

DEVELOPMENT OF SOURCE TERMS FOR GAS DISPERSION AND VAPOUR CLOUD EXPLOSION MODELLING

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Experiences with consequence modelling for COMAH safety reports showed that there was often a lack of understanding relating to the specification of source terms for modelling gas dispersion and VCE modelling. It was also apparent that there were serious inconsistencies in the approach used over a period of time on the same site.

The inconsistencies were not only in the particular models used but also in the approach used to defining the source term used. In many cases, this was attributable to a lack of understanding of the physical processes and also of the important factors in the models.

In particular, it was found that the relationship between gas dispersion and the source term for modelling a VCE was a major issue. In the EU, it was noted that a number of companies were still using the TNT Equivalence model for modelling of VCEs leading to inconsistencies in the over-pressure/distance relationships.

Another major issue was found to be the modelling of warehouse fire plumes where the materials in the warehouse contained a mixture of both flammable and toxic materials.

A rationalised and standardised methodology was developed within Haztech Consultants Ltd, which enabled a more efficient approach to consequence modelling for COMAH reports and also greater consistency of approach between individual consultants.

This paper considers the factors going into the source terms for both the gas dispersion modelling and the VCE modelling and also the inter-relation between the two separate sections of the modelling process. The development of the source term for a warehouse fire plume is also illustrated.

INTRODUCTION

Haztech Consultants Ltd were heavily involved in more than a dozen COMAH cases for upper-tier sites between 1999 and 2003. All of the COMAH cases involved aspects of gas dispersion modelling and many also involved the modelling of Vapour Cloud Explosions (VCEs) in order to be able to assess the extent and severity for identified major accident hazards^{1,2}.

Gas dispersion modelling is an essential part of hazard assessment for many scenarios and, as such, is a critical part of COMAH compliance. The source term used has a major impact on the results of the gas dispersion since it effectively defines many of the parameters in the model. Incorrect specification of the source term can

lead to significant errors in the output from the dispersion model. Explosion modelling is also highly important, especially where vapour cloud explosion (VCE) hazards were identified. Again, the source term used has a significant impact on the extent of the consequences.

At an early stage during the writing of COMAH reports, it became clear that the approach used by various companies to essentially similar problems was so diverse that it was virtually impossible to make a direct comparison between them or provide a representative set of data for submission in the COMAH safety report. Although a number of companies had had gas dispersion modelling done at some time previously, this was often not in any structured format or approach which could be linked to the identified major accident hazards. Typical of the issues encountered were:

- Diverse gas dispersion models used for the same type of release
- Improper application of models e.g. dense gas models used buoyant plumes
- Source terms not linked to major accident hazards
- Use of obsolete models e.g. TNT instead of TNO Multi Energy Model for VCE modelling
- Lack of documentation explaining choice of model, source term etc

CHOICE OF MODEL

GAS DISPERSION

There are a number of gas dispersion models available in the public domain varying in complexity many of which are described in Reference 3. Many of these public domain models originate from US Environmental Protection Agency sources. These, however, tend to be limited in their application to a very specific range of problems and it can be difficult to justify their use to the HSE due to a lack of familiarity and lack of use in the UK and EU. The limited applicability of many of the EPA models also means that several different models may be required to meet the range of scenarios found on a typical top-tier COMAH facility especially where several different processes are carried out on the site. Additionally, although the EPA models are freely available in the public domain, the user interface of the public domain versions tends to be command line based with text only output. In order to get a windows interface, it is necessary to purchase one of the third-party interfaces that have been written. It is essential that the dispersion model chosen should be appropriate to the type of release being modelled. The limitations of the chosen model should also be understood.

VAPOUR CLOUD EXPLOSION

The TNT equivalence model is generally considered obsolete for accurate VCE calculations (see below). The Baker-Strehlow model is used widely in the USA but has not found general acceptance in the EU. Within the EU, the most commonly used model is the TNO Multi-Energy Method (MEM) which has gained wide acceptance and has

been the subject of much research. Thus, for COMAH, the most appropriate model is considered to be the TNO MEM.

