



Gas dispersion model DRIFT 3.6.14: modelling the dispersion of flashing instantaneous releases of toxic substances

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HSE uses gas dispersion modelling in its assessment of the hazards and risks posed by toxic and flammable substances stored at major hazards sites. To update its dispersion modelling capability, HSE commissioned ESR Technology to develop a new version of the gas dispersion model DRIFT. The new version, DRIFT 3, includes a significant number of modelling enhancements over the version previously used within HSE (DRIFT 2.31). These include the extension of the model to treat buoyant plumes and time varying releases. Before DRIFT 3 is adopted for use by HSE, it must undergo thorough evaluation and assessment for a range of release scenarios. The initial phases of the DRIFT 3 testing programme used DRIFT 3.6.4 and are described in reports RR1100 and RR1101. Further testing is described in four reports including this one: RR1165, RR1166, RR1167 and RR1168. The four reports cover the evaluation of the model and assessment for a range of scenarios using the enhanced version DRIFT 3.6.14.

This report describes an assessment of the performance of DRIFT 3.6.14 for modelling the dispersion of flashing instantaneous releases of toxic substances. Releases of toxic pressure-liquefied gases such as chlorine, sulphur dioxide and ammonia are considered, together with flashing heated releases from pressure vessels. These scenarios are typically used by HSE to assess Hazardous Substances Consent applications and set Land Use Planning zones around major hazards sites. This report describes sensitivity tests which show that DRIFT 3.6.14 works reliably for these scenarios. As a result of this assessment and accompanying model evaluation (see RR1165), DRIFT 3.6.14 has been adopted by HSE to model instantaneous releases of toxic pressure-liquefied gases.

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Gas dispersion model DRIFT 3.6.14: modelling the dispersion of flashing instantaneous releases of toxic substances

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KEY MESSAGES

The Health and Safety Executive (HSE) uses gas dispersion modelling in its assessment of the hazards and risks posed by toxic and flammable substances stored at major hazards sites. A new version of the gas dispersion model DRIFT (Dispersion of Releases Involving Flammables or Toxics), DRIFT 3, was commissioned by HSE to update its dispersion modelling capability.

To ensure that DRIFT 3 is fit for purpose, a programme of work is being undertaken at HSE. This includes an evaluation of the dispersion modelling capabilities of DRIFT 3 and an assessment of the performance of DRIFT 3 for modelling the types of release scenario typically considered by HSE for Hazardous Substances Consent assessments.

The initial phases of the testing programme were carried out using DRIFT 3.6.4. The most recent version of DRIFT currently available to HSE is DRIFT 3.6.14. Building on the previous model testing, an assessment has been made of the use of DRIFT 3.6.14 for modelling the dispersion of instantaneous releases of toxic pressure-liquefied gases. Sensitivity tests have shown that DRIFT 3.6.14 works reliably for the types of inputs typically used by HSE.

The dispersion of such releases was previously modelled by HSE using the DENZ dispersion model, a precursor to DRIFT that was originally developed in the late 1970s. The outputs of DRIFT 3.6.14 and DENZ have been compared for a selection of chlorine, sulphur dioxide and ammonia release scenarios.

For the scenarios studied, the SLOT DTL (Specified Level of Toxicity, Dangerous Toxic Load) isopleths predicted by DRIFT 3.6.14 are shorter than those predicted by DENZ. These isopleths enclose the area within which the HSE dangerous dose of the substance, the SLOT DTL, is exceeded. Close agreement between the predicted isopleths should not necessarily be expected because there are significant differences between the modelling assumptions used in the two methodologies. DRIFT 3 contains a more sophisticated passive dispersion model than DENZ, and the smooth transition from dense to passive behaviour in DRIFT 3 is an improvement on the abrupt transition in DENZ.

The in-house HSE model IRATE was used to calculate a source term for input to DENZ. A more sophisticated source term model, ACE (Airborne Concentration Estimate), has been used to calculate a source term for input to DRIFT 3.6.14. ACE calculates the fraction of the release that becomes airborne as vapour or aerosol and assumes that the remainder of the release rains out to form a pool. Both the initial airborne component of the release and the component that rains out to form a pool may contribute to the overall risk posed by the release. DRIFT 3.6.14 does not have the capability to combine the airborne and pool components of a release into a single run to produce a single set of SLOT DTL isopleths for the overall release. Separate SLOT DTL isopleths have been calculated for the two components of each release and guidance is provided on how these isopleths should be used in subsequent risk calculations.

Flashing instantaneous releases of substances that are heated above their normal boiling point temperature in process vessels or reactors have also been considered. It has been concluded that ACE and DRIFT 3.6.14 are appropriate tools for modelling such releases.

As a result of this work and accompanying evaluation studies, DRIFT 3.6.14 has been adopted by HSE to model the dispersion of flashing instantaneous releases of toxic substances. Guidance is provided on how DRIFT 3 should be used to model the dispersion of flashing instantaneous releases of toxic substances for the purposes of Hazardous Substances Consent assessment.

This detailed technical report is aimed at technical specialists in consequence modelling and risk assessment.

EXECUTIVE SUMMARY

The Health and Safety Executive (HSE) uses gas dispersion modelling in its assessment of the hazards and risks posed to people in the vicinity by toxic and flammable substances stored at major hazards sites. To update its dispersion modelling capability, HSE recently commissioned ESR Technology to develop a new version of the gas dispersion model DRIFT (Dispersion of Releases Involving Flammables or Toxics). The new version of the model, DRIFT version 3 (DRIFT 3), includes a significant number of modelling enhancements over the version of DRIFT previously used by HSE (DRIFT 2.31). These include the extension of the model to treat buoyant plumes and time varying releases.

Under the Planning (Hazardous Substances) Regulations, the presence of hazardous chemicals above specified threshold quantities requires consent from a Hazardous Substances Authority (HSA), which is usually the local Planning Authority. HSE is a statutory consultee on all Hazardous Substances Consent applications. Its role is to consider the hazards and residual risk which would be presented by the hazardous substance(s) to people in the vicinity, and on the basis of this to advise the HSA whether or not consent should be granted. The outputs of these assessments are also used to set Land Use Planning (LUP) zones around major hazards sites. DRIFT 3 will be used by HSE in this assessment process.

To ensure that DRIFT 3 is fit for purpose, a programme of work is being undertaken at HSE. This includes an evaluation of the dispersion modelling capabilities of DRIFT 3 and an assessment of the performance of DRIFT 3 for modelling the types of release scenario typically considered by HSE for Hazardous Substances Consent assessments. The scenarios being examined include releases of toxic or flammable pressure-liquefied gases and dispersion of vapour from pools of toxic or flammable liquids.

This report describes part of this programme of work and presents an assessment of the use of DRIFT 3.6.14 for modelling the dispersion of instantaneous releases of toxic pressure-liquefied gases such as chlorine, sulphur dioxide and ammonia. This report also considers flashing instantaneous releases of substances that are heated above their normal boiling point temperature in process vessels or reactors. The results for continuous releases of toxic pressure-liquefied gases are presented in a separate report.

Prior to this work, HSE modelled the dispersion of instantaneous releases of toxic pressure-liquefied gases using the DENZ dispersion model, a precursor to DRIFT that was originally developed in the late 1970s. DRIFT 2.31 was used to model substances not available in DENZ. The in-house HSE tool, IRATE, was used to calculate a source term (e.g. initial air entrainment, initial flash fraction and final temperature of the cloud) for input to DENZ or DRIFT 2.31.

IRATE assumes that the entire inventory becomes airborne and neglects the potential for rainout and pool formation, which are likely to occur in reality. There are more sophisticated source term models now available that can account for pool formation and it was considered appropriate to identify a replacement for IRATE to use with DRIFT 3.

A number of the assumptions used for this work were identified during an earlier stage of this project, which examined the use of DRIFT 3 for modelling the dispersion of vapour from pools of toxic liquids.

Objectives

This work has four distinct objectives:

- Identify an appropriate source term model to replace IRATE and assess its suitability for use with DRIFT 3.
- Compare the previously recommended method (IRATE and DENZ) against the new methodology (new source term model and DRIFT 3).

- Use the new source term model to estimate the mass of toxic substance in the pool and the mass that becomes airborne initially (this will have aerosol and/or vapour components). Compare the SLOT DTL (Specified Level of Toxicity, Dangerous Toxic Load) dispersion isopleths from the evaporating pool against those from the fraction of the release that initially becomes airborne, to see which has the greater potential to cause harm. The SLOT DTL isopleths enclose the area within which the HSE dangerous dose of the substance, the SLOT DTL, is exceeded
- Determine whether the new source term model and DRIFT 3 are appropriate tools for modelling flashing instantaneous releases of substances that are heated above their normal boiling point temperature in process vessels or reactors.

Main Findings

The main findings are as follows:

- The ACE model (Airborne Concentration Estimate) has been identified as a suitable source term model to replace the IRATE model.
- For the releases of chlorine, sulphur dioxide and ammonia considered in this study, the SLOT DTL isopleths produced using ACE and DRIFT 3 are shorter than the isopleths generated using IRATE and DENZ. Close agreement between the predicted isopleths should not necessarily be expected because there are significant differences between the modelling assumptions used in the two methodologies. DRIFT 3 contains a more sophisticated passive dispersion model than DENZ, and the smooth transition from dense to passive behaviour in DRIFT 3 is an improvement on the abrupt transition in DENZ.
- For many of the chlorine, sulphur dioxide and ammonia releases presented here, the initial airborne component (modelled in ACE and DRIFT 3) and the pool component (modelled in ACE, the pool spreading and vaporisation model GASP and DRIFT 3) produce isopleths that are similar in length. However, for most scenarios, the isopleths for the airborne component are significantly wider than the isopleths generated for the pool component. For ammonia, no significant SLOT DTL isopleths were produced for indoor recipients when using DRIFT 3.
- ACE, GASP and DRIFT 3 are appropriate tools for modelling flashing heated instantaneous releases of toxic substances.
- For all the presented heated scenarios, the airborne component (modelled in ACE and DRIFT 3) produces longer and wider SLOT DTL isopleths than the pool component (modelled in ACE, GASP and DRIFT 3).

Outcomes

As a result of this work, ACE and DRIFT 3.6.14 have been adopted by HSE to model instantaneous releases of toxic pressure-liquefied gases. ACE and DRIFT 3.6.14 have therefore replaced IRATE, DENZ and DRIFT 2.31 for use in Hazardous Substances Consent assessments relating to such substances.

For flashing instantaneous releases, both the initial airborne component of the release (consisting of vapour and entrained liquid droplets) and the component that rains out to form a pool may contribute to the overall risk posed by the release. For the purposes of Hazardous Substances Consent assessment, the contribution from the pool component is modelled in ACE, GASP and DRIFT 3.6.14.

DRIFT 3.6.14 does not have the capability to combine the airborne puff component and the pool component of a release into a single run to produce a combined set of SLOT DTL isopleths. Therefore, for the purposes of Hazardous Substances Consent assessment, the preferred approach is to use the larger of

the two sets of SLOT DTL isopleths in the subsequent risk calculations. For ammonia scenarios which produce short, wide isopleths for the puff component and long, narrow isopleths for the pool component, an alternative option is to combine the maximum isopleth dimensions of the two release components i.e. to use the maximum isopleth width from the puff component and the maximum downwind extent from the pool component in the risk calculations.

ACE, GASP and DRIFT 3.6.14 have also been adopted by HSE for modelling superheated liquid releases of toxic substances.

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1 INTRODUCTION

The gas dispersion model DRIFT (Dispersion of Releases Involving Flammables or Toxics) was originally developed in the late 1980s, to model ground-based clouds released instantaneously or as a steady continuous source [1, 2]. DRIFT was developed for the Health and Safety Executive (HSE) by ESR Technology. ESR Technology has recently released a new version of the model, DRIFT 3.

HSE will use DRIFT 3 in its assessment of the hazards and risks posed by toxic and flammable substances stored at major hazards sites. Under the Planning (Hazardous Substances) Regulations [3] the presence of hazardous chemicals above specified threshold quantities requires consent from a Hazardous Substances Authority (HSA), which is usually the local Planning Authority. HSE is a statutory consultee on all Hazardous Substances Consent applications. Its role is to consider the hazards and residual risk which would be presented by the hazardous substance(s) to people in the vicinity, and on the basis of this to advise the HSA whether or not consent should be granted [4]. The outputs of these assessments are also used to set Land Use Planning (LUP) zones around major hazards sites [5].

DRIFT 3 includes a significant number of modelling enhancements over the version of DRIFT previously used by HSE (DRIFT 2.31) [6, 7]. These include extensions to the model to allow it to be applied to buoyant plumes and time varying releases. An overview of these enhancements is given in Section 1.1 of this report.

To ensure that DRIFT 3 is fit for purpose, a programme of work is being undertaken at HSE. This includes an evaluation of the dispersion modelling capabilities of DRIFT 3 and an assessment of the performance of DRIFT 3 for modelling the types of release scenario typically considered by HSE for Hazardous Substances Consent assessments. The scenarios being examined include releases of toxic or flammable pressure-liquefied gases and dispersion of vapour from pools of toxic or flammable liquids.

This report describes part of this programme of work and presents an assessment of the use of DRIFT 3.6.14 for modelling the dispersion of instantaneous releases of toxic pressure-liquefied gases such as chlorine, sulphur dioxide and ammonia. Instantaneous releases of these substances were previously modelled by HSE using the DENZ dispersion model, a precursor to DRIFT that was originally developed in the late 1970s [8]. This report also considers flashing instantaneous releases of substances that are heated above their normal boiling point temperature in process vessels or reactors.

The main objective of this work was to determine an appropriate methodology for modelling flashing instantaneous releases of toxic substances using DRIFT 3. Sensitivity tests were carried out to ensure that DRIFT 3 works reliably for the types of inputs typically used by HSE for Hazardous Substances Consent assessment purposes.

A further aim of this work was to determine the effect of adopting DRIFT 3 on land-use-planning decisions. This was achieved by using DRIFT 3 to model a selection of release scenarios and comparing the resulting hazard ranges to those obtained using the DENZ dispersion model.

In addition, this report describes an improved methodology for generating source terms for flashing instantaneous releases, for input to DRIFT 3. This methodology uses a new instantaneous source term model, ACE (Airborne Concentration Estimate). ACE is based on better and more up to date science than IRATE, the in-house model that was previously used by HSE to generate source terms for flashing instantaneous releases.

In this report, the new revised version of DRIFT is referred to as DRIFT 3. When the output from a specific version of DRIFT 3 is presented, the exact version number is given.

1.1 MODEL ENHANCEMENTS IN DRIFT 3

A number of additions and modelling enhancements have been implemented in DRIFT 3, expanding the scope and potential uses of the model. A comprehensive account of these changes is given by Tickle and Carlisle [6, 7]. The model enhancements include:

- The inclusion of finite duration and time varying releases in addition to the instantaneous and steady continuous releases available in DRIFT 2;
- The option to calculate initial dilution over the source and upwind spreading;
- The 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 (necessitated by the extension of the model to include buoyant plumes);
- Inclusion of a lateral meander model, which accounts for the dilution caused by fluctuations in wind direction, and a vertical meander model, which accounts for the effects of updraughts and downdraughts in unstable atmospheric conditions;
- Incorporation of a momentum jet model. The jet model is based on the stand-alone model EJECT [9], which was used in conjunction with DRIFT 2.31;
- The generalisation of the model to include multi-component mixtures;
- The facility to read in data from SPI (Substance Property Information) files [10]. HSE's substance property database is in the form of SPI files. SPI files are text files containing spot values of physical properties at specified temperatures and equation coefficients which allow the calculation of various substance physical properties at a range of temperatures. SPI files are used by the majority of HSE's in-house models;
- The facility to run DRIFT 3 either via the GUI (Graphical User Interface) or via a COM (Component Object Model) interface [11]; and
- An improved and updated user interface. Plume footprints are plotted automatically within DRIFT 3. When DRIFT 2.31 is used, a separate spreadsheet tool is required to plot the plume footprints.

The initial phases of HSE's testing programme were carried out using DRIFT 3.6.4. Since the completion of that work, DRIFT 3 has been further updated, and the most recent version of DRIFT currently available to HSE is DRIFT 3.6.14. Model enhancements implemented between DRIFT 3.6.4 and DRIFT 3.6.14 include:

- Removal of the empirical time delay for gravity spreading for non-stationary initial clouds [6]. The new non-stationary cloud option is generally considered appropriate for clouds expected to be initially moving (e.g. due to momentum associated with any ambient air entrained prior to the DRIFT 3 run);
- Inclusion of a 'stationary initial cloud' option on the release tab. This option allows for comparison with the Thorney Island trials (see for example [12]) or other instantaneous release experiments which start from rest (zero centroid velocity and zero initial radial speed). The empirical time delay discussed in the previous point is maintained for these clouds as it accounts for the initial radial acceleration of the cloud from rest [13]; and

- Modifications to allow initialisation in the case of an instantaneous cloud that is initially deeper than the mixing layer height. The mixing layer height defines the depth of the turbulent atmospheric boundary layer within which dispersion typically occurs: above this height, mixing is suppressed by the presence of a temperature inversion [14]. The new initialisation process keeps the cloud within the mixing layer and grows the lateral dimensions.

