Gas dispersion modelling using the DRIFT 3 model to assess toxic and flammable chemical major hazards

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This paper describes work undertaken to incorporate the gas dispersion model DRIFT 3 into the major hazard risk assessment process used by the Health and Safety Executive (HSE). It also presents key findings on the impact of the introduction of this model on HSE's advice. HSE undertakes risk assessments to provide advice to Local Planning Authorities (LPAs) on the safety of developments near chemical major hazards. DRIFT 3's capabilities were assessed in modelling dispersion from the wide range of release scenarios used by HSE to assess the risks from the storage and transport of hazardous chemicals. The four stages of the work looked at:

1. *Dispersion of vapour evolved from pools of toxic liquids*
   Modelling the vapour dispersion arising from liquid chemical spills, where the pool evaporation model GASP is used to generate the source term conditions.

2. *Releases of toxic pressure-liquefied gases*
   Modelling of near-instantaneous puff releases from catastrophic pressure vessel failures and modelling of jet releases from holes in pressurised vessels or pipework.

3. *Releases of toxic chemicals that disperse passively (neutral buoyancy)*
   Modelling of water reactive chemical releases that form an acid mist that disperses with the wind and modelling of spray releases where a fine mist is formed.

4. *Dispersion from releases of flammable chemicals*
   Modelling releases from major hazard chemical plant and pipelines storing and transporting flammable material.

The inputs and assumptions for DRIFT 3 were assessed for the wide range of scenarios used by HSE to calculate the risks from releases of toxic or flammable substances. Validation of the modelling results against experimental data was carried out to ensure that the model was being used correctly and to determine the appropriate modelling options.

The impact of the implementation of DRIFT 3 on HSE advice was assessed. The enhanced modelling capabilities of DRIFT 3 have enabled HSE to model release scenarios using fewer assumptions than previous approaches and have allowed a greater understanding of the key inputs required to model releases. This work programme has led to HSE updating some of the source term models used to provide inputs to DRIFT 3. The use of a single dispersion model has introduced consistency in the modelling of different releases from chemical storage and transport to allow HSE to provide safety-related advice for developments in the vicinity of major hazard sites and major accident hazard pipelines.

Keywords: gas dispersion modelling, land use planning, hazardous substance consents, source term models, model validation

Introduction

The accidental release of a gas or vapour cloud of a toxic or flammable chemical is a potential hazard to people in the vicinity of a facility storing or processing such chemicals. For a toxic substance, the gas or vapour cloud could lead to a person receiving a toxic dose of the substance leading to ill-health or death. A vapour cloud of a flammable substance could ignite leading to a *flash fire*, where the whole flammable cloud rapidly burns, which could expose people to thermal radiation from the fire potentially leading to injury and death.

Under the Planning (Hazardous Substances) Regulations (2015), the presence of hazardous chemicals above specified threshold quantities requires consent from a Hazardous Substances Authority (HSA). The Health and Safety Executive (HSE) is a statutory consultee on all Hazardous Substances Consent applications and for proposed developments which fall within HSE consultation zones. HSE is also a statutory consultee for Land Use Planning (LUP) for developments near Major Accident Hazard (MAH) Pipelines that fall under the Pipelines Safety Regulations (1996).

HSE's role is to consider the hazards and residual risks that would be presented by the hazardous substance(s) to people in the vicinity of a major hazards site. On the basis of the calculated hazards and risks, HSE advises the HSA whether or not consent should be granted. The hazard and risks calculated are used to set Land Use Planning (LUP) zones around the major hazard site plant or pipeline corresponding to specified risk levels of receiving a *dangerous dose* from the hazardous substance. A decision matrix is used to provide advice on the appropriateness of proposed developments within these zones near to the major hazard site or pipeline[1].

Historically, HSE has used a number of integral dispersion models to determine the effects of different types of release scenario. The use of multiple models evolved over time to deal with the large range of scenarios that HSE has had to

[1] http://www.hse.gov.uk/landuseplanning/methodology.pdf (accessed January 2016).

consider over the years. Different models were used for different release scenarios as no single model had sufficient capability to deal with the range of scenarios that HSE needed to model.

HSE made a decision to update the existing dispersion models used in these assessments to allow for a wider range of scenarios to be modelled using fewer and more consistent assumptions. As more sophisticated models are now available, it was decided to move, where practicable, to a single dispersion model to allow a consistent approach to be used across the range of release scenarios modelled in these assessments.

HSE commissioned ESR Technology to develop an updated version of the DRIFT model (Tickle, 2008). The revised model, DRIFT 3 (Tickle, 2012, 2013, Tickle et al., 2012, Tickle and Carlisle, 2013), includes a number of enhancements when compared to previous versions of the model (Webber, 1992a, 1992b). Significant enhancements include the introduction of *finite duration* and *time-varying* release options in the model in addition to *steady continuous* and *instantaneous* release options from previous versions of DRIFT.

- The *finite duration* release option is an extension of the *steady continuous* steady-state model which allows the effect of release duration on dispersion to be included. The finite duration model includes longitudinal spreading and dilution at the leading and trailing edges of the plume such that there is a smooth transition from steady-continuous plume-like behaviour in the near-field to instantaneous puff-like behaviour in the far-field.
- The *time-varying* release option models a release as a series of *finite duration* segments, where each segment has a different input flow rate. This allows dispersion to be modelled from a time-varying source (e.g. pool vaporisation, outflow of the depleting contents from a vessel). The concentration profiles output by each segment are summed to produce an overall time-varying concentration profile for the release.