MODELLING PACKAGE

PHAST was chosen as the consequence modelling package for several reasons:

- Unified Dispersion Model is suitable for dense, neutral and buoyant plumes and can also model lift-off of a buoyant plume released at ground level (which many more basic dispersion models cannot handle)
- Release rate calculations (including two-phase flow) built into release model
- TNT equivalence, TNO Multi-Energy & Baker-Strehlow VCE models
- PHAST is recognised by the HSE as a valid modelling package for the purposes of COMAH
- Windows based input and output with full graphical and text output available

GAS DISPERSION MODELLING

WIND/WEATHER CONDITIONS

The correct specification of wind and weather conditions is essential to maintain model accuracy. Experience has shown that this is one area which is particularly poorly understood. The important model parameters are:

Wind speed: This is the wind speed at 10 m above ground level. Wind speed varies with altitude and the wind speed profile varies with surface roughness. Two wind speeds are commonly used for modelling, these being 5 m/s and 2 m/s. Under certain circumstances, 10 m/s and 15 m/s may also need to be modelled.

Air temperature: The air temperature used in the model needs to be appropriate to the weather condition being modelled and the geographical location.

Ground

temperature: The ground temperature has an effect on the turbulence and also pool vaporisation. Again this must be appropriate for the wind/weather conditions and geographical location.

It is essential to relate the weather conditions being modelled to actual conditions experienced in terms of temperatures, solar radiation etc in order to ensure that the model is relevant. If possible, actual historical records for the location should be used. If not possible then data from the nearest Meteorological Office weather station should be used (this can be purchased directly from the Meteorological Office). Lees⁴ also contains some useful information on typical UK weather conditions although some of this data is now rather old.

The two most common wind/weather conditions used for dispersion modelling in the UK are categories D5 and F2. Category D5 relates to the most commonly experienced conditions i.e. class D stability with 5 m/s wind speed. In practice, this relates to a

“typical” day with periods of sunshine and some cloud and a moderate breeze. Thermal radiation would be in the order of 0.5kW/m^2 (average). In the UK D5 typically occurs 40–60% of the time. Category F2 relates to a “worst case” for dispersion i.e. class F stability with 2 m/s wind speed. This is a very stable atmospheric condition with low wind speed and might relate to a cold winter morning or evening with minimal wind at ground level and a temperature inversion. Thermal radiation in this case would be minimal. F2 typically only occurs $\sim 1\%$ of the time in the UK⁴.

Categories D10 and D15 both relate to windy conditions and are generally only used when modelling warehouse fires. This is because the large vertical plume from a large fire may be dragged down to ground level under high wind speed conditions although the overall size of the plume may be significantly smaller than under D5 or F2 conditions due to the increased turbulence and mixing at the higher wind speeds.

On the basis of the above, it is possible to produce a set of representative matrix of wind/weather conditions for a given location as follows:

Condition	F2	D5	D10	D15
Stability Class	F	D	D	D
Wind Speed (m/s)	2	5	10	15
Air Temperature ($^{\circ}\text{C}$)	0	10	10	10
Surface Temperature ($^{\circ}\text{C}$)	0	10	10	10

It should, however, be noted that conditions, temperatures and the frequency of their occurrence vary depending on the location e.g. conditions in Aberdeen may well be significantly different from those in London. For COMAH modelling, however, a standardised set of F2, D5, D10 and D15 weather conditions are generally acceptable to the HSE with minor variations in temperatures being the key difference required.

SURFACE ROUGHNESS

The surface roughness contributes to mixing by causing boundary layer turbulence. It also has an effect on the wind speed profile as can be seen in Lees⁴. Most models use “surface roughness length” as an input to the program. PHAST, however, has the option of surface roughness length or an internal “roughness parameter”⁵. Since PHAST, in common with virtually all conventional dispersion models, is limited to using a single value for surface roughness, it is necessary to make a best estimate based on the prevailing geographic features. In practice, most sites have a combination of features within the dispersion range of interest. Relatively few exceptions to this generalisation exist within the UK and Europe, these being generally limited to sites located in estuary areas where there is an expanse of flat land surrounding the site. Choosing the appropriate roughness length for any particular situation is, therefore, to some extent, a matter of judgement for the vast majority of cases.