Other changes relevant to DRIFT 3, which do not affect the outputs obtained when modelling flashing instantaneous releases, include:

- The addition of an 'ACE SOURCE' key word to the DRIFT vocabulary, for the purposes of handling legacy DRIFT input files (text files with extension .DIN). This is for potential future enhancements to DRIFT that depend on knowing whether the conditions correspond to a source term generated by ACE or by another source term model. The user can set ACE SOURCE = yes in the DRIFT input (.DIN) file to indicate where this is required;
- Improvements to the mathematical implementation of the time varying model, including modifications to the way in which lateral meander time averaging is applied; and
- Removal of the requirement for a user running DRIFT 3 in a Windows 7 environment to have administrator privileges, whilst maintaining compatibility with Windows XP.

In addition, improvements to how GASP (Gas Accumulation over Spreading Pools) generates DRIFT input (.DIN) files for use within DRIFT 3 have been made. GASP [15] is a source term model that calculates the evaporation rate from pools and how the pool diameter varies with time.

1.2 OVERVIEW OF DRIFT 3 VALIDATION AND VERIFICATION

The initial validation and verification of DRIFT 3 was carried out by the developers of the model at ESR Technology. Comparisons of the DRIFT 3 and DRIFT 2 outputs with experimental data are presented by Tickle [16]. The primary aim of the Tickle paper was to confirm that the two versions broadly agree rather than to carry out a comprehensive validation study of DRIFT. Areas where DRIFT 3 produces significantly different predictions from DRIFT 2 are highlighted.

Tickle et al. [17] present comparisons of DRIFT 3 model predictions with experimental measurements of hydrogen fluoride (HF) releases obtained during the EU (European Union) URAHFREP (Understanding dispersion of industrial Releases of Anhydrous Hydrogen Fluoride and the associated Risk to the Environment and People) research project. The URAHFREP project studied HF thermodynamics and lift-off of initially ground-based buoyant clouds. The focus of these comparisons was the validation and verification of the buoyant lift-off and rise related enhancements to the DRIFT model. The comparisons indicate that DRIFT 3 generally gives a good representation of the effect of buoyancy on maximum concentration, and the buoyancy at which lift-off occurs, although the ground-level concentration may be over-predicted when the cloud has significantly lifted from the ground.

The programme of work being undertaken at HSE has been designed to complement the ESR Technology studies. This programme of work considers both the validation of DRIFT 3 against experimental data and the effect of changes to the model on its predictions for the types of release scenario typically modelled by HSE for Hazardous Substances Consent assessments. To date, the following topics have been covered:

- Evaluation of the dispersion modelling capabilities of DRIFT 3

Coldrick and Webber [18] describe the evaluation of DRIFT 3.6.4 against a Model Evaluation Protocol (MEP) for dense gas dispersion models. The protocol was developed by Ivings et al. [19] for the US National Fire Protection Association (NFPA) and comprises scientific evaluation, model verification and model validation using a database of wind tunnel and field scale experimental data. The results of

these stages are recorded in a comprehensive model evaluation report which includes qualitative and quantitative criteria for model acceptance. Coldrick and Webber include additional validation of DRIFT 3.6.4 against a series of passive dispersion experiments. Following the release of DRIFT 3.6.14, Cruse and Coldrick [20] carried out a further validation and comparison exercise in which results from DRIFT 3.6.14 were compared with those obtained in the evaluation of DRIFT 3.6.4. Cruse and Coldrick also present an assessment of the performance of DRIFT 3.6.14 for modelling the dispersion of vapour from pools of toxic liquids. As a result of this evaluation and assessment, DRIFT 3.6.14 was adopted by HSE to model the dispersion of vapour evolved from pools of toxic liquids [20].

- Assessment of the use of DRIFT for modelling the dispersion of vapour from pools of toxic liquids

Cruse et al. [21] present an assessment of the use of DRIFT 3.6.4 for modelling the dispersion of vapour from pools of toxic liquids. The dispersion of such releases was previously modelled by HSE using DRIFT 2.31. Methyl iodide and ethylene oxide test scenarios were used to assess the effect on the model predictions of the enhancements implemented between DRIFT 2.3.1 and DRIFT 3.6.4. The report also provides guidance on how DRIFT 3 should be used to model the dispersion of vapour from pools of toxic liquids.

Cruse et al. modelled releases from evaporating pools of toxic liquids in D5 and F2 weather conditions for consistency with the methodology previously used by HSE to model such releases. (The letters D and F represent Pasquill stability classes: D denotes neutral conditions and F denotes stable conditions. The associated number gives the wind speed in metres per second at a reference height of 10 m.) HSE has since made a policy decision to use four weather categories when modelling releases from evaporating pools of toxic liquids for Hazardous Substances Consent assessments. These weather categories are D2.4, D4.3, D6.7 and F2.4, and have been chosen to be consistent with the weather categories used when modelling releases of toxic pressure-liquefied gases [20].

- Assessment of the use of DRIFT for modelling releases of toxic pressure-liquefied gases

Lamb and Cruse [22] describe the assessment of the use of DRIFT 3.6.14 for modelling the dispersion of continuous releases of toxic pressure-liquefied gases. The dispersion of such releases was previously modelled by HSE using CRUNCH [23]. The outputs of DRIFT 3.6.14 and CRUNCH were compared for a selection of chlorine, sulphur dioxide and ammonia release scenarios.

This report presents an assessment of the use of DRIFT 3.6.14 for modelling the dispersion of flashing instantaneous releases of toxic substances. The dispersion of such releases was previously modelled by HSE using DENZ [8]. The outputs of DRIFT 3.6.14 and DENZ are compared for a selection of chlorine, sulphur dioxide and ammonia release scenarios. Releases of substances heated above their normal boiling point in process vessels are also considered. Both Lamb and Cruse [22] and this report provide guidance on how DRIFT 3 should be used to model releases of toxic pressure-liquefied gases.

- Assessment of the use of DRIFT for modelling flammable releases

Chaplin and Cruse [24] present an assessment of the use of DRIFT 3.6.14 for modelling the dispersion of flammable vapour, considering both releases of flammable pressure-liquefied gases and the dispersion of vapour from pools of flammable liquids. The dispersion of vapour from pools of flammable liquids was previously modelled by HSE in DRIFT 2.31. Liquefied hydrogen and liquefied natural gas (LNG) test cases were used to assess the effect on the model predictions of changing from DRIFT 2.31 to DRIFT 3.6.14. Continuous flashing releases of flammable substances were previously modelled by HSE using either DRIFT 2.31 (holes in vessels or pipework) or CRUNCH [23] (holes in pipelines). The CRUNCH and DRIFT 3.6.14 predictions were compared for releases from ethylene and liquefied petroleum gas (LPG) pipelines. Instantaneous flashing releases of flammable substances were previously modelled by HSE in DRIFT 2.31. The effect on the model predictions of changing from DRIFT 2.31 to DRIFT 3.6.14 was assessed for a selection of isobutane and propane release scenarios.

The report also provides guidance on how DRIFT 3 should be used to model the dispersion of flammable vapour.

1.3 DISPERSION MODELLING USING DRIFT 3

DRIFT 3 has a series of input tabs, onto which information about the conditions of the release, the source geometry and the atmospheric conditions should be entered. These inputs can either be imported from a source term model or directly input by the user.

The user can also input harm criteria of interest, which are used to determine the hazard ranges for the release. For flammable substances the harm criterion is expressed as a fraction of the lower flammable limit (LFL), whereas for toxic substances a concentration or dose of interest should be entered. Within HSE, the dose of interest is generally chosen to be the SLOT DTL (Specified Level of Toxicity, Dangerous Toxic Load) of the substance. The SLOT DTL is assumed to be equivalent to the LD1 (Lethal Dose 1), the dose that causes approximately 1% mortality in a normal population [25]. The SLOT DTL is also referred to as the HSE Dangerous Dose for toxic substances, which is defined as the dose which is sufficient to cause:

- Severe distress to almost everyone exposed to it;
- 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.

A large range of outputs is available in DRIFT 3, in both tabular and graphical format. The main outputs of interest to HSE are:

- The variation with downwind distance of the width of the isopleth enclosing the area within which the target level of interest is exceeded; and
- The maximum downwind dispersion distance to the target level of interest.

A Hazardous Substances Consent assessment relating to toxic substances requires the calculation of SLOT DTL isopleths for an appropriate range of release scenarios and weather conditions. The downwind extent and widths of the isopleths at a series of distances up to the maximum downwind extent are used as inputs to a risk calculation model, together with local weather data and failure frequencies. Using this model, the risk that a hypothetical individual at a given location will receive the HSE Dangerous Dose can be calculated, and this is then used to inform HSE's Hazardous Substances Consent advice to Hazardous Substances Authorities.

Further guidance on the model input parameters and on how to run the model and extract results is provided in the DRIFT User Guide [26].

1.4 MODELLING METHODOLOGY FOR FLASHING INSTANTANEOUS RELEASES

HSE has previously modelled the dispersion of instantaneous releases of pressure-liquefied gases using the model DENZ [8]. DENZ is an integral dense gas dispersion model used for modelling instantaneous releases and, along with its continuous release counterpart CRUNCH, forms the hazard modelling part of the calculations in RISKAT version 3.1.1 (RISK Assessment Tool) [27], HSE's risk assessment suite of programs. Prior to this work, DENZ and CRUNCH were recommended for use in HSE for modelling releases of ammonia, chlorine, bromine, phosgene and sulphur dioxide, but in some instances, the use of DRIFT 2.31 [1, 2] was necessary. DRIFT 2.31 was also used for substances not available in RISKAT. During the IFRLUP (Implementation of the Fundamental Review of Land Use Planning) [28] process, DENZ and CRUNCH were identified as in need of improvement or replacement. DRIFT version 2 was marked as a potential replacement for DENZ and CRUNCH in the IFRLUP report.

HSE has previously used the in-house model IRATE to generate a source term for flashing instantaneous releases, for input to either DENZ or DRIFT 2.31. A review by Tickle [29] highlights areas for improvement within IRATE. One example is that IRATE assumes that the entire inventory becomes airborne and neglects the potential for rainout and pool formation, which are likely to occur in reality. Despite this, the IRATE outputs compare well with those from ACE [30], another source term model applicable for instantaneous releases, but one that has a better established scientific basis.

ACE [30] is a source term model that can model the initial stages of a flashing instantaneous release from a catastrophic failure of a vessel storing a pressure-liquefied gas. ACE predicts both the properties of the airborne cloud that is generated and the amount of released material that will form a pool. ACE was originally written for HSE by WS Atkins in 1999.

Initial ACE validation studies were carried out by Shepherd and Deaves [31], but a lack of experimental data prevented a more detailed study. Coldrick [32] expanded the validation studies and found that the ACE predictions are in reasonable agreement with the data available from large-scale tests.

Tickle [33] presents a detailed examination of the science behind the ACE tool and reports no significant problems that would affect its use by HSE. Tickle [33] also examines the practicalities of using the ACE output as a source term for DRIFT 3 and gives a set of recommended inputs; these can be found in Section 2 of this report.

HSE has developed a new version of ACE based on the science described in [30] and taking into consideration recommendations made by Coldrick [32] and Tickle [33]. The reauthoring of the code has enabled HSE to implement further changes to ACE to allow it to be more easily integrated into HSE's hazard and risk assessment processes. It has also allowed modifications to be made to the code to ensure the calculations within ACE are consistent with similar calculations in other models used by HSE.

1.4.1 Generating a source term for a flashing instantaneous release

Figure 1 illustrates the consequences of an instantaneous release of a flashing (superheated) material. Superheat is the term used to describe when a liquid is stored at a temperature in excess of its normal boiling point, for example, by pressure liquefaction. If there is insufficient material superheat, not all of the inventory will become airborne as a vapour and/or aerosol and a portion will rain out to form a pool. The proportions that go into the air and into the pool depend on parameters such as the storage conditions and the flash fraction (which is dependent on the degree of superheat).

The IRATE source term model does not account for pool formation and does not produce any output if the superheat is less than 15 K (as significant rainout would be expected under these conditions). If the superheat is greater than 15 K, IRATE assumes that 100% of the inventory becomes airborne (as a vapour and/or aerosol), and rainout is neglected. However, significant rainout can occur even if the superheat is greater than 15 K [31]. In recent years, models that are more sophisticated have been developed that attempt to predict rainout, pool formation and evaporation, and it is prudent to bring HSE's methodology up to date. A model that has the ability to predict rainout, pool formation and subsequent evaporation of the pool into the airborne plume may represent reality more closely than the approach used in IRATE. The use of the IRATE model for a release where the superheat is greater than 15 K would mean that the entire inventory goes into the red plume marked 'AIRBORNE' in Figure 1. DRIFT 3 would model the subsequent dispersion and the 'POOL' and 'POOL EVAPORATION' processes would be neglected.

The ACE source term model [30, 31] can account for rainout and subsequent pool formation. It calculates the fraction of the stored liquid inventory that becomes airborne and assumes that the remainder (1 – airborne fraction) forms a pool. ACE calculates the radius of the pool and the mass of material that is contained within it. Referring to Figure 1, this means that ACE calculates how much of the inventory goes into the red puff marked 'AIRBORNE' and how much goes into the green shaded pool marked 'POOL'. ACE can also account for evaporation from the pool that is formed. However, the pool evaporation process in

ACE is a simple model that assumes that either no evaporation occurs and the pool (plus any rained out material) is neglected from further calculations, or that the entire contents of the pool evaporate back into the cloud. Therefore, in this study, the pool evaporation model in ACE has not been used and more sophisticated pool evaporation modelling has been carried out using the GASP source term model, as described below.

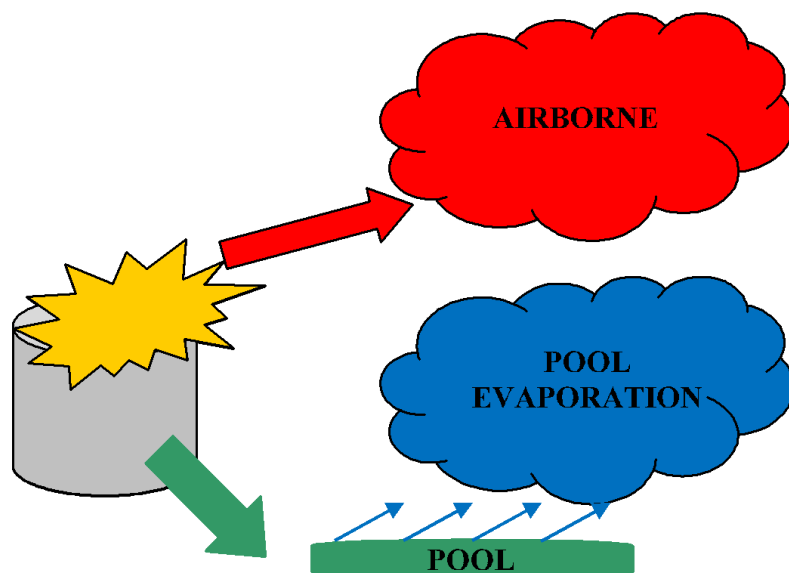


Figure 1 The potential scenarios that could occur from an instantaneous release of flashing material

GASP [15] is a source term model written specifically to calculate pool spreading and pool evaporation and it therefore produces a more realistic pool source term than ACE. Referring to Figure 1, ACE outputs the dimensions and mass of the green shaded pool and these are subsequently used as an input to GASP. GASP calculates the evaporation rate (blue arrows) as well as the total mass evaporated into the blue plume marked 'POOL EVAPORATION' in Figure 1. The dispersion of the 'POOL EVAPORATION' plume can then be modelled using DRIFT. This process neglects the contribution from the initial airborne component.

Figure 1 shows equally sized 'AIRBORNE' and 'POOL EVAPORATION' clouds, and although there is a chance this may occur in reality, for many releases one mechanism will lead to a larger cloud than the other mechanism. Ideally, the contributions from the airborne puff and the pool should be recombined and modelled together in DRIFT 3 but this is not currently possible. In most cases, the preferred approach is to model the puff and pool components separately and use the larger of the two sets of SLOT DTL isopleths for Hazardous Substances Consent assessment purposes. This is one of the key changes to the methodology for modelling flashing instantaneous releases.