Both of these methods have been tested as part of this programme of work. Other enhancements in DRIFT 3 when compared to the previous version of the model include:

- The option to calculate initial dilution and upwind dense gas spreading over a continuous area source;
- Extension of the model to include buoyant lift-off and buoyant rise;
- Allowance for the effect of the vertical variation of atmospheric pressure, temperature and humidity on the cloud thermodynamics;
- A concentration averaging-time model that is included to account for the dilution caused by lateral meander induced by fluctuations in the wind direction, together with a vertical meander model which accounts for the effects of updraughts and downdraughts in unstable atmospheric conditions;
- A momentum jet model that is integrated with the dispersion model to allow modelling of flashing jets entirely and smoothly within DRIFT 3; and
- The generalisation of the model to include multi-component, multi-phase mixtures.

This paper describes the validation and verification studies that were carried out by HSE prior to the adoption of DRIFT 3 into HSE's hazard and risk assessment processes.

DRIFT 3 model evaluation and validation

An evaluation of the DRIFT 3 model was made in accordance with a Model Evaluation Protocol (Ivings, 2007). The protocol sets out a method of scientific assessment, verification and validation for heavy gas dispersion models where the results are recorded in a model evaluation report (MER). The validation stage is carried out by running the model against a carefully selected database of dense gas dispersion experiments and calculating a number of Statistical Performance Measures (SPM). These SPM are then compared against performance criteria for an acceptable model. Figure 1 shows an example comparing DRIFT 3 predictions against Thorney Island experimental measurements (Coldrick, 2012).

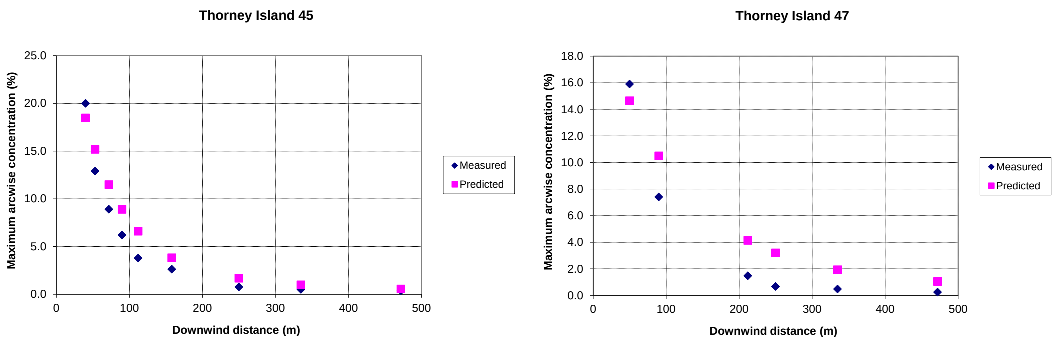

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Figure 1 Measured and DRIFT 3 predicted maximum arcwise concentrations for Thorney Island

The model evaluation of DRIFT 3 identified that this version implemented a number of improvements in the modelling capability compared to the original version of the model. The validation exercise found that DRIFT 3 generally compared well with the experimental data with validation results comparable to (or better than) other similar models.

The model evaluation report identified that DRIFT 3 was a complicated model:

> *"In attempting to get a physically well-founded understanding of the behaviour of heavy clouds into the form of an integral model (whose solutions can be found very rapidly on a computer) the original DRIFT 1 was a more complicated model than most of its contemporaries. The extended scope of [DRIFT 3] follows the same aims and it is more complicated still."*

A concern raised in the evaluation report was that care would be required to ensure that the model was being used appropriately, suggesting that it would be useful to have guidance on how to use the model in certain situations to ensure that a consistent approach was applied to dispersion modelling.

The programme of work within HSE to assess and test DRIFT 3 was informed by the findings of the model evaluation report. HSE took the opportunity to review how best to use the model including assessing the source terms' input conditions and assessing the most appropriate outputs to be used from the model. Working closely with the model developers allowed guidance on the use of the model to be developed to ensure that the enhanced capabilities of DRIFT 3 were being used consistently and appropriately.

DRIFT 3 verification and sensitivity studies

A programme of work was devised within HSE to assess how the DRIFT 3 model should be used in LUP hazard and risk assessments. This was an iterative process, working closely with the model developers. This programme was initiated to understand how the model operates, to allow for model capabilities to be reviewed, and to allow modifications to be made to the model to fit with HSE's needs more closely.

A four stage project was initiated to assess how to use the DRIFT 3 model for different types of release scenario. The four stages were:

1. *Dispersion of vapour evolved from pools of toxic liquids.*
   Modelling the vapour dispersion arising from liquid chemical spills, where the pool evaporation model GASP (Webber, 1990) is used to generate the source term conditions.
2. *Releases of toxic pressure-liquefied gases.*
   Modelling of near-instantaneous puff releases from catastrophic pressure vessel failures and modelling of jet releases from holes in pressurised vessels or pipework.
3. *Releases of toxic chemicals that disperse passively (neutral buoyancy).*
   Modelling of water reactive chemical releases that form an acid mist that disperses with the wind and modelling of spray releases where a fine mist is formed.
4. *Dispersion from releases of flammable chemicals.*
   Modelling releases from major hazard chemical plant and pipelines storing and transporting flammable material.