Type of Surface	Roughness Length (m)	PHAST Surface Roughness Parameter
Sea surface	0.013	0.06
Flat land, few trees	0.013	0.06
Open farmland	0.117	0.09
Open countryside	0.263	0.11
Woods, rural area or industrial site	0.951	0.17
Urban area	2.976	0.33

It should be noted that values between the numbers may be used if necessary although this again requires a certain amount of judgement.

RELEASE MATERIAL PARAMETERS

A clear understanding of the process from which the release occurs is essential for the accurate specification of the source term. Obviously, the material composition being released must be known but also the temperature and pressure are also critical e.g. gas, liquid, liquefied gas under pressure etc. The release condition should also take account of any process deviation that may be the cause of the release if appropriate.

The material parameters in conjunction with the line size, hole size etc define the release rate and velocity which are used in the dispersion source term.

ELEVATION

The effect of the elevation of the release above ground level is often neglected but can have a significant effect on the gas dispersion. This is due to the presence of a boundary layer of slow moving air close to the ground caused by the drag of the ground and any obstructions on the wind. Thus, wind speed increases with elevation and dispersion tends to be faster the higher above ground level a release occurs. A release at ground level may travel further if it remains entrained in the boundary layer than the same release at say 3 m elevation. It is, therefore, important to specify the release elevation correctly. This, of course, should be clearly related to the plant configuration and scenario being modelled.

ORIENTATION

The orientation of a release can also have a significant effect on the release, especially if the release impinges on another surface. Vertical upward releases tend to disperse quicker because of the increased wind speed at higher altitude. Horizontal releases are usually assumed to occur in the same direction as the wind i.e. downwind as this usually gives

the furthest hazard ranges. A release upwind would reduce the hazard range due to better mixing. A release which impinges on an adjacent surface tends to disperse more slowly than a free jet because the velocity of the jet is reduced and thus jet mixing is less giving a larger plume.

It is essential to consider the orientation of a release for the system being modelled. E.g. for a guillotine failure of a pipeline between adjacent plants it may be appropriate to use a horizontal release whilst for a release from the vent line of a tank with a “swan neck” then an impingement model might be appropriate. The selection of the appropriate orientation should be made based on the identified Major Accident Hazard scenario, taking into account any relevant details of the plant layout.

EXPLOSION MODELS

Three of the best known models for modelling of VCEs are:

1. TNT Equivalence
2. Baker-Strehlow
3. TNO Multi-Energy Model

There are also a number of lesser known models e.g. insurance models¹⁶ but these are not relevant to COMAH consequence modelling.

TNT EQUIVALENCE

The TNT equivalence model is based on an energy comparison between the flammable vapour cloud and a calculated amount of TNT. This model was used for many years to model VCEs since the explosion parameters for TNT are well known and the blast overpressure radii are well defined. The TNT model is⁵:

$$M_{TNT} = \left[\frac{H_{COMB}}{H_{TNT}} \right] M_{CLOUD} \times Eff \times R$$

Where:

- M_{TNT} = Equivalent mass of TNT (kg)
- H_{COMB} = Combustion energy (J/kg)
- H_{TNT} = Combustion energy of TNT (J/kg)
- M_{CLOUD} = Mass of flammable gas in cloud (kg)
- Eff = Explosion Efficiency
- R = Ground reflection factor

The explosion efficiency for typical hydrocarbons is usually set to a value of 0.1 but other values may be used. The ground reflection factor = 1 for an air burst or 2 for ground burst. This is to take account of the reflection of the blast from the ground.

Whilst the TNT method is useful for its' simplicity, it is limited in that the pressure/time and pressure/distance characteristics of blast waves from TNT detonations

differ significantly from industrial accidental explosions (VCEs) which are usually deflagrations.

The blast from TNT is a point source whereas the blast from a VCE is dispersed over a potentially large area. Thus, there are significant differences in the decay of the blast waves from TNT and VCE explosions with distance and a TNT explosion produces a higher pressure close to the source.