The flowchart in Appendix 1 shows how ACE and GASP should be used to generate a source term for use in DRIFT 3.

1.5 STRUCTURE OF REPORT

This report presents a comparison of DRIFT 3.6.14 with the model DENZ, which was previously used by HSE for modelling instantaneous releases of pressure-liquefied gases. The remainder of the report is structured as follows:

- Section 2 gives an overview of the recommended inputs for the ACE source term model. The recommended input values for use in DRIFT 3 when modelling flashing instantaneous releases are also presented.
- In Section 3, chlorine, sulphur dioxide and ammonia release scenarios have been modelled using DENZ and DRIFT 3.6.14. The hazard ranges obtained using the two methodologies have been compared, to assess the impact of adopting DRIFT 3 on HSE's land-use planning advice. Possible reasons for the differences between the predicted hazard ranges, such as differences in the mathematical models and modelling assumptions, are discussed.
- In Section 4, a discussion of the results is presented and a comparison is made between the old and new methodologies.
- Section 5 describes the modelling of heated releases of methyl chloroformate, propionitrile and 2-chloroethanol in DRIFT 3.6.14, to test the performance of the model when considering releases of superheated liquids.
- The conclusions from this work are presented in Section 6.

2 RECOMMENDED INPUTS FOR ACE AND DRIFT 3

This section presents the recommended ACE version 3.15 inputs for use in DRIFT 3, as described by Tickle [33]. Some of the input values that were agreed during the earlier phase of work that investigated the dispersion of vapour from pools of toxic substances [21] are also applicable for flashing instantaneous releases; these are summarised in Section 2.2.

2.1 RECOMMENDED ACE INPUTS

ACE requires the following site-specific values:

- Substance;
- Mass;
- Storage temperature; and
- Storage pressure.

Where possible, these inputs will be populated based on information in the Hazardous Substances Consent Application submitted to HSE. In cases where the storage pressure is the saturated vapour pressure of the substance, this will be calculated automatically by ACE.

Generic HSE assumptions are normally used for the following ACE inputs¹, unless there is site-specific information available:

- Ambient temperature;
- Ambient pressure;
- Wind speed;
- Pasquill stability category; and
- Roughness length.

The Pasquill stability category is not used directly by ACE but is passed through to DRIFT 3. Table 1 gives the recommended values for the remaining ACE inputs that are not covered by the site-specific and generic inputs given above. These values are based on recommendations from Tickle [33] and should always be used.

Table 1 Recommended ACE input values for use with DRIFT 3

ACE parameter	Value
Release direction	Down
Airborne fraction	Upper curve
Droplet option	Aerosol
Pool formation	Yes
Pool evaporation	No

Tickle [33] gives a detailed examination of each of the inputs in Table 1. The key points are summarised below:

- Release direction: *omni* or *down*. The release direction affects the shape of the initial expansion. An *omni* release is assumed to be spherical in shape whereas a *down* release is assumed to be

¹The wind speed and roughness length are used to calculate the cloud velocity in ACE, but this does not affect any of the outputs that are written to the DRIFT input file. The wind speed, Pasquill stability, and roughness length input to ACE are written directly to the DRIFT input file.

hemispherical. Tickle recommends that the release direction should be set to *down* because the instantaneous puff is likely to interact with the ground at some stage and become hemispherical in shape. The *omni* release is only realistic for smaller masses released at height where a spherical-shaped puff is possible.

- Airborne fraction: *upper curve* or *lower curve*. The airborne fraction is used as the basis for determining the initial aerosol content of the cloud. In ACE, the airborne fraction is determined from a plot of experimental measurements of the airborne fraction (as aerosol) as a function of the flash fraction. Two curves have been fitted to the data: an *upper curve* representing the upper part of the data (the measurements with the highest airborne fractions for a particular flash fraction) and a *lower curve* representing the lower part of the data (the measurements with the lowest airborne fractions for a particular flash fraction). For simple modelling Tickle [33] considers these correlations to be reasonable approximations. In ACE version 2.0, the *omni* release direction was coupled with the *upper curve* and the *down* release was coupled with the *lower curve*. The release directions are no longer coupled to the airborne fraction curves within ACE version 3.15. For both release directions, ACE version 3.15 defaults to the *upper curve*, which reflects observations that superheated releases with flash fractions of 0.3 or higher generally result in negligible pool formation [33]. The *upper curve* also better represents the commonly used assumption of the airborne fraction being three times the flash fraction [33].
- Droplet option: *rainout*, *aerosol* or *vaporisation*. In reality, airborne droplets are likely to be present (at least initially) from flashing releases. ACE's liquid droplet model is used to determine how the evaporation of airborne droplets contributes to the enthalpy balance of the cloud. It is not used to calculate the initial liquid rainout fraction; this is based on the calculated airborne fraction. The liquid material that becomes airborne can either *rainout* to form a pool, remain as an *aerosol*, or there can be complete *vaporisation* of the droplets within the cloud; these are the three droplet options available in ACE. Pools that form immediately on release are considered separately. An ACE run terminates when the cloud transitions to gravity-slumping behaviour and at this point the *rainout* option adds any remaining droplets in the cloud to the pool. In reality, fine droplets may remain airborne and forcing rainout is not a scientifically robust assumption. The *vaporisation* option adds extra air into the cloud to ensure complete evaporation of any remaining droplets before the ACE run terminates. The *aerosol* option allows any liquid remaining in the cloud at the end of the ACE run to remain airborne as a liquid aerosol. This option allows more flexibility and because DRIFT 3 is capable of modelling aerosol components, the *aerosol* option is the most appropriate ACE selection.
- Pool formation: *yes* or *no*. The pool formation option accounts for pool formation immediately on release and does not account for pool formation due to rainout of liquid droplets; droplet rainout is accounted for using the Droplet option in ACE. The pool formation option should be selected. Materials such as chlorine are usually stored above their normal boiling point temperature and under their own vapour pressure resulting in a liquefied state. When a material is stored above its boiling point temperature it is considered to be superheated, with low superheats occurring when the difference between the storage temperature and the normal boiling point temperature is small. Pool formation is considered to be more likely for instances of low superheats because the resulting flash fraction is low and there is more liquid initially available to enter the pool. Previously, pool formation was rarely considered by HSE when modelling flashing instantaneous releases, due to the limitations of the IRATE source term model.
- Pool evaporation: *yes* or *no*. ACE has the option to include or exclude pool evaporation. However, ACE does not include a pool evaporation model; it assumes that either all the material in the pool evaporates or none of it evaporates. Neither of these modelling assumptions can be completely justified and the best option is considered to be the use of a designated pool spreading and pool

evaporation model, such as GASP, to perform these calculations where required. The pool evaporation option should not be selected in ACE.

2.2 DRIFT 3 INPUTS FROM EARLIER WORK ON TOXIC POOLS

Table 2 summarises the recommended values for the DRIFT 3 inputs that are applicable to flashing instantaneous releases. The table has been split into those inputs applicable to the initial airborne puff (ACE generated source terms) and those applicable to the pool component (GASP generated source terms). Guidance on using the ACE output to specify appropriate inputs for modelling the pool component in GASP is provided in Appendix 2. In DRIFT 3, the wind direction (the wind angle from North parameter in Table 2) is defined as the direction from which the wind is blowing. This is the convention used by the Met Office.

Justification for the assumptions used for generic DRIFT 3 inputs, such as those relating to the weather conditions, is provided in Cruse et al. [21]. One notable difference between the recommendations given in Table 1 and those described in Cruse et al. is the choice of weather categories. Cruse et al. [21] recommended that the D5 and F2 weather categories should be used to represent daytime and night-time conditions, respectively, when modelling the dispersion of vapour evolved from pools of toxic substances. This approach was consistent with the methodology previously used by HSE to model such releases. However, it is recommended that four weather categories be used when modelling continuous releases of toxic pressure-liquefied gases. Daytime weather should be represented by the D2.4, D4.3 and D6.7 categories, and night-time weather should be represented by the F2.4 weather category. In this nomenclature, the letter corresponds to the Pasquill category, a measure of atmospheric stability. This ranges from unstable (category A) to stable (category F/G), with neutral stability (category D) occurring in the middle of the range. The number corresponds to the wind speed in metres per second at a reference height of 10 m.

Turner et al. [34] carried out test risk assessment calculations for selected sites across the UK using representative sets of weather categories. The conditional probability of a person being exposed to the HSE dangerous dose or greater (a metric that is proportional to the individual risk) was calculated as a function of distance from source for typical release scenarios. The outputs of the calculations using the representative weather sets were compared to those obtained when the full set of UK Meteorological Office wind speed and Pasquill stability data for each site was used. The D2.4, D4.3, D6.7 and F2.4 weather set provided a better correlation than the D5 and F2 weather set to the risk versus distance profiles obtained using the full set of weather data. Since the publication of Cruse et al. [21], HSE has made a policy decision to use the D2.4, D4.3, D6.7 and F2.4 weather categories when modelling the dispersion of vapour evolved from pools of toxic substances [20]. This policy change has been implemented to ensure that all types of toxic release are modelled using the same weather categories.

Table 2 Recommended input values for use in DRIFT 3 when modelling flashing instantaneous releases

<i>Input</i>	<i>Recommended value for ACE generated source term</i>	<i>Recommended value for GASP generated source term</i>
Release type	Instantaneous	Finite duration
Phase	Superheated liquid/two-phase: Imported from DRIFT input (.DRIFT) file generated by ACE	Gaseous: Imported from DRIFT input (.DIN) file generated by GASP
Substance, temperature, liquid fraction and contaminant fraction	As imported from the DRIFT input file generated by ACE	As imported from the DRIFT input file generated by GASP
Release amount	Contaminant mass: Imported from DRIFT input file generated by ACE	Release rate and duration: Imported from DRIFT input file output by GASP, except for releases that satisfy both the following criteria: 1. The substance has a toxic exponent (<i>n</i>) greater than 1; and 2. The peak vaporisation rate is greater than twice the mean vaporisation rate over the release duration. In such cases, refer to Cruse et al. [21]
Stationary initial cloud	No	N/A
Location	(x,y,z) = (0,0,0) (z = 0 m corresponds to ground level)	(x,y,z) = (0,0,0) (z = 0 m corresponds to ground level)
Source type	N/A	Low momentum area source
Source size	Initial cloud radius: Imported from DRIFT input file generated by ACE	Source diameter: Imported from DRIFT input file generated by GASP
Include dilution over source	N/A	Yes
Weather scheme	Pasquill	Pasquill
Input inversion height	No (the model determines this from a look-up table when the Pasquill weather scheme is selected)	No (the model determines this from a look-up table when the Pasquill weather scheme is selected)
Ambient temperature	288.15 K (D weather conditions); 278.15 K (F weather conditions)	288.15 K (D weather conditions); 278.15 K (F weather conditions)
Relative humidity	60%	60%
Reference height	10 m	10 m
Roughness length	0.1 m (rural); 0.3 m (urban)	0.1 m (rural); 0.3 m (urban)
Wind angle from North	270° (towards the positive x-direction)	270° (towards the positive x-direction)
Pasquill stability and wind speed	D2.4, D4.3, D6.7 and F2.4	D2.4, D4.3, D6.7 and F2.4
Time averaging	N/A	Yes – set equal to release duration
Maximum exposure duration	1800 s	1800 s
Ventilation rate	2 ac/h (air changes per hour) for wind speeds ≤ 5 m/s; 3 ac/h for wind speeds > 5 m/s	2 ac/h (air changes per hour) for wind speeds ≤ 5 m/s; 3 ac/h for wind speeds > 5 m/s
Indoors lag time	600 s	600 s
Levels of interest	SLOT DTL (LD ₁) dose isopleths	SLOT DTL (LD ₁) dose isopleths
Receiver height	Use centreline height (default option)	Use centreline height (default option)

3 COMPARISON OF THE OUTPUTS OF DRIFT 3 AND DENZ

HSE has previously assessed the hazards posed by flashing instantaneous releases using IRATE and DENZ. This section describes a study comparing the SLOT DTL isopleths produced using the previous methodology with those generated using ACE and DRIFT 3, to assess the impact of adopting ACE and DRIFT 3 on HSE's land-use-planning advice.

Four sets of scenarios were modelled and compared:

- i. Review of previous method – IRATE and DENZ;
- ii. Review of previous source term method and new dispersion method – IRATE and DRIFT 3;
- iii. Review of new method – ACE and DRIFT 3; and
- iv. Consideration of rainout – ACE, GASP and DRIFT 3.

The first set of scenarios modelled (i) shows the isopleths produced using the method recommended by HSE prior to the implementation of DRIFT 3. The second set (ii) shows the effects of changing the dispersion model from DENZ to DRIFT 3. The effect of changing the source term model from IRATE to ACE can be examined by comparing set (ii) to set (iii). Comparison of set (i) and set (iii) shows the effect of changing from the previous approach to the new approach. The fourth set of scenarios modelled (iv) considers the pool component of the release. The relative contributions of the airborne component of the release and the pool component of the release can be determined by comparing set (iii) to set (iv).

The DRIFT 3 results presented in Section 3.2 to Section 3.4 are all plotted on different scales. The maximum usable area of the plot is used to allow the results to be viewed more easily.

3.1 SCENARIOS

For this study, chlorine, sulphur dioxide and ammonia were chosen as exemplars (representative substances) because they were available in the previous method (DENZ) and in SPI file form for input to the new method (DRIFT 3).

The release masses were chosen based on typical vessel sizes at small and large scale chlorine facilities. The masses identified are: 1 te, 7.5 te, 10 te, 15 te, 50 te and 100 te.

Table 3 lists the full range of variables that were considered in this study. For conciseness, only a representative set of results is presented within this report.

Table 3 Scenarios used for the assessment of DRIFT 3

<i>Parameter</i>	<i>Value</i>
Release size (te)	1, 7.5, 10, 15, 50 and 100
Substances	Chlorine (Cl ₂), Sulphur dioxide (SO ₂) and Ammonia (NH ₃)
Weather	D2.4, D4.3, D6.7 and F2.4

Section 3.2 presents the chlorine results, Section 3.3 the sulphur dioxide results and Section 3.4 the ammonia results.

3.2 CHLORINE RELEASES

The chlorine results are split into two sections. Section 3.2.1 presents the comparison of ACE/DRIFT 3 with IRATE/DENZ and IRATE/DRIFT 3. This is a comparison of Sets (i), (ii) and (iii) as described at the start of Section 3. Section 3.2.2 presents the comparison of the contribution from the initial airborne

component (modelled in ACE/DRIFT 3) and the contribution from the pool component (modelled in ACE/GASP/DRIFT 3). This is a comparison of Sets (iii) and (iv) as described at the start of Section 3.

A SLOT DTL of 1.08×10^5 ppm².min (i.e. a toxic *n* value of 2) [25] was used in DRIFT 3 for chlorine.

3.2.1 A comparison of results: ACE/DRIFT 3 against IRATE/DENZ and IRATE/DRIFT 3

The source term models ACE and IRATE generate source terms that are based on the airborne component only. Appendix 3 gives some example ACE outputs.

Although ACE accounts for pool formation, in this study, evaporation of the pool into the cloud has not been modelled using ACE. A more sophisticated pool evaporation and spreading model, GASP, has been used for this purpose, and the results obtained using GASP are discussed in Section 3.2.2 for releases of chlorine.

The legends in Figures 2 to 9 describe the scenarios that were modelled and Table 4 summarises what is shown in the figures. SLOT DTL isopleths were produced for all the scenarios modelled.