The work involved identifying appropriate methodologies for modelling these different hazardous release scenarios. As part of this work, the source term models used to generate the input conditions to DRIFT 3 were also reviewed. An assessment was made of how best to use the source term models to realistically represent the release mechanism and to ensure appropriate interaction between the source term model and DRIFT 3. During the course of this work it was necessary to adjust some of the source term models to meet these requirements.

Sensitivity tests were carried out to ensure that DRIFT 3 works reliably and produces scientifically sound results for the types of inputs typically used by HSE for Hazardous Substances Consent LUP purposes and for Pipelines Safety Regulations LUP assessment purposes.

The impacts on HSE's LUP advice from the use of the DRIFT 3 model were assessed by re-evaluating risk assessments for a number of sites to see what difference this would make to the hazard and risk zones generated.

This work programme is ongoing and is investigating the use of DRIFT 3 to model passive (neutral buoyancy) gas clouds. There is also a plan to investigate the use of DRIFT 3 to model buoyant clouds that could give rise to ground-level impacts e.g. when buoyant rise is limited by high wind speeds. This will complement the other workstreams in this programme which consider mainly dense or heavy (negative buoyancy) gas dispersion.

For assessments of toxic chemical releases, HSE uses a dose of interest referred to as the SLOT DTL (Specified Level Of Toxicity Dangerous Toxic Load). The SLOT DTL is assumed to be equivalent to the LD1 (Lethal Dose 1%), which is the toxic load that causes approximately 1% mortality in a normal population[2] (HSE website, *Toxicity levels of chemicals*). This HSE *dangerous dose* is sufficient to cause:

- Severe distress to almost everyone exposed to it;

[2] http://www.hse.gov.uk/chemicals/haztox.htm (accessed January 2016).

- A substantial fraction of the exposed population to require medical attention;
- Serious injuries to some people, requiring prolonged treatment; and
- Possible fatalities to highly susceptible people.

The Toxic Load for exposure to the toxic substance in air is given by:

$$\text{Toxic Load} = C^n t \quad (1)$$

Where *C* is the concentration of the toxic substance in the air in parts per million (ppm) by volume, *n* is the toxic exponent derived for the substance from the toxicological assessment of the substance[3], *t* is the duration of exposure (mins) and the Toxic Load is calculated in units of ppm^n.min.

The DRIFT 3 dispersion model can calculate the hazard footprints generated to the SLOT DTL criterion value. These hazard footprints are referred to as the SLOT DTL isopleths.

For the dispersion of flammable chemical releases that could lead to a *flash fire*, the concentration of interest is taken as the Lower Flammability Limit (LFL), also commonly referred to as the Lower Explosion Limit (LEL). Above this concentration, it is assumed that the cloud is flammable. The LFL contour has therefore been used to indicate the maximum footprint over which the cloud could ignite and burn.

Dispersion of vapour evolved from pools of toxic liquids

The first stage of the work programme investigated the use of DRIFT 3 to model the dispersion of vapour clouds that evolve from pools following spills of volatile toxic liquids. The model used by HSE to generate the source term conditions for these types of spills is the GASP model (Webber, 1990). GASP is a pool spreading and evaporation model that can calculate the time evolution of parameters such as the pool size, pool temperature, vaporisation rate and the total mass of vapour generated. GASP outputs are in a format that can be easily read by DRIFT 3. An updated Microsoft Windows version of GASP (version 4) has been produced by ESR Technology for HSE.

The existing methodology used within HSE to model pool spills was reviewed, taking into consideration the improvements available from the GASP 4 source term model interface and the enhanced modelling capabilities of DRIFT 3. Where appropriate, changes were made to the inputs and assumptions used by HSE to model such releases (Cruse, 2012).

Time-varying pool vaporisation

Given that vaporisation from a spreading pool is usually time-varying, the *time-varying* release option in DRIFT 3 was identified as giving the most appropriate representation of the source for a vaporising pool. However, the *time-varying* option in DRIFT 3 is a complex model that takes considerably longer to run a scenario than the other release types that can be modelled by the software. Some other issues were also identified relating to the implementation of the *time-varying* release option in DRIFT 3 when it was first tested. It was therefore decided not to use the *time-varying* release option initially until further development of the model could resolve some of the issues identified. ESR Technology has continued to improve this release model throughout the DRIFT 3 implementation work programme. The intention is to revisit the review of the *time-varying* release option to identify how best to use this option within DRIFT 3.

A simple methodology was devised to approximate the time-varying GASP pool source output for input to the DRIFT 3 *finite duration* model. This methodology identifies ‘peaky’ cases where the time-variation of the vaporisation rate from the pool is too great to model using a simple average rate. The methodology is used for substances that have a toxic exponent, *n*, greater than one, e.g. chlorine[3], where the contribution of the concentration peak is of greater significance to the toxic load calculation.

The method used involves assessing the vaporisation time profile output by the GASP model. The ‘peaky’ method is applied if the peak vaporisation rate is at least twice the mean vaporisation rate over the duration of the release.

For releases where the ‘peaky’ method is applied, the total mass vaporised, M_T, output by GASP over the release duration is used to determine a representative release duration, T_{RD}:

$$T_{\mathrm{RD}} = \frac{M_{\mathrm{T}}}{V_{\mathrm{peak}}} \quad (2)$$

where V_{peak} is the maximum (peak) vaporisation rate (kg s^{-1}) from the release.

