n° 1, pp. 52-61.

Franke,J. Hellsten, A. Schlünzen, H. Carissimo, B. (2007) “Best Practice Guideline for the CFD simulation of flows in the urban environment” Action COST 732 – Quality Assurance and Improvement of MicroScale Meteorological Models

HSE Health & Safety Laboratory, F. a. (2002). A Review of the State of the Art in Gas Explosion Modelling. HSE.

UFIP (2003) "Guide méthodologique pour la réalisation des études de dangers en raffineries, stockages et dépôts de produits liquides et liquéfiés" (Guide Bleu)

Rew, P.J. & Hulbert, W.G. (1996), Development of a pool fire thermal radiation model’, HSE Contract research report no. 96

Yellow Book (2005). Methods for the calculation of physical effects due to the release of hazardous materials. The Hague: Committee for the Prevention of Disasters, third edition, 2nd revised print,

Appendix A. Tabular representations of resulting model description spreadsheet

(note that the full spreadsheet also contains columns with references, tools using this, and validation references which are not listed here because of readability)

Liquid outflow models			
Model name	**Model description**	**Field of application**	**Limits in application**
Bernouille model	Calculates outflow rate from vessel. Driving forces is liquid height. Input is hole diameter, substance and storage conditions. Result is time depending rate, time to empty vessel etc.	Outflow from vessel	Suitable for liquids only, by default not applicable for supercritical conditions. Supercritical fluids require an EOS (Costald)
Outflow with pipe friction	Includes flow reducing effects due to friction losses in pipe	Outflow from pipeline connected to vessel	Suitable for liquids only

Gas outflow models			
Model name	**Model description**	**Field of application**	**Limits in application**
Yellow book model	A model based on ideal gas behaviour.	Pressurised gas discharge	Inaccurate for supercritical conditions, no negative JouleThompson effects (H2)
DISC / ATEX model	Disc = orifice modelling outflow, Atex models expansion phase	Gas, Liquid and two phase	Inaccurate for supercritical conditions
Maytal model real gasses	based on real gasses (non-ideal)	Pressurised gas release	Inaccurate for supercritical conditions
Wilson model	Calculates flowrate from a blocked length of pipeline, pressure wave traveling upwards with speed of sound. Full rupture or leak	Long gas pipelines	Assumes blocked length of pipeline. Only first order effects

Gas expansion model	Calculates adiabatic or isentropic expansion of an compressed gas resulting in initial dimensions and conditions of the gas cloud.	Instantaneous gas release	Inaccurate for supercritical conditions
GASPIPE model	Long pipeline model based on Fannelop-Ryhming model	Long gas pipelines	Assumes blocked pipeline

Pressurised Liquefied outflow models			
Model name	**Model description**	**Field of application**	**Limits in application**
TPDIS model	a Homogenous Equilibrium Model: assumes equilibrium between vapour and liquid at any location in pipe. Most implementations include model for vessel depresssurization including vapour generation	2 phase outflow= storage temp > normal boiling point	Mixture: vapour has same constant composition as liquid. Inaccurate for supercritical conditions
LEUNG model	a Homogenous Equilibrium Model	2 phase outflow	Mixture: vapour has same constant composition as liquid. Inaccurate for supercritical conditions
Homogeneous Non-equilibrium Model	Not applicable for outflow through pipes	2 phase outflow	Neither pipe friction nor vapour creation taken into account
Morrow model	Calculates flowrate from a blocked length of pipeline, pressure wave traveliing upwards with speed of sound. Full rupture or leak	Long PLG pipelines	Assumes immediate blocking, based on contents of blocked length
Vapour release model	Release above liquid level	Simple vapour outflow model, incorporating vessel dynamics	No liquid, pure dry vapour

Diers vapour release	Release above liquid level, includes potential liquid outflow due to bubbling / foaming effects	Outflow through PRV, including potential liquid outflow	Requires knowledge occurrence "Champagne bubbling effect" for substance
DISC / ATEX model	Disc = orifice modeling outflow, Atex = modeling expansion phase	Gas, Liquid and two phase	Inaccurate for supercritical conditions