Table 4 Key for figures showing a comparison of the previous and new methodologies for chlorine releases

<i>Figure #</i>	<i>Substance</i>	<i>Weather</i>	<i>Recipient location</i>
2	Cl ₂	D2.4	Outdoor
3	Cl ₂	D2.4	Indoor
4	Cl ₂	D4.3	Outdoor
5	Cl ₂	D4.3	Indoor
6	Cl ₂	D6.7	Outdoor
7	Cl ₂	D6.7	Indoor
8	Cl ₂	F2.4	Outdoor
9	Cl ₂	F2.4	Indoor

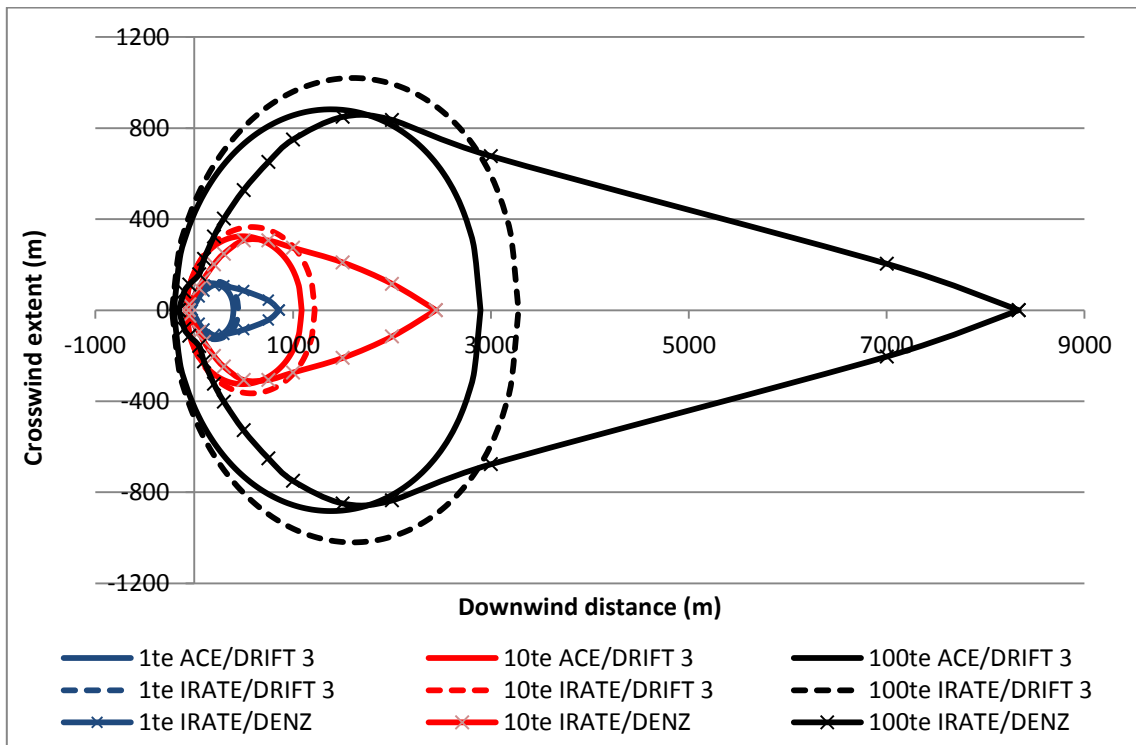


Figure 2 SLOT DTL isopleths obtained for instantaneous chlorine releases in D2.4 weather for an outdoor recipient. The results show dispersion of the airborne puff.

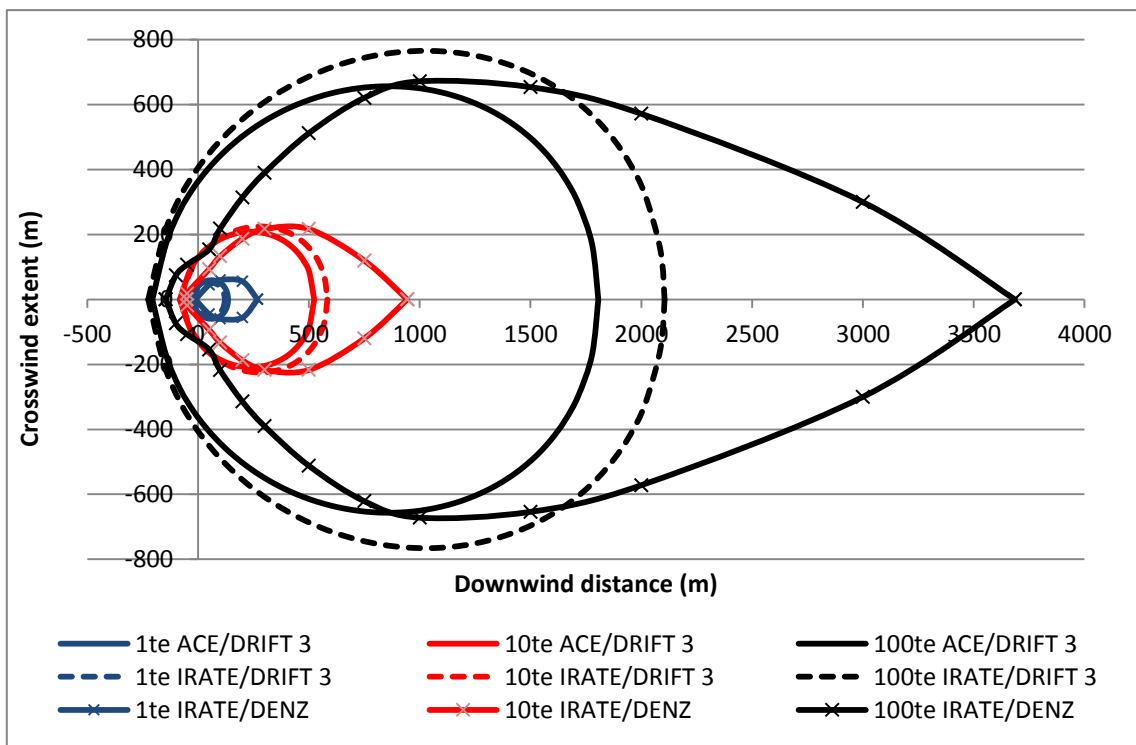


Figure 3 SLOT DTL isopleths obtained for instantaneous chlorine releases in D2.4 weather for an indoor recipient. The results show dispersion of the airborne puff.

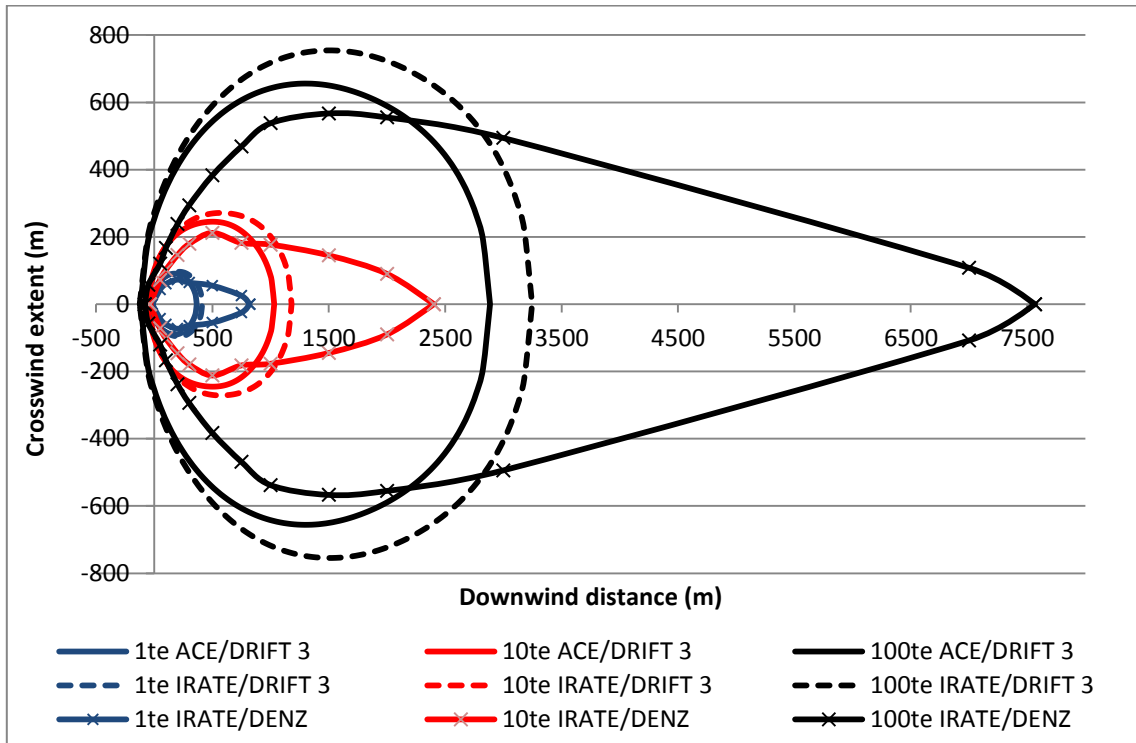


Figure 4 SLOT DTL isopleths obtained for instantaneous chlorine releases in D4.3 weather for an outdoor recipient. The results show dispersion of the airborne puff.

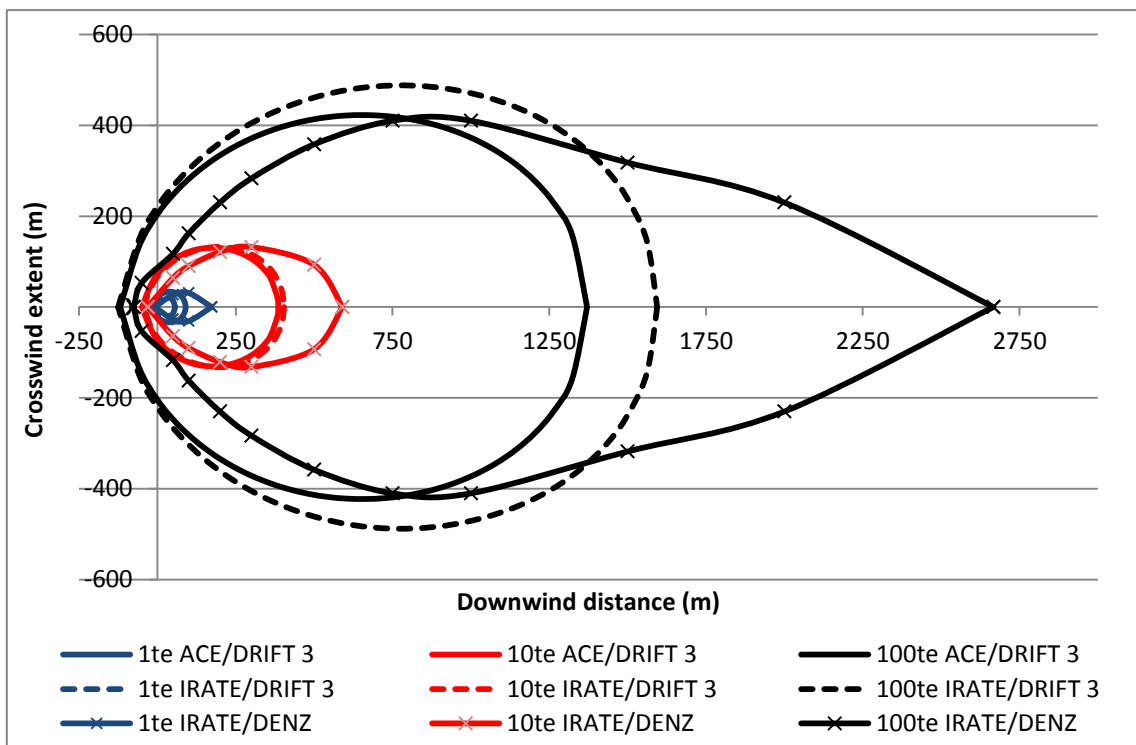


Figure 5 SLOT DTL isopleths obtained for instantaneous chlorine releases in D4.3 weather for an indoor recipient. The results show dispersion of the airborne puff.

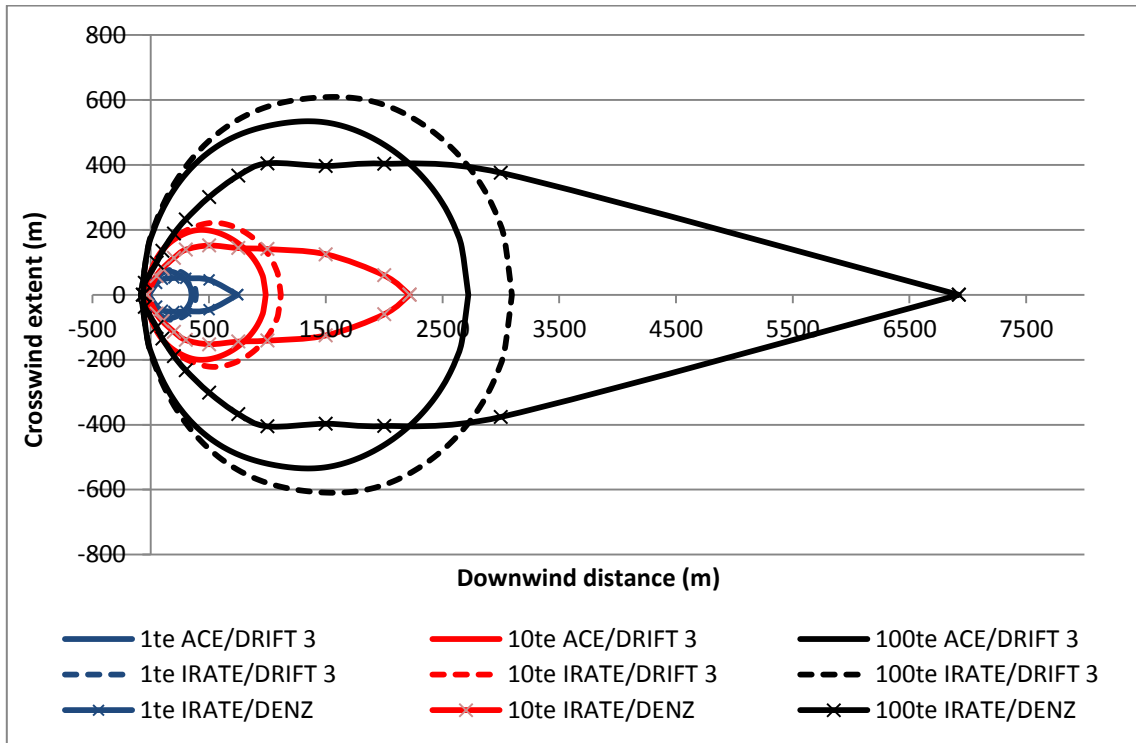


Figure 6 SLOT DTL isopleths obtained for instantaneous chlorine releases in D6.7 weather for an outdoor recipient. The results show dispersion of the airborne puff.

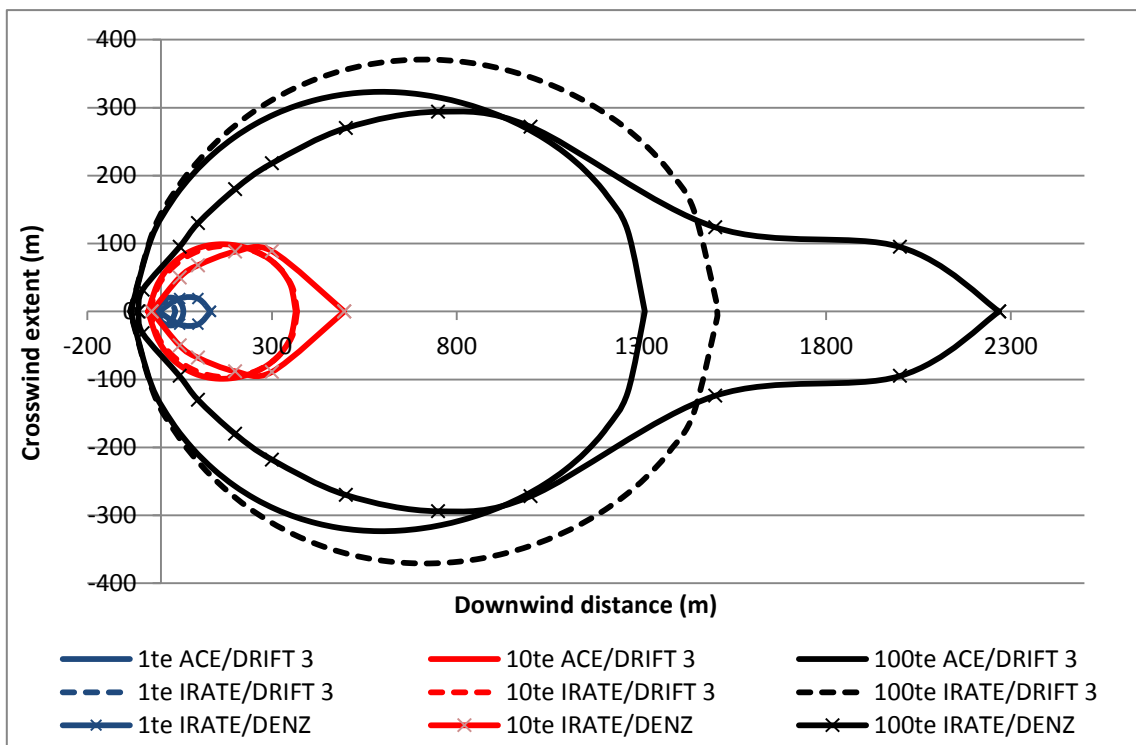


Figure 7 SLOT DTL isopleths obtained for instantaneous chlorine releases in D6.7 weather for an indoor recipient. The results show dispersion of the airborne puff.