The release is modelled in DRIFT 3 using a mass flow rate equal to V_{peak} for the representative duration T_{RD}. This ensures that the toxic load calculation captures high concentrations from the release whilst conserving the mass of the release.

Sensitivity and testing

The *finite duration* methodology in DRIFT 3 was used to assess methyl iodide and ethylene oxide releases to allow a comparison between the results generated using DRIFT 3 and the results generated using the previous HSE methodology for these types of release. Representative sets of scenarios were used to carry out the comparison:

[3] http://www.hse.gov.uk/chemicals/haztox.htm (accessed January 2016).

- A catastrophic vessel failure leading to a near-instantaneous large pool of the released substance; and
- A leak from a hole in a storage vessel.

Although HSE generally considers a more comprehensive set of scenarios when undertaking a risk assessment, the representative sets chosen for this study are sufficient for assessing the impact of using the new DRIFT 3 methodology.

Sensitivity analyses were carried out varying the size of the release and the new DRIFT 3 input parameters to ascertain the impact that these would have on the results generated and input to HSE's LUP advice.

Figure 2 shows an example of the SLOT DTL isopleths from ethylene oxide generated using DRIFT 3 compared with those generated from the previous HSE methodology using the DRIFT 2 model. The testing found that the SLOT DTL isopleths generated by DRIFT 3 did not have as large a downwind or crosswind extent as the SLOT DTL isopleths generated using the DRIFT 2 methodology. This means that the risk levels calculated from a release will be reduced as there is a smaller chance of a person being affected by a release. DRIFT 3 does calculate an upwind effect from a release, whereas DRIFT 2 did not calculate any upwind effects for such releases. This is due to DRIFT 3 being able to model upwind gravity driven spreading from dense area sources, which DRIFT 2 did not take into account. For this case, the upwind extent is closely related to the pool source size and is not likely to lead to a significant contribution to the risk levels calculated for persons off-site from the release point. Generally the differences between the results obtained from the two versions of the model were identified as being due to DRIFT 3's improved ability to model real physical processes, such as upwind spreading from a dense source, or the effect of a finite release duration.

Based on the findings of this work package, the new methodology using DRIFT 3 to model spills of toxic liquids for LUP assessments has been agreed within HSE and is now in use.

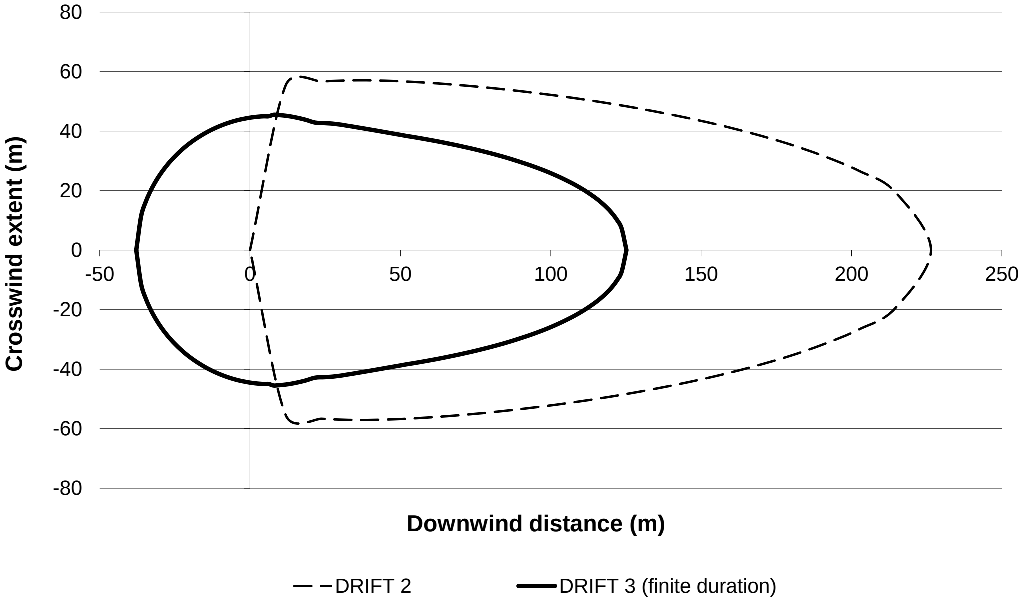

Figure 2 SLOT DTL isopleths for outdoor recipients calculated for a pool generated from a 50 mm hole in an ethylene oxide vessel in D5 weather conditions (D Pasquill atmospheric stability; 5 ms^{-1} wind speed)

Releases of toxic pressure-liquefied gases

The second stage of the work programme concentrated on the use of DRIFT 3 to model the dispersion from releases of toxic chemicals from pressurised storage. This stage of the work programme was split into two distinct workstreams: one workstream investigating the dispersion of continuous flashing jet releases from holes in storage vessels or pipework; the other workstream investigating the dispersion of near-instantaneous puff releases following catastrophic vessel failure.

Modelling flashing continuous releases of toxic substances from holes in vessels and pipework

Work was undertaken to examine the behaviour of DRIFT 3 in modelling flashing jets from holes in vessels and pipework (Lamb, 2013).

This workstream included investigating the source terms for modelling flashing continuous releases. The previous HSE methodology used the in-house CREATE model (Carter, 1991) to model the jet expansion phase of a release from an orifice of a pressure-liquefied gas. The results from the CREATE model were used as inputs to the CRUNCH dense gas dispersion model (Jagger, 1983).