The importance of this was highlighted after the VCE at Decatur⁶ in which there were serious discrepancies between the predicted overpressures from the TNT model and the observed blast effects. Similarly, analysis of the Flixborough VCE also indicated discrepancies between the damage observed and TNT model predictions⁷. Flixborough represents something of a decisive moment in the understanding of the generation of explosion overpressure in that it became apparent that there were other mechanisms at work e.g. flame acceleration and turbulence caused by pipework, which had a significant contribution to overpressure^{8,9}.

The TNT method is not now generally used for explosion modelling except to provide a very quick approximate estimate of blast damage and overpressure radii as stated in the introduction. It was found that several companies were still reliant on the TNT equivalence model for estimation of VCE overpressure. This model has been known to be inaccurate for VCE modelling for some considerable time and has generally been superseded by the TNO Multi-Energy Method (TNO MEM) in the EU and the Baker-Strehlow method in the USA. Again, several instances were found in which the model parameters were not linked to a MAH scenario and in some cases there was no clear justification for the quantities of flammable gas or constants used in the equation¹⁰.

BAKER-STREHLOW VCE MODEL

The Baker-Strehlow method was developed in the early 1980s in the USA¹¹. This is a much more sophisticated method than the TNT equivalence. The energy of the explosion must first be defined and the scaled distance (dimensionless) calculated. The dimensionless pressure and impulse can then be read from graphs or lookup tables. The calculation is based on the flame speed of the gas mixture. The equation is:

$$R = \left(\frac{rP_0^{2/3}}{E^{1/3}} \right)$$

Where: R = Scaled distance
 r = Distance from centre of vapour cloud (m)
 P_0 = Atmospheric pressure (Pa)
 E = Energy (J)

R is then used with the data for flame speed to select a curve on the graph and the dimensionless side-on overpressure (P_s/P_0) can be read from the graph. The blast impulse can also be calculated using the Baker-Strehlow correlation^{12,13}.

TNO MULTI-ENERGY METHOD (TNO MEM)

Research during the 1980s¹⁴ showed that the blast overpressure was extremely difficult to correlate with the amount of vapour in the cloud using the TNT methodology. It was, however, noted that there was a strong correlation of blast with the amount of the flammable cloud which was in a confined or congested environment. The portion of the cloud not in a congested area was found not to contribute significantly to the blast overpressure. The blast was found to decay in a similar manner to an acoustic wave.

The explosion parameters are defined by the congested region and the strength is defined primarily by the amount of congestion and it is assumed that the cloud is all at stoichiometric concentration. Thus the main parameters of interest are the volume of the congested region containing the flammable mixture and the explosion strength factor.

Once the congested volume has been defined and the congestion factor, the calculation uses a series of equations to calculate the blast overpressure. The explosion strength is represented on a set of curves from 1–10 where 10 is the strongest. For “typical” chemical plants, a value of 7 is recommended for use. TNO ran two major projects (GAMES and GAMES II) into the strength of VCEs in structures. GAMES II is available from the HSE website as a contract research report¹³. Whilst these reports contained much useful research and information, it is relatively difficult to apply the findings to typical chemical plant situations due to the amount of data required. Unless there is a significant reason to deviate from strength 7 then this is the value recommended for use with typical chemical plant structures.

WAREHOUSE FIRE MODEL

In several COMAH cases it was necessary to model toxic gas dispersion from warehouse fires where the building contained a mixture of both toxic and flammable materials stored in drums and IBCs. The key problems with the source term for this type of model are:

- Definition of survival rates for toxic species in the plume
- Material properties for toxic species in the plume where a mixture of toxic and very toxic materials were stored
- Initial specification of plume composition for use in PHAST (composition, diameter, velocity, temperature)

Survival rates for toxic materials in a warehouse plume can be problematic since the manner in which materials are stored can vary in terms of racking, packaging etc. Guidance for survival rates of various species can be found in Reference 17, although a more crude assumption of 5% or 1% survival by mass is usually

adequate for first pass modelling and often adequate for COMAH depending on the results including toxicity of the materials being modelled and the potential effects on local population.