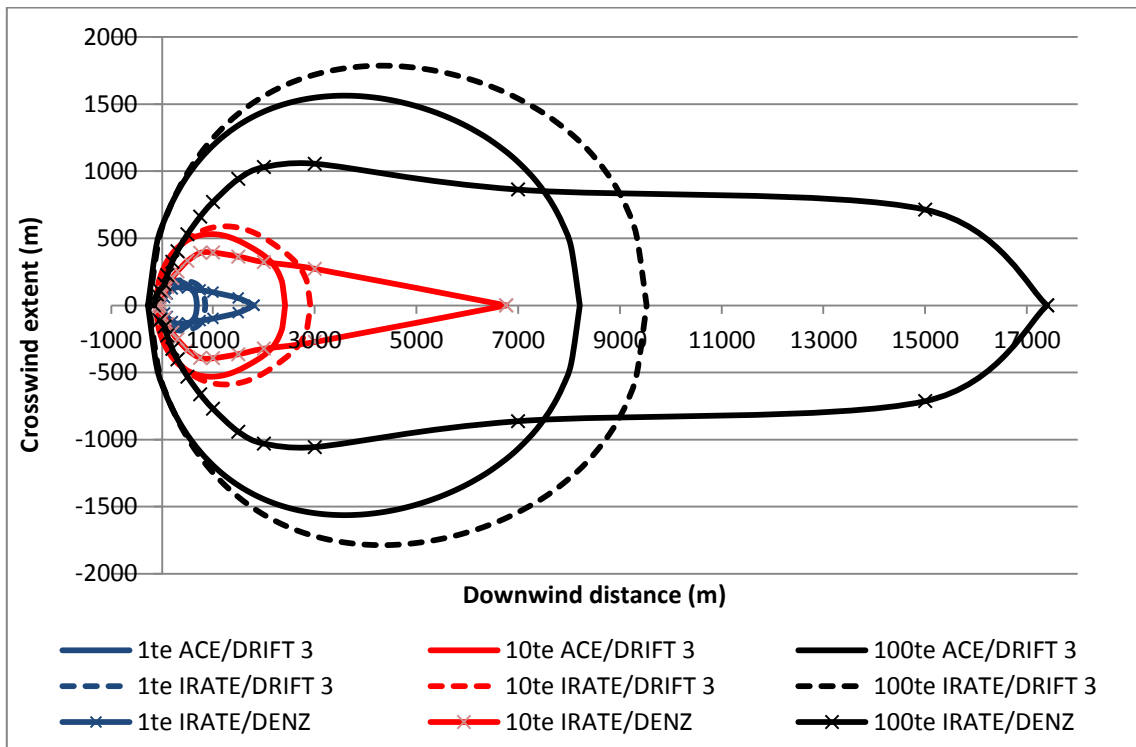


Figure 8 SLOT DTL isopleths obtained for instantaneous chlorine releases in F2.4 weather for an outdoor recipient. The results show dispersion of the airborne puff.

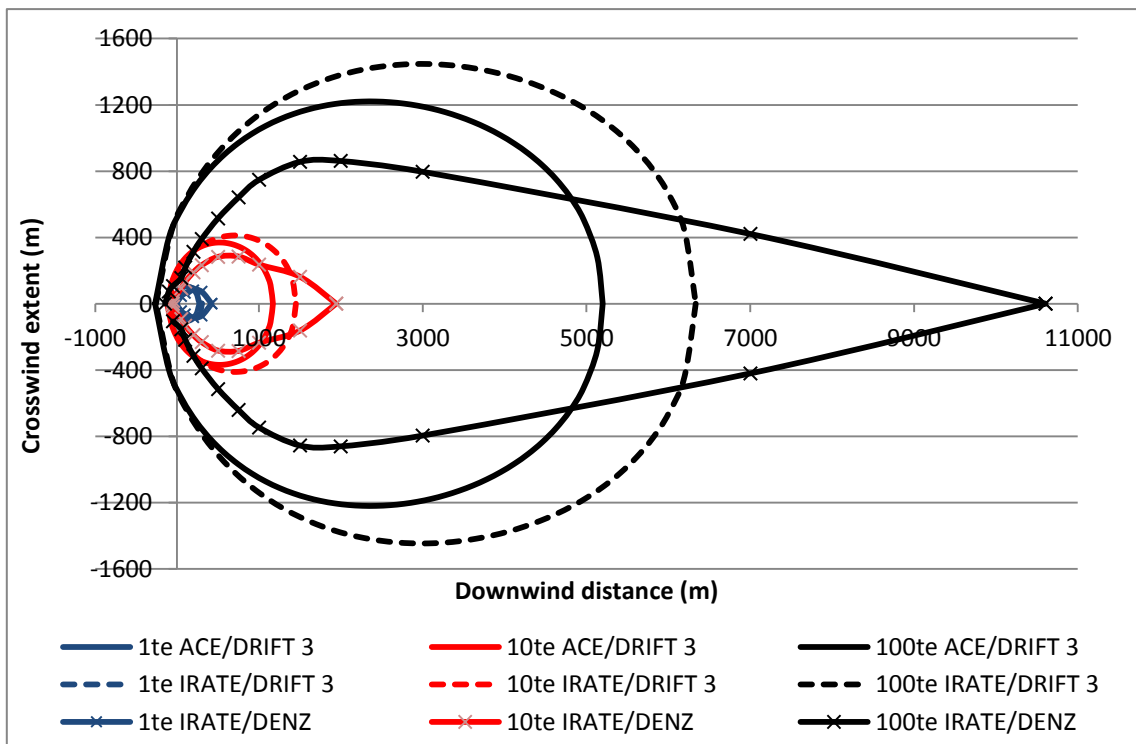


Figure 9 SLOT DTL isopleths obtained for instantaneous chlorine releases in F2.4 weather for an indoor recipient. The results show dispersion of the airborne puff.

Overall, the chlorine results follow similar patterns regardless of the size of the release, the weather conditions and the location of the recipient. The IRATE/DENZ results give the longest downwind extent isopleths, followed by IRATE/DRIFT 3 and then ACE/DRIFT 3 with the shortest. The widest isopleths (measured at the widest point) are produced by IRATE/DRIFT 3. The differences in the maximum widths produced by the three methodologies are more pronounced for the larger releases. In general, the isopleths produced using the DRIFT 3 dispersion model are shorter and wider than those produced using DENZ.

3.2.2 A comparison of results: ACE/DRIFT 3 and ACE/GASP/DRIFT 3

The source terms used for Figures 2 to 9 are based on the airborne component only. To estimate the importance of the contribution from the pool component, GASP was used to calculate the pool evaporation rate for use in DRIFT 3. The pool properties, such as the pool radius and mass of liquid within the pool, were taken from the ACE output files and input to GASP. Further information about the recommended inputs for use in GASP is provided in Appendix 2. Figures 10 to 13 show the comparison between the airborne component (ACE/DRIFT 3) and the pool component (ACE/GASP/DRIFT 3) and indicate which source term is potentially the worst-case. Ideally, the contributions from the airborne puff and the pool should be combined and modelled together in DRIFT, but this is not possible in DRIFT 3.6.14.

Figures 2 to 9 show similar patterns regardless of the weather and the location of the recipient. As there was little variation in the results obtained, a smaller set of GASP scenarios is shown in Figures 10 to 13. The legends in Figures 10 to 13 describe the scenarios that were modelled and Table 5 summarises what is shown in the figures. SLOT DTL isopleths were produced for all the scenarios modelled.

Table 5 Key for DRIFT 3 figures showing a comparison of the airborne and pool components for chlorine releases

<i>Figure #</i>	<i>Substance</i>	<i>Weather</i>	<i>Recipient location</i>
10	Cl ₂	D4.3	Outdoor
11	Cl ₂	D4.3	Indoor
12	Cl ₂	F2.4	Outdoor
13	Cl ₂	F2.4	Indoor

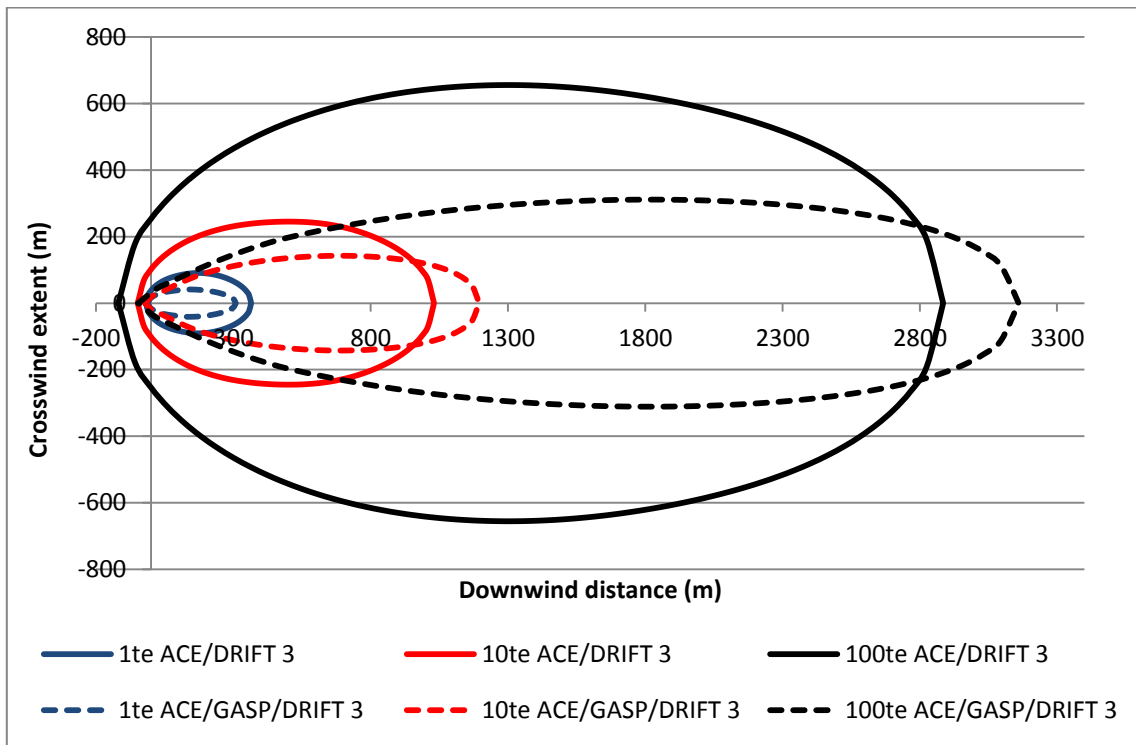


Figure 10 SLOT DTL isopleths obtained for instantaneous chlorine releases in D4.3 weather for an outdoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

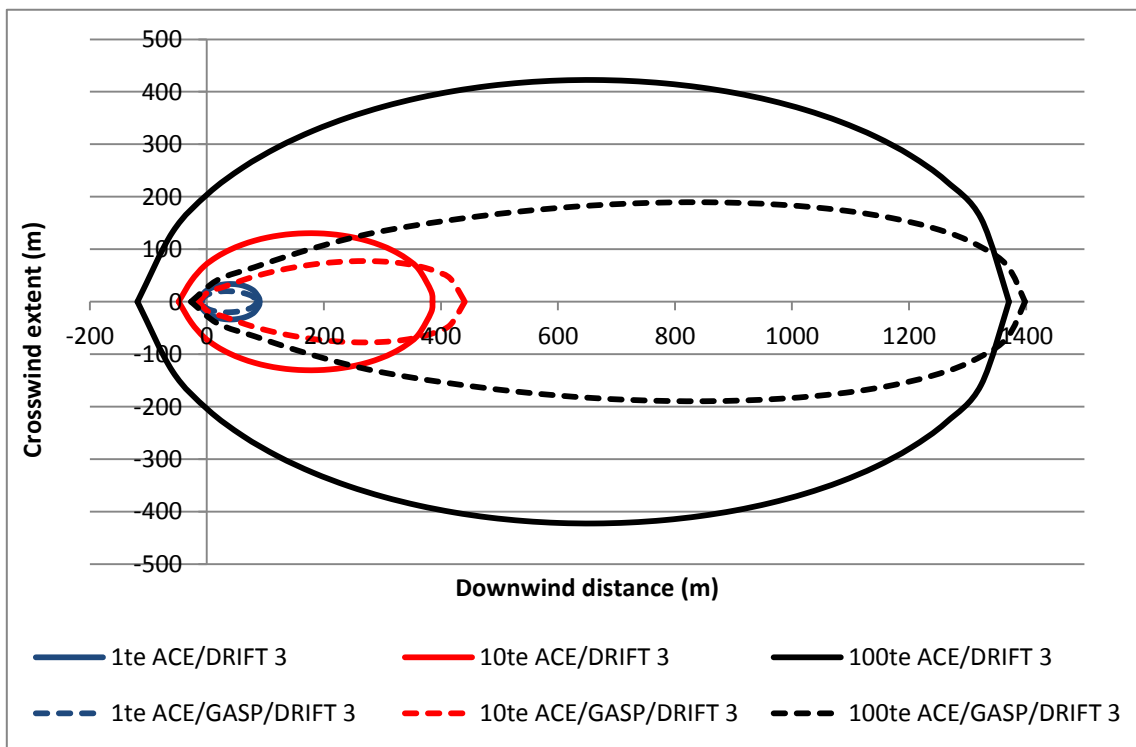


Figure 11 SLOT DTL isopleths obtained for instantaneous chlorine releases in D4.3 weather for an indoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

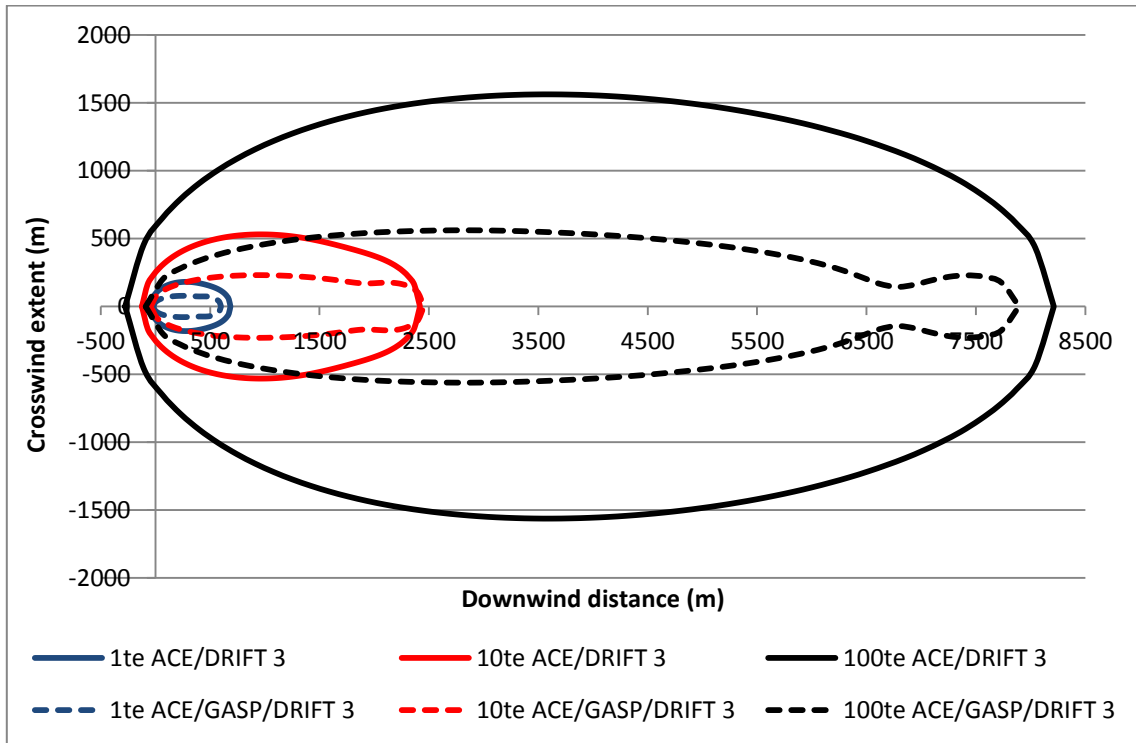


Figure 12 SLOT DTL isopleths obtained for instantaneous chlorine releases in F2.4 weather for an outdoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