This workstream also considered the potential rainout of droplets from the momentum jet (Tickle, 2015c). Rainout of material from the jet can reduce the range of any hazardous impact of the toxic material. However, the rainout can also lead to a secondary vapour source: an evaporating pool that could last longer than the jet release and also contribute to any off-site harm effects following the release.

A review of the CREATE model (Tickle, 2015a) indicated that there are now better models available to determine the source terms for continuous flashing releases. As DRIFT 3 directly incorporates a momentum jet model, based on the EJECT model (Tickle, 1998), use of the DRIFT 3 jet model was investigated to ensure that it could be used appropriately for the types of release that HSE required.

Consideration was given to whether different jet orientations could be modelled and whether different orientations would make a significant impact on the footprint of the SLOT DTL isopleths. It was found that some different release orientations could be modelled in DRIFT 3 but that, for the release cases considered, the differences made in the SLOT DTL isopleth extents was minimal. This, together with uncertainties in the likelihoods of different release orientations, suggested that the modelling of different release orientations required a large amount of extra work for no significant gain in modelling accuracy. It was therefore decided to base assessments on releases in the same direction as the wind and this approach was subsequently used for the sensitivity testing of flashing continuous releases using DRIFT 3.

Continuous flashing releases from holes in vessels and pipework were modelled using DRIFT 3 for chlorine, sulphur dioxide and ammonia releases and compared against the results obtained from using the CREATE/CRUNCH methodology previously used by HSE.

Sensitivity analyses were also carried out to ascertain whether the modelling of a pool generated from rainout near to the source would contribute to the harm effects experienced by nearby populations.

For the modelled cases, the SLOT DTL isopleths generated from the use of DRIFT 3 extended further downwind and to a larger crosswind extent than those generated using the CREATE/CRUNCH methodology (see e.g. Figure 3). This means that the risk levels calculated will be greater when using DRIFT 3 compared to the previous method due to the larger hazardous footprint from a release.

For all the scenarios modelled in this study, the SLOT DTL isopleths obtained from modelling the plume arising from the continuous jet were significantly larger than the SLOT DTL isopleths generated from pools formed from rainout near to the source.

Figure 3 SLOT DTL isopleths for outdoor recipients for the plume component of a chlorine release from a 50 mm hole in the liquid space of a 15 te vessel in D2.4 weather conditions (D Pasquill atmospheric stability; 2.4 ms^{-1} wind speed)

Modelling flashing near-instantaneous releases of toxic substances following catastrophic vessel failure

Work was undertaken to examine the behaviour of DRIFT 3 in modelling flashing near-instantaneous releases following the catastrophic failure of a pressure vessel storing a pressure-liquefied toxic gas (McGillivray, 2013).

This workstream included an investigation of how best to model the source term conditions for input into DRIFT 3. The previous HSE methodology used the outputs from the in-house IRATE model to determine the inputs to the DENZ dense gas dispersion model (Fryer, 1979) following the initial expansion phase of a puff release. Consideration was also given to any potential rainout of droplets during the initial phases of a release and also to any remaining toxic liquid pool following a catastrophic vessel failure. Both of these conditions could lead to a secondary pool event that could contribute to off-site harm effects following the release (see Figure 4).

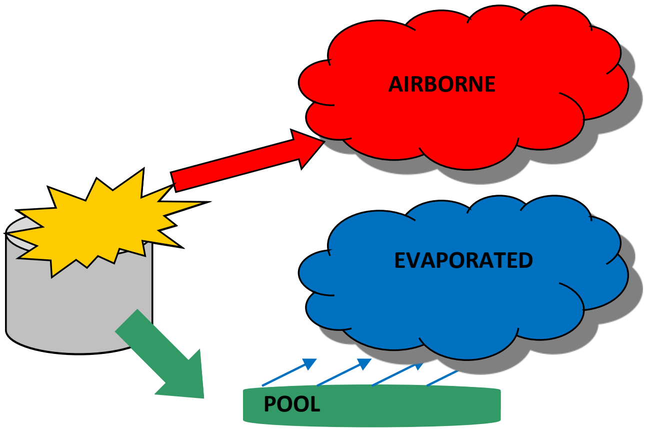

Figure 4 The potential scenarios that could occur from an instantaneous release of flashing material

A review of the IRATE model (Tickle, 2015a) indicated that there are now better models available for source terms for a near-instantaneous puff release. The ACE model was developed by WS Atkins for HSE in the late 1990s (Gilham, 1997a, 1997b, Shepherd, 2000). WS Atkins had provided HSE with a software version of the ACE model and this allowed some initial testing of the model. As part of the HSE review of the ACE model, the results generated by ACE were validated against experimental data (Coldrick, 2013). The ACE model methodology was also reviewed (Tickle, 2015b) and recommendations made for improvements that could be made to the model to allow it to be used with DRIFT 3. HSE used the WS Atkins methodology described in Gilham (1997a, 1997b) and Shepherd (2000) to code up a new version of ACE. The results from this new version were verified by comparison with the results generated by the WS Atkins version of ACE. The recommended modifications to the model were then implemented and this version of ACE was validated against the experimental results.