Where multiple toxic materials are stored in the same warehouse (as is commonly the case) it may be extremely difficult to define the composition of toxic materials in the fire plume. Since PHAST has a reasonably large database of material properties, many of the more common toxic materials may be found and used directly in the model. In many cases, however, there will be a number of materials that are not available in the database. These can be dealt with by using an exemplar compound which has similar properties. For example, toxic materials may be represented by Lindane and very toxic materials by Paraquat, both of which are in the PHAST database.

PHAST has limitations on the source term for maximum temperature and cannot deal with temperatures above 600°C. This is well below the combustion temperature of typical hydrocarbons that would be achieved in a warehouse fire where temperatures greater than 1,000°C might be expected. It is, therefore, necessary to calculate the source term for the gas dispersion at a point where the temperature is below 600°C. Reference 18 gives equations which can be used to estimate the initial plume temperature and air dilution factor from a given source. This method was used to estimate a source term with a temperature of less than 600°C and the figures for composition, velocity etc were used in the PHAST source term.

A “reality check” was also carried out on this model in order to see if it represented the actual plume behaviour that might be expected from a fire. Graphs of the shape of the plume produced by PHAST were compared with photographs of several warehouse fires and the overall shape of the smoke plume was found to be very similar to that produced by PHAST. Taking into account the variables of wind, weather and source terms, it was felt that the Haztech methodology produced an acceptable representation of the behaviour of a warehouse fire plume. This can be seen in Picture 1 and Graph 1 below.

COMAH METHODOLOGY

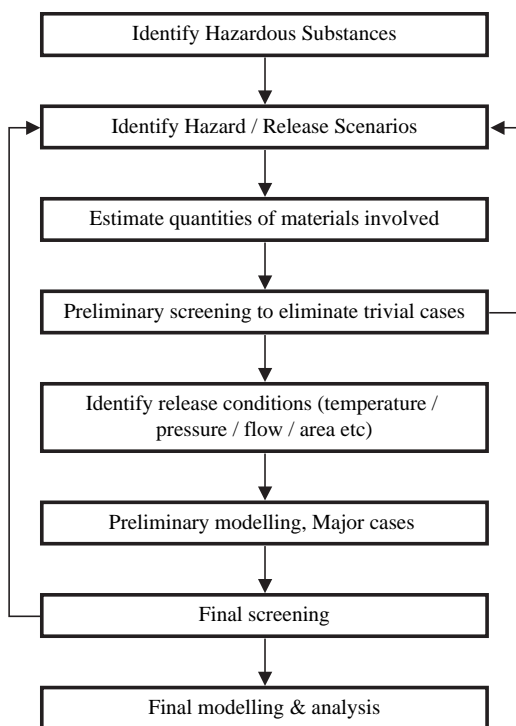
The linkage of source terms to identified Major Accident Hazard (MAH) scenarios is a key part of COMAH^{1,2}. In many cases it was found that modelling had been carried out for scenarios which were either not the worst credible incident or else were not clearly linked or related to identified MAH scenarios. In one particular example, a pool size and temperature had been used for gas dispersion which could not be linked to any of the physical or geographical features of the site or to the process conditions of the material. It is essential that a well defined set of conditions are used for dispersion modelling based as far as possible on prevailing conditions.

Due to the diversity in the way that consequence modelling had been carried out, it was decided at an early stage that a rational methodology was required in order to provide a consistent approach to modelling that would be acceptable to the HSE. This was doubly important where COMAH cases were being written for several sites within the same company.

Flow chart No. 1 below outlines the main steps in the modelling process:

The identification of hazardous materials, process conditions and release scenarios was accomplished using a tool developed by Haztech Consultants Limited, known as the “Major Accident Hazard Risk Assessment Tool” or MAHRAT which uses a guide word approach similar to Hazard Study stage 2. This tool was also developed based on information from references 18–22.

Toxic and flammable materials are treated differently because of the differing analysis required. A preliminary screening process is carried out on all scenarios in order to ensure that they meet the necessary MAH criteria and are directly related to identifiable scenarios. At this stage it is something of a “reality check”. Only after the preliminary screening is full gas dispersion modelling carried out. After the main part of the gas dispersion has been carried out a second screening process is carried out in order to eliminate the scenarios that fall below the threshold of the MAH definition. The release scenarios are also reviewed at this stage in order to ensure that they are relevant and appropriate.