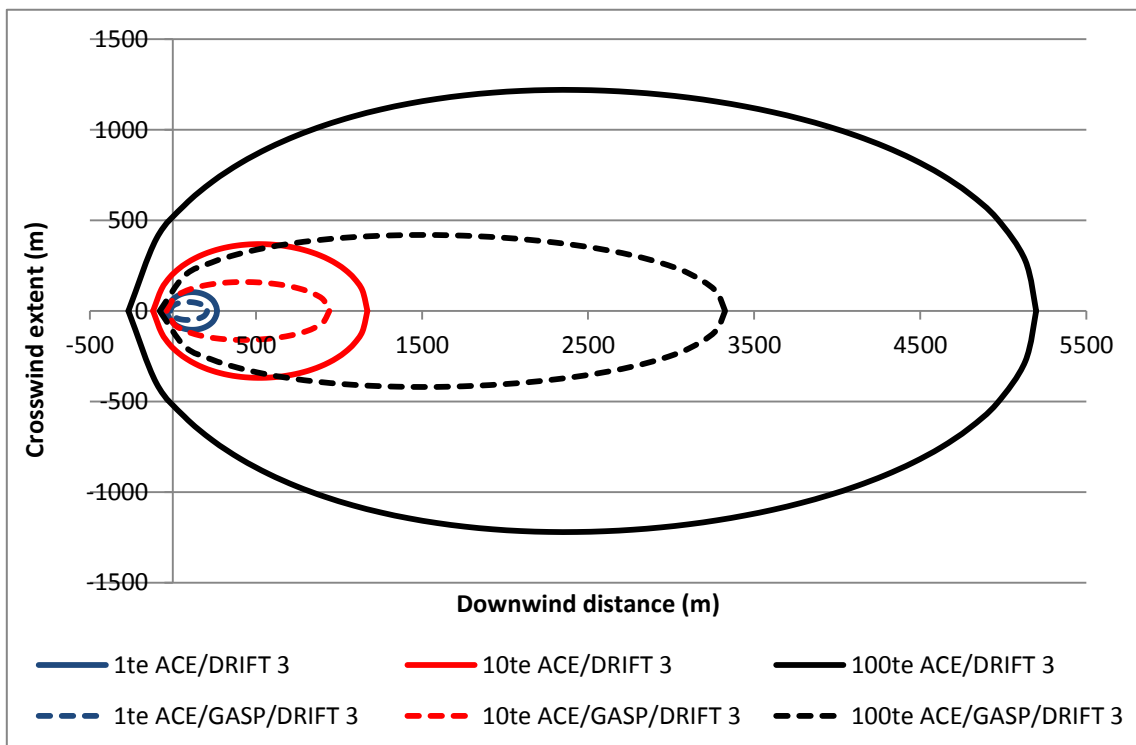


Figure 13 SLOT DTL isopleths obtained for instantaneous chlorine releases in F2.4 weather for an indoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

For chlorine releases of 10 te and above in D4.3 weather, the isopleths from the pool component (ACE/GASP/DRIFT 3) extend slightly further downwind and are narrower than those from the airborne

component (ACE/DRIFT 3). In F2.4 weather for an outdoor recipient, the isopleths for the airborne and pool components are similar in length, although the airborne component isopleths are wider. In F2.4 weather for an indoor recipient, the isopleths for the airborne and pool components are of a similar length for the two smaller releases (1 te and 10 te), but for the 100 te release, the airborne component is dominant in terms of both width and length. A possible reason for this is that due to the greater dense gas spreading of the 100 te release in F2.4 conditions, there is a longer cloud passage time for the airborne puff than for the pool release. This causes the maximum concentration built up indoors for the airborne puff to be greater than that for the pool component, and results in a larger SLOT DTL isopleth being predicted for the airborne puff.

In this study, it has been assumed that chlorine is stored at ambient temperature. If a lower storage temperature were used, the rainout fraction would be higher, and the contribution of the pool component relative to the airborne component would increase.

The bulb shape at the end of the 100 te release isopleth in Figure 12 is believed to be an artefact of the dense to passive transition in DRIFT 3. The cloud leans over due to wind shear and the maximum concentration at ground level lags behind the cloud centroid, which affects the toxic dose. This shear leaning effect is greater in stable conditions, i.e. F Pasquill stability [6].

3.3 SULPHUR DIOXIDE RELEASES

The sulphur dioxide results are split into two sections. Section 3.3.1 presents the comparison of ACE/DRIFT 3 with IRATE/DENZ and IRATE/DRIFT 3. This is a comparison of Sets (i), (ii) and (iii) as described at the start of Section 3. Section 3.3.2 presents the comparison of the contribution from the initial airborne component (modelled in ACE/DRIFT 3) and the contribution from the pool component (modelled in ACE/GASP/DRIFT 3). This is a comparison of Sets (iii) and (iv) as described at the start of Section 3.

A SLOT DTL of 4.655×10^6 ppm².min (i.e. a toxic *n* value of 2) [25] was used in DRIFT 3 for sulphur dioxide.

3.3.1 A comparison of results: ACE/DRIFT 3 against IRATE/DENZ and IRATE/DRIFT 3

The source term models ACE and IRATE generate source terms that are based on the airborne component only. Appendix 3 gives some example ACE outputs.

Although ACE accounts for the pool formation, in this study, evaporation of the pool into the cloud has not been modelled using ACE. A more sophisticated pool evaporation and spreading model, GASP, has been used for this purpose, and the results obtained using GASP are discussed in Section 3.3.2 for releases of sulphur dioxide.

The legends in Figures 14 to 21 show all the scenarios that were modelled. Table 6 summarises what is shown in the figures and shows which scenarios could not be plotted because DRIFT 3 did not produce isopleths for the chosen harm criterion. For indoor recipients, few of the model combinations predict SLOT DTL isopleths for the smaller releases.

Table 6 Key for figures showing a comparison of the previous and new methodologies for sulphur dioxide releases

Figure #	Substance	Weather	Recipient location	Release masses where the dispersion model produces no isopleths for the SLOT DTL harm criterion
14	SO ₂	D2.4	Outdoor	-
15	SO ₂	D2.4	Indoor	ACE/DRIFT 3: 1 te; IRATE/DENZ: 1 te
16	SO ₂	D4.3	Outdoor	-
17	SO ₂	D4.3	Indoor	ACE/DRIFT 3: 1 te; IRATE/DRIFT 3: 1 te, 10 te; IRATE/DENZ: 1 te
18	SO ₂	D6.7	Outdoor	-
19	SO ₂	D6.7	Indoor	ACE/DRIFT 3: 1 te, 10 te; IRATE/DRIFT 3: 1 te, 10 te; IRATE/DENZ: 1 te, 10 te
20	SO ₂	F2.4	Outdoor	-
21	SO ₂	F2.4	Indoor	ACE/DRIFT 3: 1 te; IRATE/DENZ: 1 te

Figures 14 to 21 show the isopleths generated using the different combinations of source term and dispersion model.

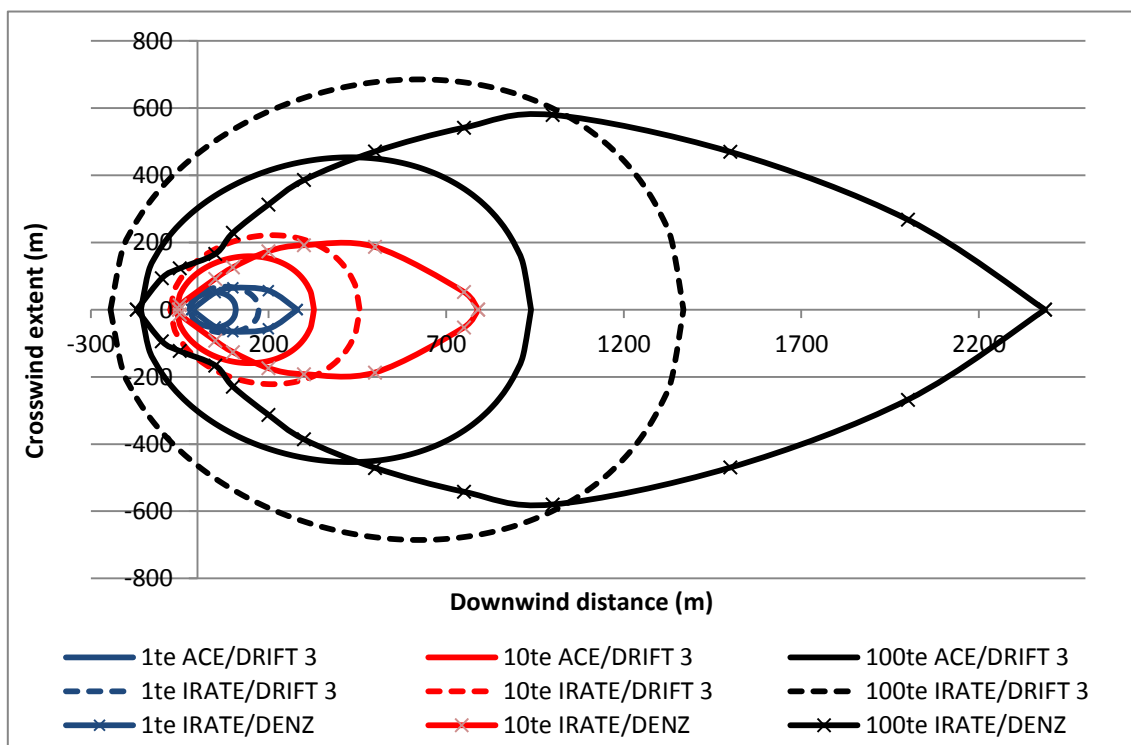


Figure 14 SLOT DTL isopleths obtained for instantaneous sulphur dioxide releases in D2.4 weather for an outdoor recipient. The results show dispersion of the airborne puff.

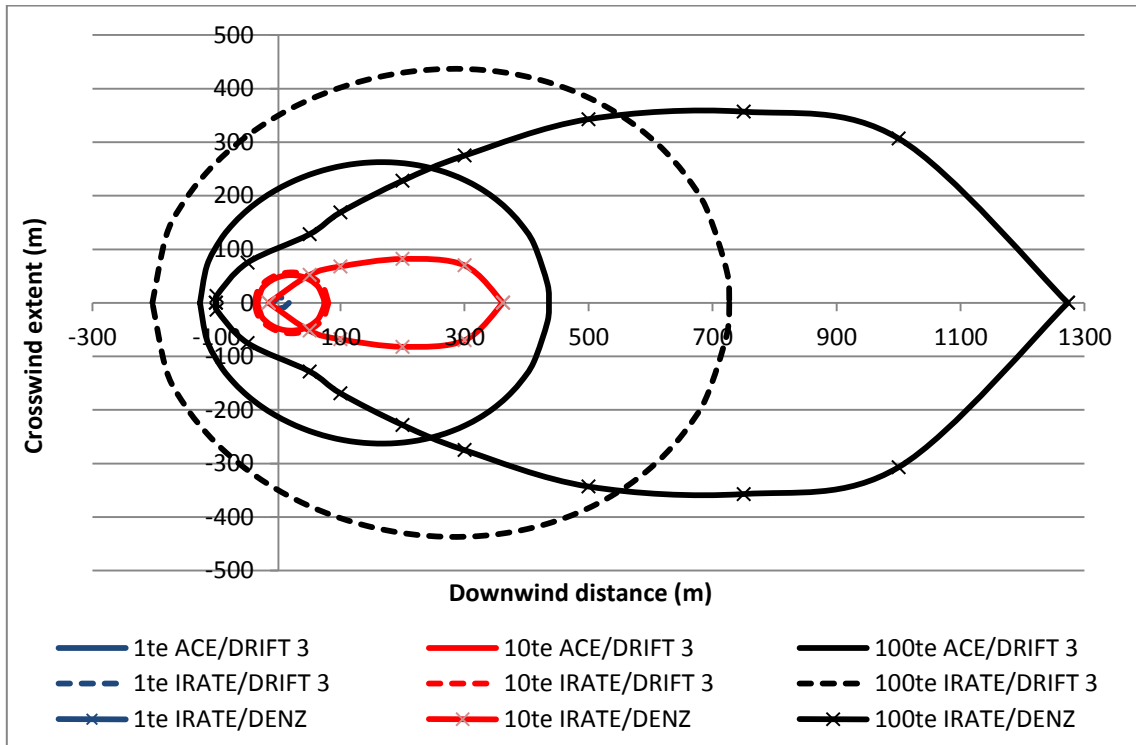


Figure 15 SLOT DTL isopleths obtained for instantaneous sulphur dioxide releases in D2.4 weather for an indoor recipient. The results show dispersion of the airborne puff.

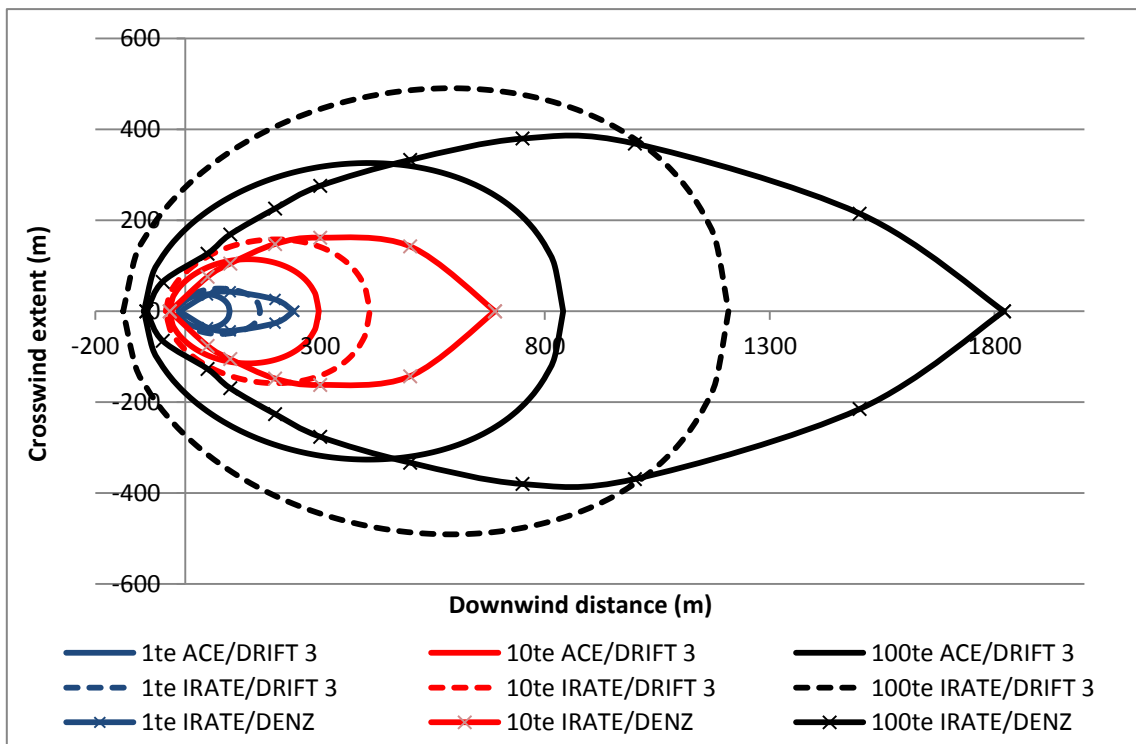


Figure 16 SLOT DTL isopleths obtained for instantaneous sulphur dioxide releases in D4.3 weather for an outdoor recipient. The results show dispersion of the airborne puff.

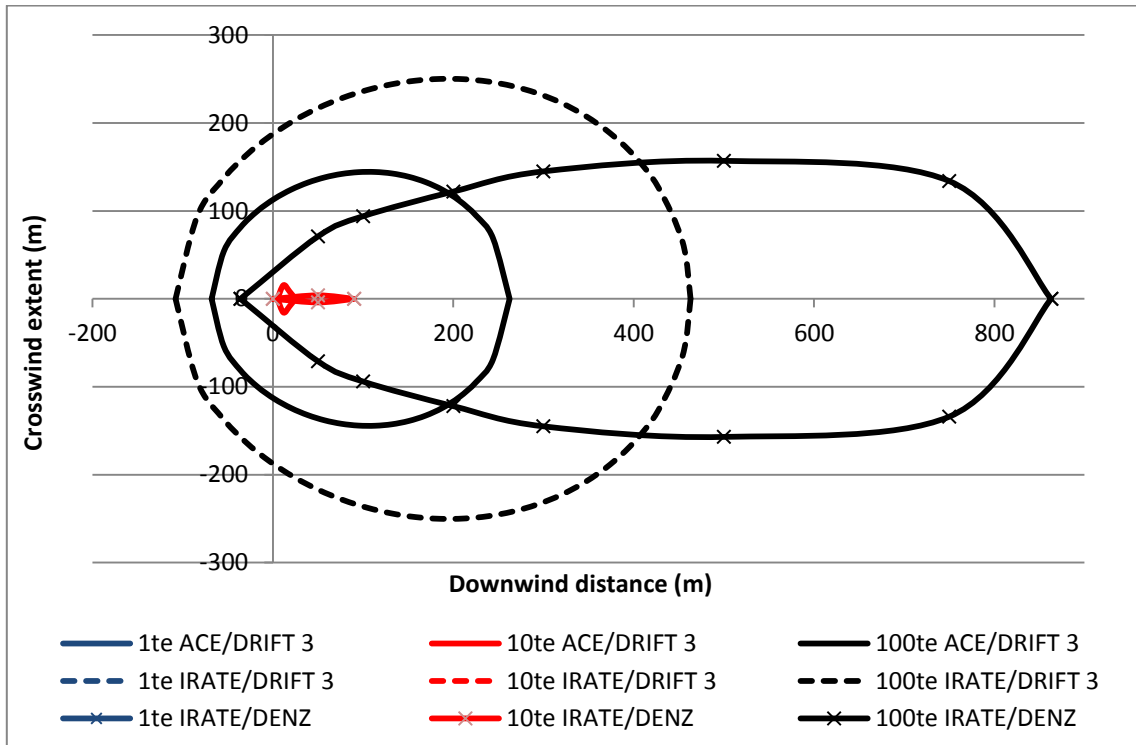


Figure 17 SLOT DTL isopleths obtained for instantaneous sulphur dioxide releases in D4.3 weather for an indoor recipient. The results show dispersion of the airborne puff.