ACE models an explosion (rapid-expansion) phase followed by a (slower) turbulent growth phase. To allow validation against both large and small scale experiments (and to accommodate the different scales of the experimental data recorded), a non-dimensional approach was used as outlined in Makhviladze (2004). Non-dimensional expansion velocity (U/U_*) versus time (t/t_*) plots were obtained for the ACE predictions against the experimental data (Coldrick, 2013). Experimental data from Makhviladze (2004), Hardee (1975), Pettitt (1990), Bettis (1992) and Schmidli (1992) have been used in the validation of the ACE model predictions as shown in Figure 5. Comparison of overall cloud radius predictions against experiments at a range of scales showed that the ACE predictions were in reasonable overall agreement with the data.

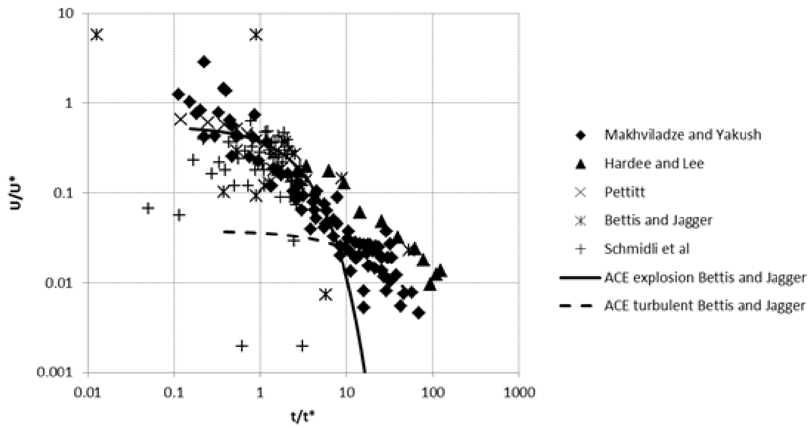

Figure 5 ACE predictions of Bettis (1992) experiments plotted against all data

The HSE version of ACE was used in all of the subsequent sensitivity testing of the use of DRIFT 3 for flashing near-instantaneous puff releases.

Representative sets of releases from pressurised storage vessels of chlorine, sulphur dioxide and ammonia were modelled to allow a comparison of the results generated using the ACE and DRIFT 3 models with those generated using the previous HSE methodology (IRATE and DENZ). The impact of any pool evaporation was also considered for these releases, where the toxic material in the vessel that did not form part of the airborne aerosol cloud was modelled using the GASP pool model and the methodology derived in stage 1 of this programme for modelling pool evaporation using DRIFT 3.

Representative sets of releases from heated vessels storing methyl chloroformate, propionitrile and 2-chloroethanol were also modelled and compared against the results from the previous HSE methodology for modelling these releases. Once again, the pool component of a release was modelled alongside the puff component and the SLOT DTL extents compared to assess whether HSE would need to model pools alongside the instantaneous release puff following a catastrophic vessel failure.

The SLOT DTL isopleths produced using ACE and DRIFT 3 for the puff releases (storage vessels and heated vessels) were significantly shorter than the isopleths generated using IRATE and DENZ, but were generally wider in the crosswind extent. The impact that this would have on the risk levels calculated is that close to the release source the risk levels calculated will be slightly greater as there is a greater chance that a person would be within the wider isopleth extent, but the downwind distances at which there would be a risk from a release would be significantly reduced in length.

The SLOT DTL isopleths for the pool scenarios modelled did not extend as far downwind or to as great a crosswind extent as the isopleths generated for the corresponding puff scenarios modelled.

Figure 6 shows the comparison between the SLOT DTL isopleths generated using the IRATE/DENZ methodology and the isopleths from the ACE/DRIFT 3 methodology for 10 te and 100 te chlorine vessel failures.

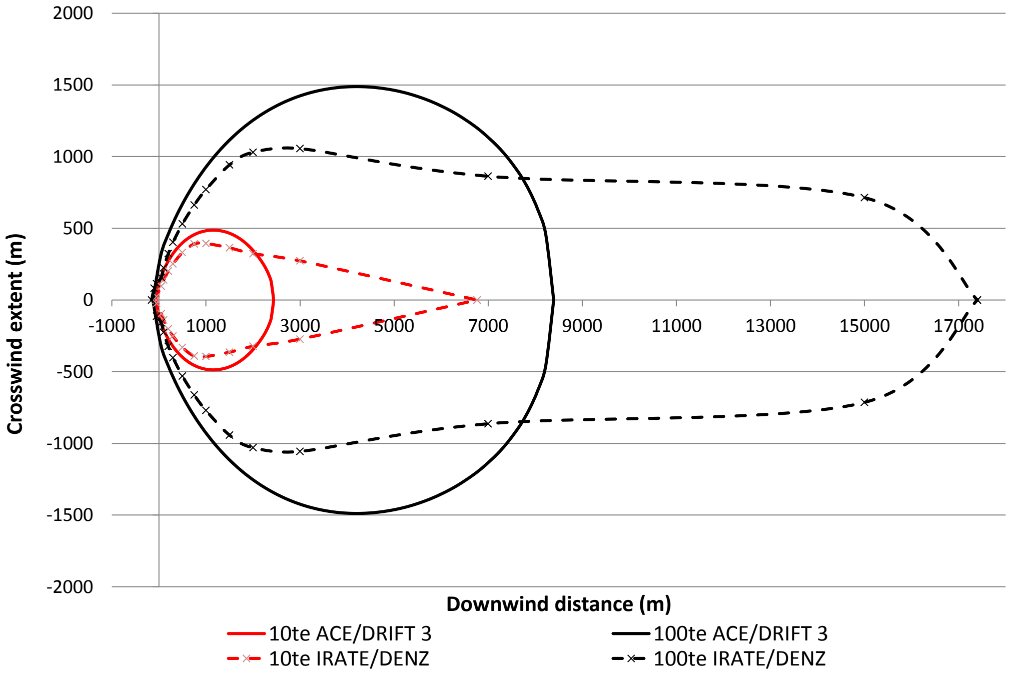

Figure 6 SLOT DTL isopleths for outdoor recipients generated for 10 te and 100 te chlorine vessel instantaneous puff releases in F2.4 weather conditions