Flash and Evaporation models			
Model name	**Model description**	**Field of application**	**Limits in application**
GASP pool evaporation	Pool evaporation model	Pool evaporation from land or water	
Brighton model	Pool evaporation model with correction for wind speed profile, including Kawamura-MacKay relations for heat transfer	Pool evaporation from land	
Aminal model	An empirical model based on correction of adiabatic flash with spray fraction	2 phase outflow flash	
Spray release model	Calculates rain-out and liquid fraction of vapour outflow resulting from PLG release	2 phase outflow flash	Not suitable for CO2 with solid/vapour equilibrium
Statistical Spray release model	Using droplet size distribution to calculate rainout/liquid fraction	2 Phase outflow, including CO2	
ATEX SMD model	Using droplet size distribution to calculate rainout/liquid fraction	2 Phase outflow, including CO2	
Sutton-Pasquill model	Pool evaporation model with mass transfer coefficient determination	Pool evaporation from land	
Mackay-Matsugu model	Pool evaporation model with mass transfer coefficient determination	Pool evaporation from land	
Yellow book	Pool evaporation	Boiling and Non-	Calculation of

poolevaporation model	boiling / non boiling liquids based on Mackay-Matsugu, extended for pools on water	boiling pools both from water / land	Schmidt number needs mass diffusivity in air, requiring knowledge of conditions at critical point
Vapour Cloud Formation model	Predicts the vapour cloud formation from a cascading liquid (tank overfilling) release	Liquid cascade in case of tank overfilling	Non boiling liquids with low flash point below ambient temp, limited amount of substances
STAWaRS	Pool evaporation of water reactive substances	Pool evaporation from land or water	
Clancey Model	Pool evaporation model with mass transfer coefficient determination	Pool evaporation from land	
Deutsch Model	Pool evaporation model with mass transfer coefficient determination	Pool evaporation from land	
TÜV Rheinland Model	Pool evaporation model with mass transfer coefficient determination	Pool evaporation from land	
Brötz Model	Pool evaporation model with mass transfer coefficient determination	Pool evaporation from land	
PVAP Model	Pool evaporation model based on GASP and Yellow Book pool spreading equations	Pool evaporation from land and water	

Jet fire models			
Model name	**Model description**	**Field of application**	**Limits in application**
Chamberlain model	The Chamberlain model calculates a representation of a flame with solid body (conical frustum) emitting radiation from its surface. The model predicts the flame shape and radiation field of flares from flare	Gas jet fires, originally designed for flares (vertical jets) but adapted for tilted flames.	Does not take into account flame bending effect of horizontal flames. Only applicable for gas jets

	stacks. The flame represents the flame as a frustum (part of cone or pyramid that remains after top is cut off) of a cone, radiating as a solid body with uniform surface emissive power.		
API 521 model	A point source model describing the flame as a serie of point emitters. These models are only applicable to vertical torches and when the point source is enough far away from the emitter.	Vertical Gas jet fires	Only applicable for vertical torches at longer distances
Cook Model	The general approach of the Cook model is similar to the Chamberlain model. The correlations for the determination of the width of the base of the frustum (W1), the determination of the effective source diameter (De) and lift-off distance (B) are slightly modified from the Chamberlain's model. The model is specifically adapted to use for two-phase releases.	An adaptation of Chamberlain, suitable for gaseous AND 2 phase jet fires.	Does not take into account flame bending effect of horizontal flames (thermal draft effects).
Johnson model	The Johnson model describes the burning torch as a result of (almost) horizontal gas phase release.	Gaseous horizontal jet fires	Only applicable for gaseous horizontal jets
Barker jet fire model	The Barker model is suitable for two phase releases of propane, butane and LPG. The flame	PLG horizontal jet fires	Applicable for PLG and horizontal jets only, proprietary model and non-public references

	shape is described as a horizontal part and a tilted flame part representing 50% occurrence of the flame		
Cracknell model	A general jet fire model for gaseous, two-phase and liquid releases of hydrocarbons, describing the jet as a tilted solid flame cone.	Liquid, gas and 2-phase jet fires	Proprietary model, non-public references
Dome fire model	The dome fire models the interaction of two jets within a crater where a highly turbulent volume of gas is formed by jets emerging in random, time varying directions. The approximation to this type of release was assumed to be a hemispherical flame centred over the break at ground level.	Gas jet fire of double sided outflow pipeline	Only applicable for 2 collisioning jets inside crater (underground gas pipelines)