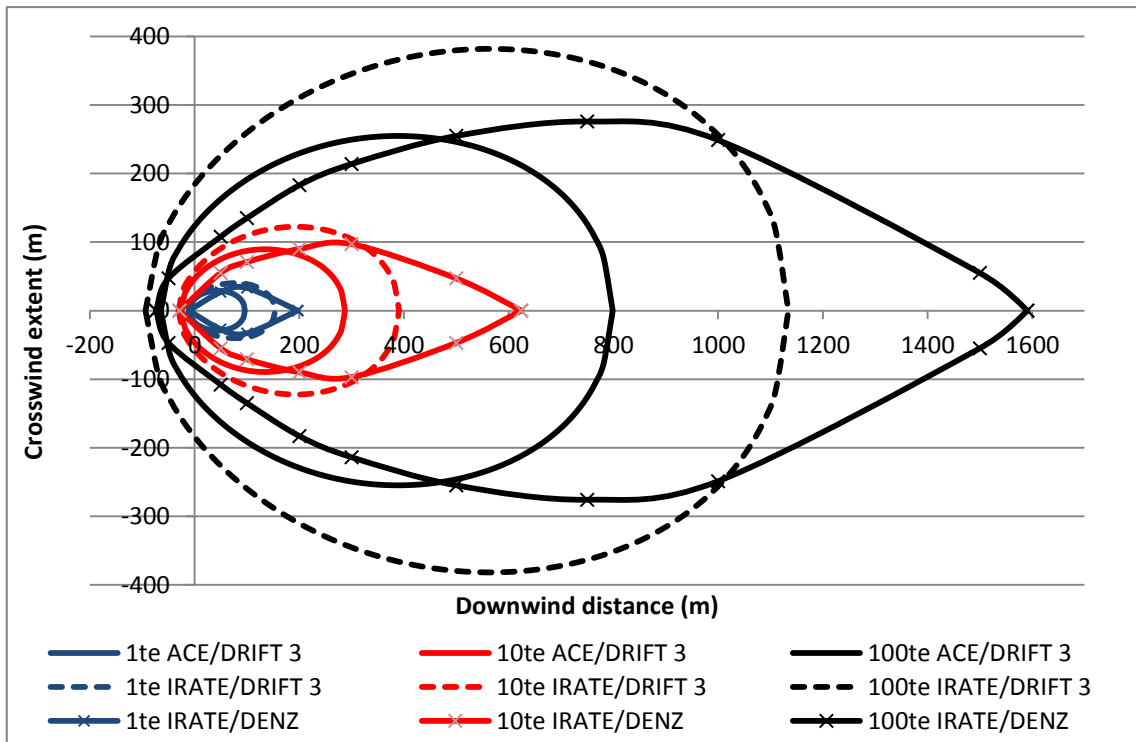


Figure 18 SLOT DTL isopleths obtained for instantaneous sulphur dioxide releases in D6.7 weather for an outdoor recipient. The results show dispersion of the airborne puff.

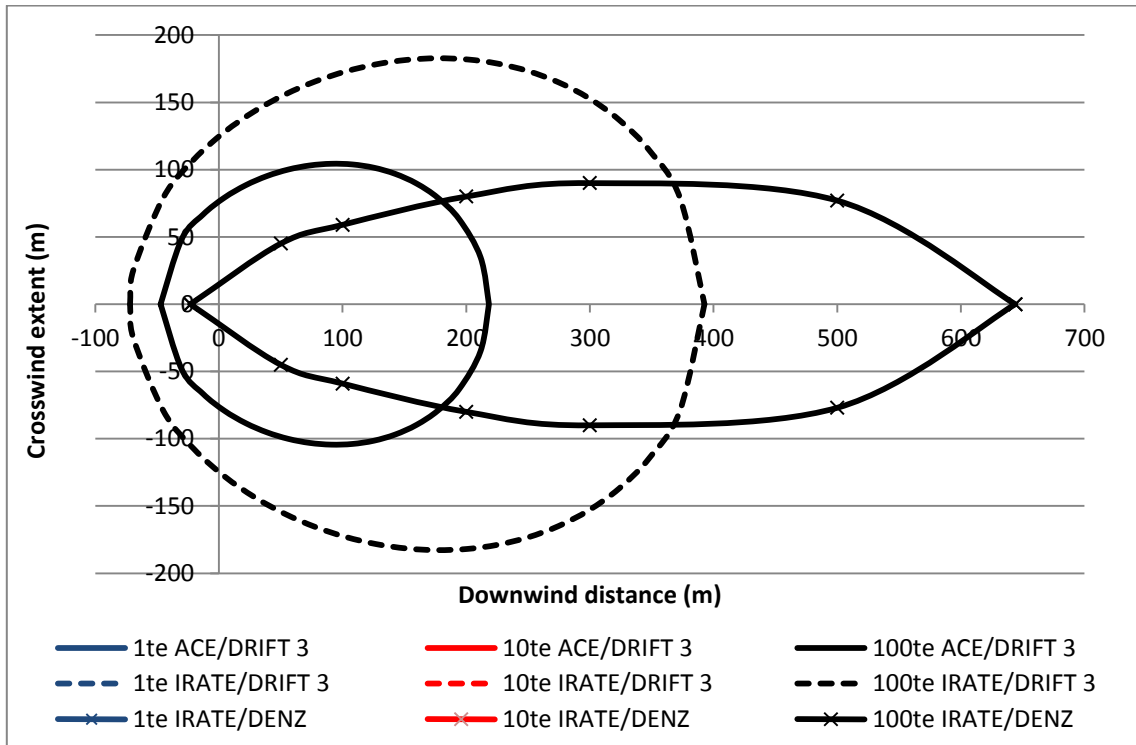


Figure 19 SLOT DTL isopleths obtained for instantaneous sulphur dioxide releases in D6.7 weather for an indoor recipient. The results show dispersion of the airborne puff.

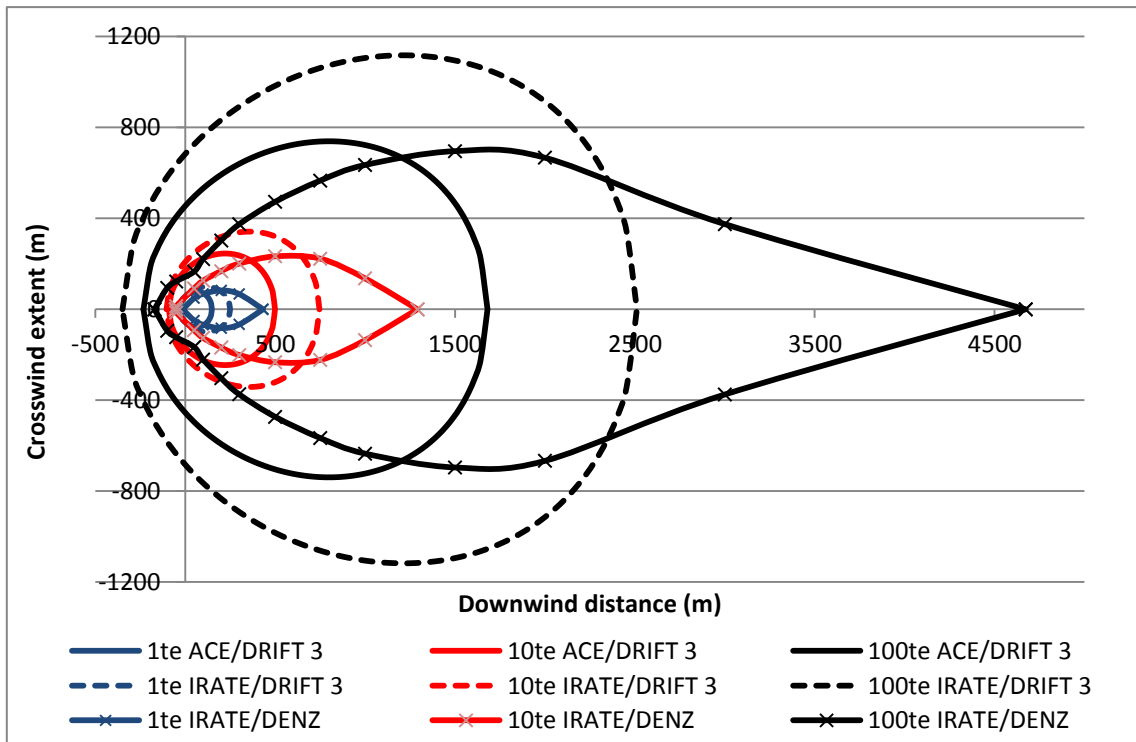


Figure 20 SLOT DTL isopleths obtained for instantaneous sulphur dioxide releases in F2.4 weather for an outdoor recipient. The results show dispersion of the airborne puff.

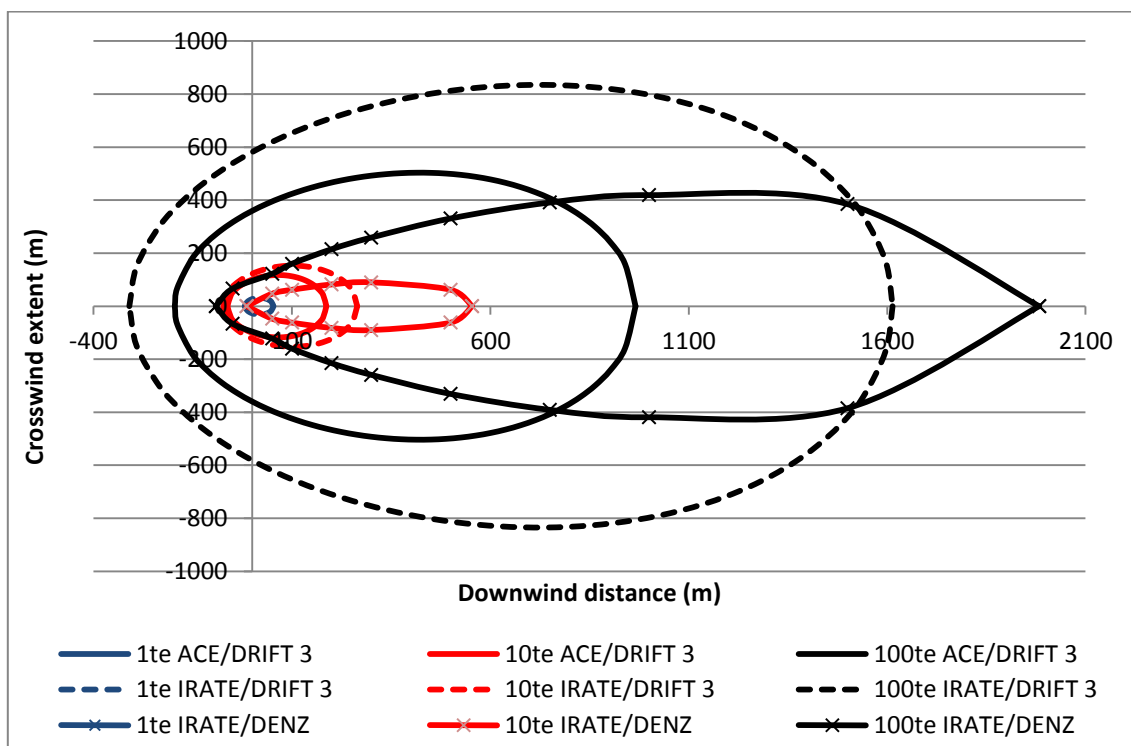


Figure 21 SLOT DTL isopleths obtained for instantaneous sulphur dioxide releases in F2.4 weather for an indoor recipient. The results show dispersion of the airborne puff.

Overall, the sulphur dioxide results follow a similar pattern to those of chlorine. The IRATE/DENZ results give the isopleths with the longest downwind extent, followed by IRATE/DRIFT 3 and then ACE/DRIFT 3 with the shortest downwind isopleths. All the model combinations produce results for outdoor recipients. For indoor recipients, SLOT DTL isopleths were produced for all of the 100 te releases, but were not produced for most of the 1 te releases and some of the 10 te releases (as summarised in Table 6 and illustrated in Figures 15, 17, 19 and 21). When the smaller releases of sulphur dioxide are modelled with the ventilation rates used by HSE for housing, then this leads to low concentrations and doses being modelled indoors, such that the toxicity criterion is never reached.

The IRATE/DRIFT 3 results generally produce the widest plumes, for both indoor and outdoor recipients. Further discussion can be found in the sulphur dioxide conclusions in Section 4.3.

3.3.2 A comparison of results: ACE/DRIFT 3 and ACE/GASP/DRIFT 3

The source terms used for Figures 14 to 21 are based on the airborne component only. To estimate the importance of the contribution from the pool, GASP was used to calculate the evaporation rate for use in DRIFT 3. The pool properties, such as the pool radius and mass of liquid within the pool, were taken from the ACE output files and input to GASP. Figures 22 to 25 show the comparison between the airborne component (ACE/DRIFT 3) and the pool component (ACE/GASP/DRIFT 3) and indicate which source term leads to potentially the worst-case dispersion results. Appendix 2 gives some example GASP inputs.

Figures 14 to 21 show similar patterns regardless of the weather and the location of the recipient. As there was little variation in the results obtained, a smaller set of GASP scenarios is shown in Figures 22 to 25. The legends in Figures 22 to 25 describe the scenarios that were modelled. Table 7 summarises what is shown in the figures and shows which scenarios could not be plotted because DRIFT 3 did not produce isopleths for the chosen harm criterion. DRIFT 3 produced isopleths for the pool component for all scenarios.

Table 7 Key for DRIFT 3 figures showing a comparison of the airborne and pool components for sulphur dioxide releases

Figure #	Substance	Weather	Recipient location	Release masses where the dispersion model produces no isopleths for the SLOT DTL harm criterion
22	SO ₂	D4.3	Outdoor	-
23	SO ₂	D4.3	Indoor	ACE/DRIFT 3: 1 te
24	SO ₂	F2.4	Outdoor	-
25	SO ₂	F2.4	Indoor	ACE/DRIFT 3: 1 te

Figures 22 to 25 show the isopleths generated for the puff and pool components of the scenarios modelled.