Releases of toxic chemicals that disperse passively (neutral buoyancy)

The third stage of work involved investigating the ability of DRIFT 3 to model scenarios leading to passive gas or vapour dispersion of a toxic chemical. The modelling of spray releases was also investigated. This was to ascertain a way to deal with cases where a small pressurised liquid leak from a flange or a crack leads to fine mist being generated that can disperse a normally non-volatile substance off-site thereby affecting nearby populations.

The existing HSE dispersion modelling approach for sprays, developed in the 1990s, used a Gaussian dispersion model and assumed that all of the spray remained airborne. Whilst this approach may be adequate for small spray releases, a concern is that it may be overly cautious when applied to larger releases or for releases that involve highly toxic substances. One of the aims of this stage of the work programme was to try to provide a better modelling solution for these cases.

A study was undertaken to develop a spray screening tool to identify conditions under which releases should be modelled as toxic sprays, rather than pools, and to ascertain whether there was a suitable approach that could be adopted for input to DRIFT 3. The screening tool includes consideration of droplet size distributions and droplet dry out times. The droplet dry out times are based on the height of the release and the volatility of the substance. In some cases hazard ranges can effectively be limited by using standard deposition algorithms available within DRIFT. Recently published experimental work on droplet sizes and rainout from sub-cooled liquid sprays (Witlox, 2013, Bettis, 2013) is useful, but extrapolation to hole sizes and hole configurations outside the range of the experimental conditions remains a major uncertainty.

The next phase of this work stage is to investigate the use of DRIFT 3 to model the dispersion of passive (neutrally buoyant) clouds of toxic chemicals. This includes investigating the use of DRIFT 3 to model the dispersion of acid mists generated from spills of water reactive chemicals. Acid mists from water reactive spills may display complex thermodynamic behaviour due to the combined effects of increased density due to possible liquid/solid aerosol and decreased density due to the heat generated from reaction of airborne water reactive substances with atmospheric moisture. In an actual release, an acid mist cloud generated from a water reactive spill may go through initial phases of dense gas dispersion and buoyant dispersion before eventually dispersing passively.

Given that these clouds tend to disperse passively following the initial phases of the release, HSE has historically assumed that the entire release is treated as a passive cloud when assessing the off-site risk from an accident to allow these releases to be modelled. This part of the work programme is ongoing with a review of existing literature on the behaviour of observed acid mist dispersion being the first task.

Dispersion from releases of flammable chemicals

The fourth stage of work investigated how the methodologies identified in stages 1 and 2 for toxic substances could be adapted and implemented for assessing the hazards and risks for flammable substance releases (Chaplin, 2014). In this case, the DRIFT 3 model was used to output to the Lower Flammable Limit (LFL) concentration rather than outputting the isopleth to where a person would receive the SLOT DTL *dangerous dose*. The LFL footprint output from DRIFT 3 can then be used to determine the potential extent of a *flash fire* event.

As well as investigating releases from vessels and pipework, the modelling of releases from holes and ruptures in major accident hazard pipelines that fall under the Pipelines Safety Regulations (1996) was also considered as part of this stage of the work programme.

This work stream investigated three distinct release types corresponding to the releases investigated in stages 1 and 2 of the DRIFT 3 implementation work programme:

- Dispersion from vaporisation of a spreading pool of a flammable liquid;
- Dispersion from a flashing jet release of a flammable substance from a hole or rupture in pressurised vessels, pipework or major accident hazard pipelines; and
- Dispersion from a near-instantaneous puff of flammable vapour following a catastrophic vessel failure.

Each of these work areas is discussed in more detail in the following sections.

Evaporating pools of flammable liquids

Work was undertaken to investigate the modelling of continuous releases of flammable substances that form a spreading evaporating pool that generates a dispersing flammable cloud. How this scenario could best be modelled using GASP and DRIFT 3 was investigated.

The evolution of vapour from the flammable pool was modelled using the *finite duration* release option in DRIFT 3 using the mean vaporisation rate over the release duration from the pool. The sensitivity of this approach was investigated by comparing the results generated using the *finite duration* option with the results generated from the use of the *time-varying* release option in DRIFT 3 and from the use of the ‘peaky’ methodology developed for toxic pools (as described in more detail earlier).

It was found that, for the scenarios considered, the mean vaporisation rate gave a reasonable approximation to model a release apart from cases where there was a significant change in the pool vaporisation rate over time. Guidance has been written to allow HSE to determine when to employ the ‘peaky’ method to calculate the pool vaporisation rate and duration in preference to the use of the mean vaporisation rate across the entire duration of the release (Chaplin, 2014).

In some scenarios modelled, the clouds became buoyant downwind from the pool. Checks have been included to ensure that realistic hazard ranges are being calculated given the buoyancy of the dispersing cloud.