Pool fire models			
Model name	**Model description**	**Field of application**	**Limits in application**
POLF model	Modelling a tilted cylindrical flame surface. Burning rate based on Burgess formulation	Liquid pool fire radiation	Fraction heat radiated & Estimated soot fraction highly influences results
Yellow book model	Modelling a tilted cylindrical flame surface. Burning rate based on Burgess & Hertzberg, 1974 , Thomas formula for flame length	Liquid pool fire radiation	Fraction heat radiated & Estimated soot fraction highly influences results
Rew & Hulbert 2 zone model	Modelling a tilted cylinder with elliptical top part. Flame contains a clear bottom part and a sooted top part with a lower SEP, specific SEP clear and SEP soot enlisted for various chemicals.	Liquid pool fire radiation, validated clear and sooty flame SEP	Approx. 20 substances with listed values for burning rate/SEPmax/SEPso ot
Mudan & Groce model	Flame geometry based on a tilted elliptical cylinder. Combustion rate calculated using Burgess & Hertzberg, 1974. It is stated that the specific combustion rate for boiling water puddles (including LNG and LPG) are typically 2 to 3 times higher than the combustion rate on land.	Liquid pool fire radiation	Fraction heat radiated & Estimated soot fraction highly influences results
SAVE II model	Flame geometry is based on a straight vertical cylinder, no tilt due to wind	Liquid pool fire radiation	No flame tilt incorporated
LNGFIRE3	Calculating thermal exlusion zones around LNG fires	Dedicated to LNG fires	Not suitable for generic hydrocarbon pool fires

Flash Fire models			
Model name	**Model description**	**Field of application**	**Limits in application**
LFL footprint model	100% damage assumed within the footprint of the LFL or 50% LFL cloud. Outside this cloud there is no damage due to the short duration of the heat load.	Flash fire with infinite short fire duration	Basically a damage models based on atmospheric dispersion model calculation a flammable cloud
CCPS model	Flash fire model describing the flame as a two dimensional turbulent flame propagating at constant speed	Flash fire incorporating flame propagation and radiation exposure	Requires atmospheric dispersion model to calculate concentration distribution

Explosion models			
Model name	**Model description**	**Field of application**	**Limits in application**
TNT equivalency method	Explosive energy of VCE is translated into equivalent charge weight of TNT, using equivalence factor and heat of combustion of substance	Originally developed for solid explosions, extended for usage on VCE's	Requires estimation of TNT equivalence factor, with wide statistical distribution. Not very suitable for VCE (lower amplitude and longer duration shockwave)
Baker Strehlow Tang blast method	A blast curve method, providing curves with dimensionless overpressure/impulse vs. dimensionless distance	Developed for vapor cloud explosions	Selection of appropriate blast curve involves expert judgement on congestion level, fuel reactivity and confinement.
TNO Multi Energy method	A blast curve method, providing curves with dimensionless overpressure/impulse vs. dimensionless distance	Developed for vapour cloud explosions	Selection of appropriate blast curve involves expert judgement on congestion level. GAME correlation provides quantifiable relation but requires detailed knowledge congestion area

Congestion Assessment Method	Estimation of overpressure and impulse form VCE based on congestion characteristics and "fuel factor" F	Developed for vapour cloud explosions, using calibration against large number of tests	Severity Index calculation requires detailed knowledge of congestion parameters
Numerical (CFD) models	Full calculation of transport equations in 4D, resulting in flammable cloud dimensions and mass, flame acceleration and overpressure data	Detailed modelling of complex environment, e.g. off-shore platforms	Requires detailed 3D geometries to be entered, time consuming procedure, only valid in 1 wind direction, 1 atmospheric stability condition

Pressure Vessel Burst models			
Model name	**Model description**	**Field of application**	**Limits in application**
Baker model	A model for the determination of overpressure and fragments damage upon failure of a presure vessel	Suitable for vessel burst due to: External impact, runaway reaction, decomposition and internal explosion	Calculation of liberated energy is complex, fraction of energy translated into kinetic energy has big influence
BLEVE blast model	A model for the determination of overpressure due a to a BLEVE phenomenon	Only for overpressure due to BLEVE	Only provides overpressure information, no fragment damage incorporated