Flow Chart No.1



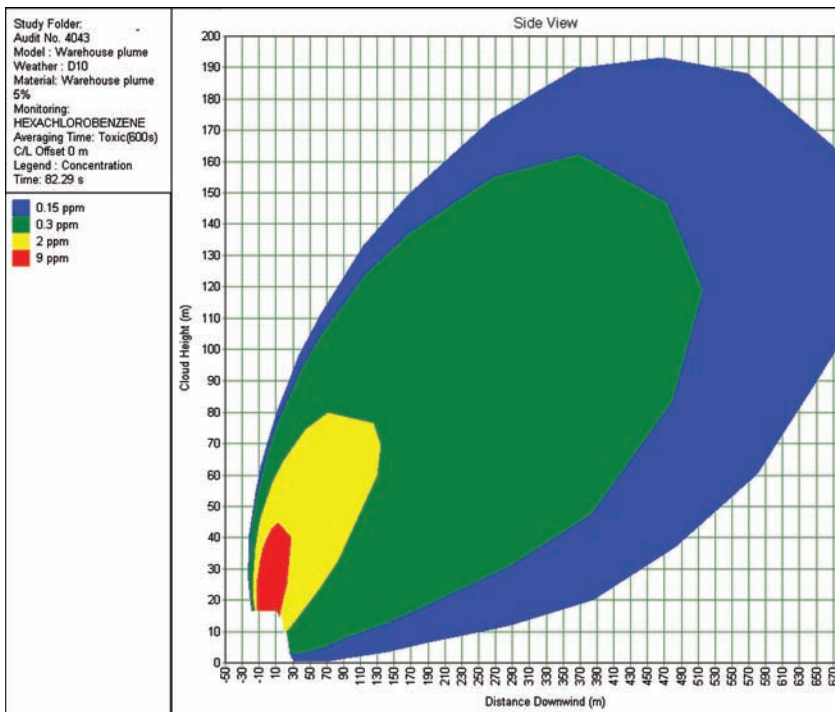
Picture 1 – Typical Warehouse Fire Plume

For flammable releases, there are four potential scenarios as follows:

1. Pool fire (liquid pool formed by the release)
2. Jet fire (ignition of gas/vapour release)
3. Flash fire (delayed ignition of large release without congestion or confinement)
4. VCE (delayed ignition of release in congested or confined space)

Of these, the first three are relatively straightforward to model although the size of the pool may need to be modified for the particular geographical location features e.g. bunds, kerbs, obstructions etc. VCE is usually more complex since there are confinement and congestion aspects to factor in to the model.

For a VCE, if the release completely fills a confined space then this scenario is relatively straightforward to model. If, however, the release is outdoors and only partially confined then the situation is less clear. For open structures then an estimate can be made



Graph 1 – PHAST Warehouse Fire Model Output

of the volume of the flammable cloud which enters the structure. This is dependent on the cross sectional area of the cloud, wind direction and the volume of the congested structure. It is necessary to make an estimate of the largest volume of flammable volume that can be generated based on the geometry of the flammable cloud and the geographic features of the site.

It should be noted that, since gas dispersion is a statistical model, the cloud may have pockets of flammable material down to the half LFL boundary. Thus, when considering the size of the flammable cloud entering a confined space or structure, it may be necessary to use the LFL/2 boundary when calculating the explosive volume.

SUMMARY

This paper has attempted to address the inconsistencies that were found in the modelling of gas dispersion and vapour cloud explosions prior to the submission of top-tier COMAH reports. A key requirement of the legislation was that all hazards should be assessed for

their “extent and severity”. This paper also attempts to address the lack of direct guidance relating to the use of consequence models or consequence modelling methodology.

A structured approach was developed by Haztech and the methodology was applied consistently across all of the COMAH cases in which the company were involved. The key factors of the Haztech approach were:

- Consistent approach to the identification of MAH scenarios
- Direct linkage from MAH scenarios to the consequence modelling output
- Consistent application consequence modelling across the full range of problems

This ensured that an appropriate and sufficient set of data were presented in the COMAH safety report and that these data would be directly comparable with any other similar scenarios modelled for any other company by Haztech.

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