Flashing releases of flammable chemicals from holes in vessels, pipework and pipelines

This workstream investigated how to use DRIFT 3 to model a continuous release of a flammable substance from a vessel, pipework or a pipeline resulting in a dispersing flammable cloud.

Releases from ethylene and propane pipelines were undertaken as part of this workstream and the results compared to the LFL distances generated from the previous HSE methodology using the CRUNCH dense gas dispersion model.

The CRUNCH methodology generated maximum downwind extents to the LFL that were much larger than those generated by DRIFT 3. This is believed to be due to the importance of jet dilution for these releases, which is included in DRIFT 3 but not included in CRUNCH.

Sensitivity analyses were undertaken to ascertain the most suitable inputs required to model such releases. This included investigating inputs such as release height, release angle, release temperature and relative humidity. Guidance was written to allow HSE to assess these types of releases consistently (Chaplin, 2014).

Flashing releases of flammable chemicals from catastrophic vessel failure

Releases where the contents of a vessel are lost almost instantaneously and a flammable cloud is formed were also investigated in this stage of the work programme. The release mechanisms are the same as those investigated for toxic releases in stage 2. A vaporising pool of flammable liquid can be formed alongside the flammable vapour cloud following a vessel failure. The impact of any secondary pool event was examined alongside the impact of the near-instantaneous puff dispersion.

The ACE model was used to generate the source term inputs for DRIFT 3. The methodology developed in stage 2 to model near-instantaneous flashing releases for toxic chemicals was investigated to determine whether it could also be applied to near-instantaneous flammable puff releases. A sensitivity analysis of the use of ACE as an input to DRIFT 3 was carried out, considering the impact of different input options on the results generated. It was found that the user inputs in ACE can have a significant impact on the hazard ranges to the flammable substance LFL produced by DRIFT 3.

This workstream also identified that the resultant pool caused by rainout from the initial release can lead to hazard ranges to the substance LFL of a similar magnitude to the hazard range footprint from the initial puff cloud, when using DRIFT 3 to model both releases. The recommendation from this work is for HSE to consider both the cloud and the pool when performing a Hazardous Substances Consent assessment for flammable substances.

Guidance was produced on how to model near-instantaneous flashing releases following the catastrophic failure of a pressurised vessel storing or processing a flammable chemical (Chaplin, 2014). This guidance specifies how to use the ACE model to generate the inputs for DRIFT 3 and gives a methodology for comparing the results generated using the instantaneous release type in DRIFT 3 with the results from DRIFT 3 based on pool vaporisation following liquid rainout.

DRIFT 3 has recently been enhanced to allow both the dispersion from a direct source (e.g. airborne aerosol cloud) and from a vaporising pool (predicted by GASP) to be combined within a single DRIFT run thus avoiding the need to manually combine the results from these two sources.

Conclusion

HSE embarked on a programme of work to update its dispersion modelling capability using the DRIFT 3 model. This programme of work has led to improved modelling capability within HSE. It has clarified the dispersion modelling process in HSE by moving away from multiple dispersion models to one dispersion model that is applied consistently across a range of different release scenarios.

The programme of work has given confidence that the DRIFT 3 model is being used in an appropriate manner and the outputs are being used correctly to generate HSE's Land Use Planning (LUP) advice regarding developments near hazardous substance installations.

DRIFT 3 has undergone a rigorous testing regime as part of its adoption into HSE's hazard and risk assessment processes. The ways that DRIFT 3 could be used to model different types of release scenario have been comprehensively explored to ascertain the best way for HSE to model such releases. The model has been evaluated following an existing model evaluation protocol and has been further validated against experimental data by HSE (in addition to the validation undertaken by ESR Technology as part of the model development). The review of source term models and the assumptions used in HSE's modelling processes has improved the quality of inputs used in the dispersion model, thereby further improving HSE's modelling capabilities.

The results generated using DRIFT 3 and the associated new source term models and assumptions were compared against the results generated from the previous methodology for each type of release scenario examined. The aim was to assess the difference the new model would make to HSE advice with regards to LUP developments near to hazardous substance plant or pipelines.

In most cases, the use of DRIFT 3 has led to a reduction in the size of the hazard zone isopleths generated for the release types investigated. This consequently reduces the risk levels calculated in the vicinity of a hazardous substance plant or pipeline. For flashing continuous releases, DRIFT 3 predicted slightly larger hazard zone isopleth footprints than the previous methodology. However, for this type of release, the differences in isopleth footprint size were not significant and, therefore, the overall trend for a full risk assessment, taking into account different potential release mechanisms, is still likely to be a reduction in the risk levels calculated near to a hazardous installation.

Ongoing work in this area is investigating how best to use DRIFT 3 to model the dispersion of acid mist releases from spills of water reactive chemicals. The use of DRIFT 3 for scenarios where the dispersion of a buoyant hazardous substance could impact on nearby populations is also to be investigated further. The *time-varying* release model has been improved by ESR Technology throughout this work programme. Testing of this method is to continue, to determine when it would be appropriate to use this method and to identify the best methodology to ensure that HSE uses this method consistently in the generation of its advice.

A test plan to validate and verify any new versions of the model has been drafted. This is to ensure that any future modifications to the model do not invalidate the results from the testing of the previous versions of the model. The test plan includes looking at verifying predictions against aspects from all of the four stages of the work programme undertaken.

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