Gaussian dispersion models			
Model name	**Model description**	**Field of application**	**Limits in application**
DRIFT	Dispersion model for releases of heavy or passive materials	Hazard assessment	
VDI 3783/1	Dispersion of light or neutrally buoyant gases	Hazard assessment	No obstacles, distances below 100 m with high uncertainties
ALOHA	Dispersion of light or neutrally buoyant gases	Hazard assessment	No obstacles, distances below 100 m with high uncertainties

UDM (Unified Dispersion Model)	Dispersion model for releases of heavy or passive materials	Hazard assessment, including toxic dose and explosive mass calculations	No obstacles, distances below 100 m with high uncertainties
Neutral Gas Dispersion model	Dispersion of neutrally buoyant releases	Hazard assessment, including toxic dose and explosive mass calculations	No obstacles, distances below 100 m with high uncertainties

Heavy gas dispersion models			
Model name	**Model description**	**Field of application**	**Limits in application**
UDM model	Unified Dispersion Model includes both heavy and neutral gas dispersion modelling	Hazard assessment of neutral and heavy gasses, instantaneous, jet and pool sources, including toxic dose and explosive mass calculations	Plume to puff transitions can give inconsistant results, Semicontinuous releases don't use σx. No obstacles distances < 100 m with high uncertainty. Proprietary model
DEGADIS	Degadis is an adaptation of the HEGADIS model by Colenbrander.	Heavy gas dispersion, puff and plume mode	No support available, no longer maintained code, no dose calculations, no explosive mass calculations, No obstacles, distances < 100 m with high uncertainty
HEGADIS	Shell HEGADIS is a dense gas model for puff and plume releases at ground level	Heavy gas dispersion, puff and plume mode	No support available, no longer maintained code, no dose calculations, no explosive mass calculations, No obstacles, distances < 100 m with high uncertainty
SLAB	A steady state plume and transient puff model for heavy gas dispersion	Heavy gas dispersion	No support available, original code is no longer maintained. No dose calculations, no explosive mass calculations, No obstacles, distances < 100 m with high uncertainty
TNO-DENSEGAS	A densegas model based on SLAB	Heavy gas dispersion for instantaneous, pool evaporation, horizontal and vertical jet, including toxic dose and explosive mass calculations	Plume to Puff transition can give inconsistent results. Slightly different results compared with validated SLAB, No obstacles, distances < 100 m with high uncertainty

Britter & McQuaid model	A dense gas model for continuous and instantaneous releases	Heavy gas dispersion	No semi continuous releases, no dose calculation, no post-release thermodynamic behaviour (droplet evaporation)
VDI 3783/2	A model based on wind tunnel experiments of heavy gas dispersion	Hazard assessment	Only "model" dispersion areas available, so that the one has to be chosen which is the "closest" to the real case
ALOHA-DEGADIS	ALOHA-DEGADIS is simplified as compared to original DEGADIS. ALOHA-DEGADIS is limited to releases at ground level, and does not account for the initial momentum from a jet release	Heavy gas dispersion	No jet releases (initial impulse). No dose calculations. No explosive mass calculations, No obstacles, distances < 100 m with high uncertainty
TRACE	A densegas model from SAFER Systems. TRACE also includes release models	Heavy gas dispersion	No public documentation. No obstacles distances < 100 m with high uncertainty. Proprietary model.
HGSYSTEM	A suite of models including HEGADAS for densegas area sources and HEGABOX for instantaneous densegas	Heavy gas dispersion	No support available, no longer maintained code, no dose calculations, no explosive mass calculations, No obstacles, distances < 100 m with high uncertainty

Short distance / Complex Terrain dispersion models			
Model name	**Model description**	**Field of application**	**Limits in application**
Separated windfield	These type of models use a separated (3D) windfield calculation method, where this windfield is subsequently forced upon a dispersion code module. This type of approach is much faster than CFD but includes wind field disturbance by urban buildings	Hazard assessment in Urban and Industrial area, thus including obstacle influence. Dispersion module can also include support for dense gas situations	Detailed geometry definition required. Separate validation of windfield required, Recalculation of windfield required for all potential wind-directions/ stability class situations

Eulerian CFD	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.		Results highly dependent of user defined boundary conditions, mesh geometry chosen. Stabilising effect of density gradients not reproduced
Lagrangian	Langrangian Particle model with input flow data either on-line or off-line (precomputed flow field)	Air pollution models, Prediction radioactive fallout, Volcanic ashes, Emergency response	No heavy gas yet