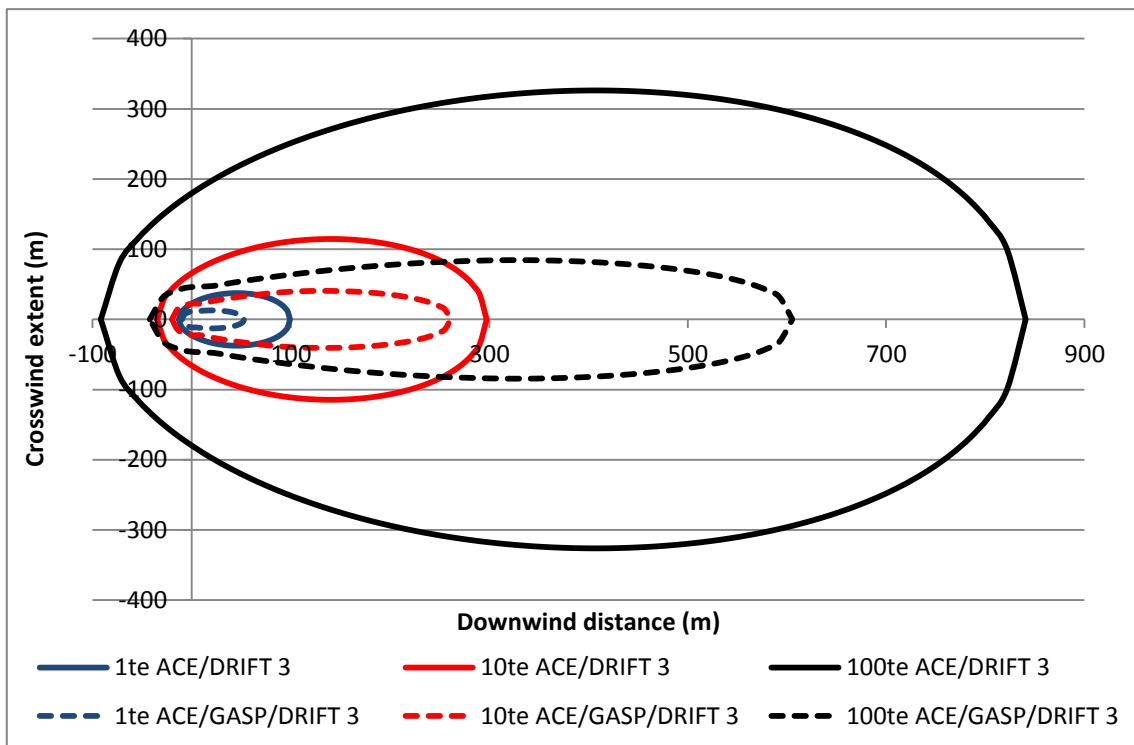


Figure 22 SLOT DTL isopleths obtained for instantaneous sulphur dioxide releases in D4.3 weather for an outdoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

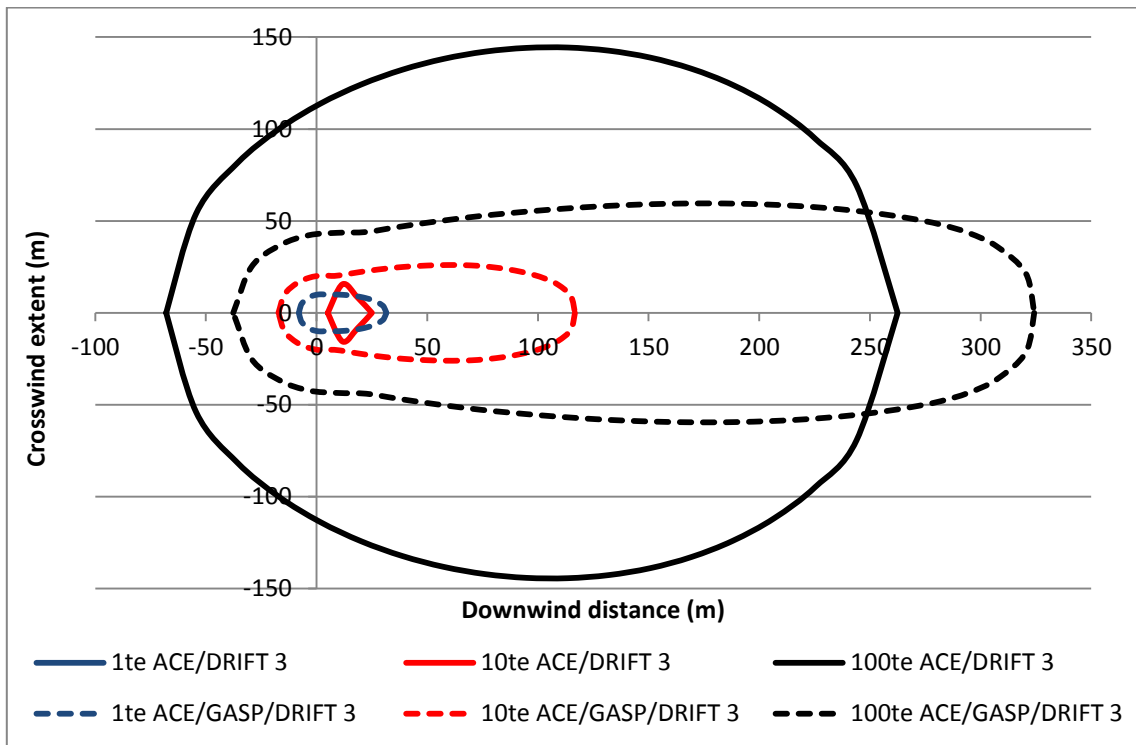


Figure 23 SLOT DTL isopleths obtained for instantaneous sulphur dioxide releases in D4.3 weather for an indoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

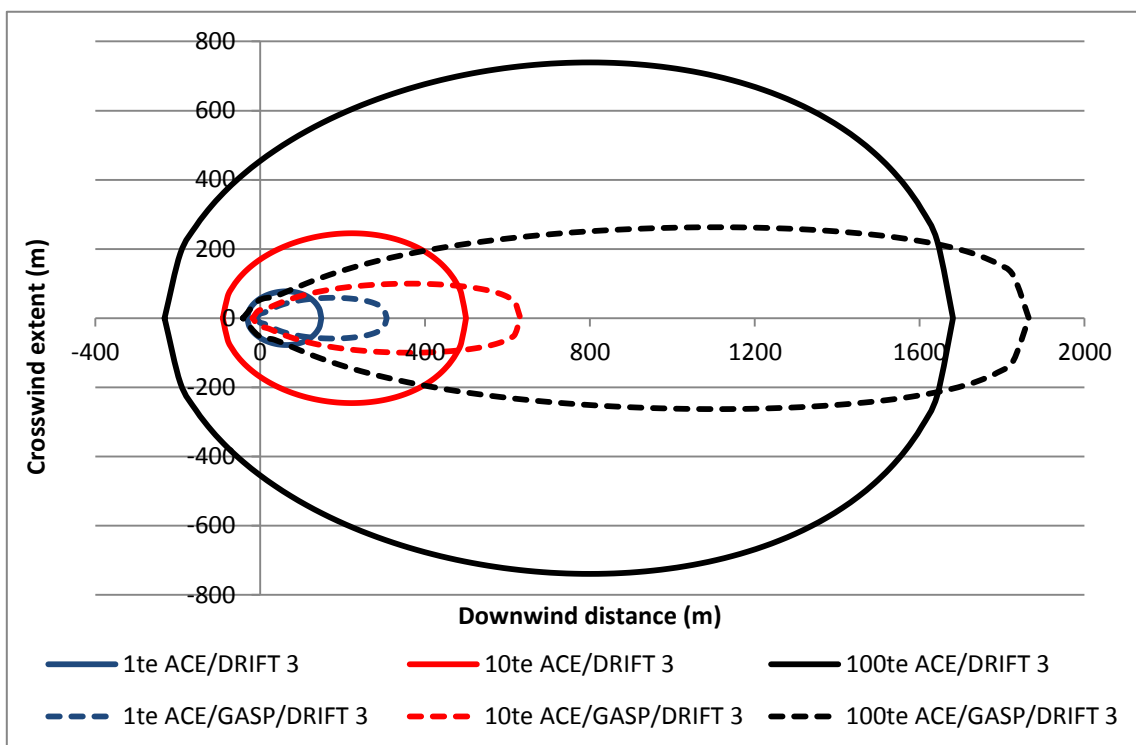


Figure 24 SLOT DTL isopleths obtained for instantaneous sulphur dioxide releases in F2.4 weather for an outdoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

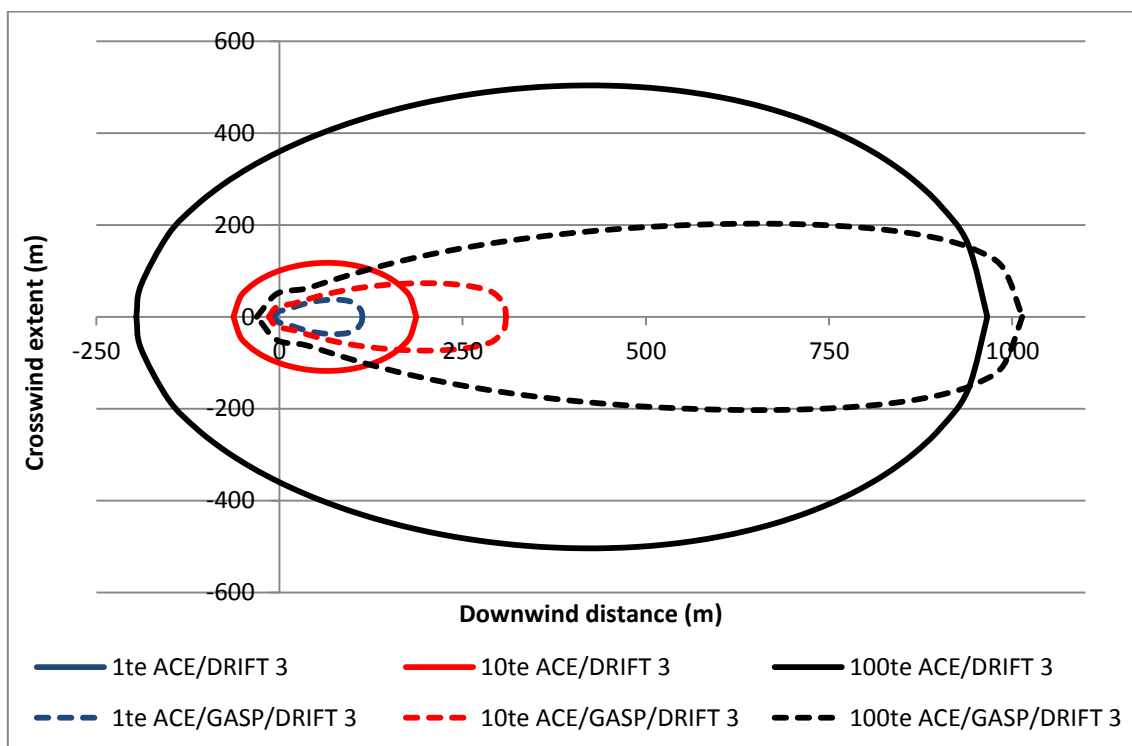


Figure 25 SLOT DTL isopleths obtained for instantaneous sulphur dioxide releases in F2.4 weather for an indoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

For all the sulphur dioxide release scenarios considered in this study, the airborne component (modelled in ACE and DRIFT 3) produces significantly wider isopleths than the pool component (modelled in ACE, GASP and DRIFT 3). For all cases except D4.3 weather for outdoor recipients, the pool component predicts slightly longer downwind extent isopleths than the airborne puff. Further discussion can be found in the sulphur dioxide conclusions section, Section 4.3.

3.4 AMMONIA RELEASES

The ammonia results are split into two sections. Section 3.4.1 presents the comparison of ACE/DRIFT 3 with IRATE/DENZ and IRATE/DRIFT. This is a comparison of Sets (i), (ii) and (iii) as described at the start of Section 3. Section 3.4.2 presents the comparison of the contribution from the initial airborne component (modelled in ACE/DRIFT 3) and the contribution from the pool component (modelled in ACE/GASP/DRIFT 3). This is a comparison of Sets (iii) and (iv) as described at the start of Section 3.

A SLOT DTL of 3.78×10^8 ppm².min (i.e. a toxic *n* value of 2) [25] was used in DRIFT 3 for ammonia.

3.4.1 A comparison of results: ACE/DRIFT 3 against IRATE/DENZ and IRATE/DRIFT 3

The source term models ACE and IRATE generate source terms that are based on the airborne component only. Appendix 3 gives some example ACE outputs.

Although ACE accounts for the pool formation, in this study, evaporation of the pool into the cloud has not been modelled using ACE. A more sophisticated pool evaporation and spreading model, GASP, has been used for this purpose, and the results obtained using GASP are discussed in Section 3.4.2 for releases of ammonia.

The legends in Figures 26 to 31 describe the scenarios that were modelled. Table 8 summarises what is shown in the figures and shows which scenarios could not be plotted because DRIFT 3 did not produce

isopleths for the chosen harm criterion. Only some of the model combinations predict SLOT DTL isopleths for the airborne component and usually only for outdoor recipients. Isopleths are generally not produced for the lower release masses. Figures are not presented for indoor recipients in D4.3 and D6.7 weather because none of the model combinations predicted SLOT DTL isopleths.

Table 8 Key for figures showing a comparison of the previous and new methodologies for ammonia releases

Figure #	Substance	Weather	Recipient location	Release masses where the dispersion model produces no isopleths for the SLOT DTL harm criterion
26	NH ₃	D2.4	Outdoor	ACE/DRIFT 3: 1 te; IRATE/DRIFT 3: 1 te
27	NH ₃	D2.4	Indoor	ACE/DRIFT 3: 1 te, 10 te, 100 te; IRATE/DRIFT 3: 1 te, 10 te, 100 te; IRATE/DENZ: 1 te, 10 te
28	NH ₃	D4.3	Outdoor	ACE/DRIFT 3: 1 te; IRATE/DRIFT 3: 1 te
-	NH ₃	D4.3	Indoor	ACE/DRIFT 3: 1 te, 10 te, 100 te; IRATE/DRIFT 3: 1 te, 10 te, 100 te; IRATE/DENZ: 1 te, 10 te, 100 te
29	NH ₃	D6.7	Outdoor	ACE/DRIFT 3: 1 te; IRATE/DRIFT 3: 1 te
-	NH ₃	D6.7	Indoor	ACE/DRIFT 3: 1 te, 10 te, 100 te; IRATE/DRIFT 3: 1 te, 10 te, 100 te; IRATE/DENZ: 1 te, 10 te, 100 te
30	NH ₃	F2.4	Outdoor	IRATE/DRIFT 3: 1 te
31	NH ₃	F2.4	Indoor	ACE/DRIFT 3: 1 te, 10 te, 100 te; IRATE/DRIFT 3: 1 te, 10 te, 100 te; IRATE/DENZ: 1 te, 10 te

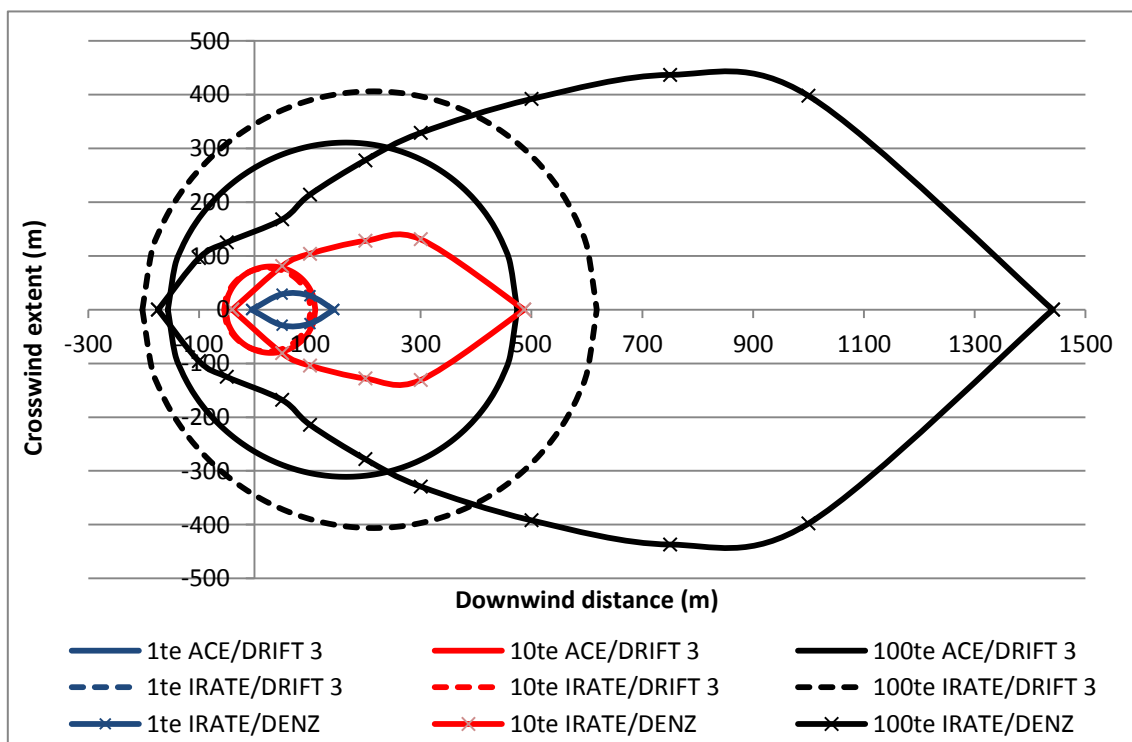


Figure 26 SLOT DTL isopleths obtained for instantaneous ammonia releases in D2.4 weather for an outdoor recipient. The results show dispersion of the airborne puff.

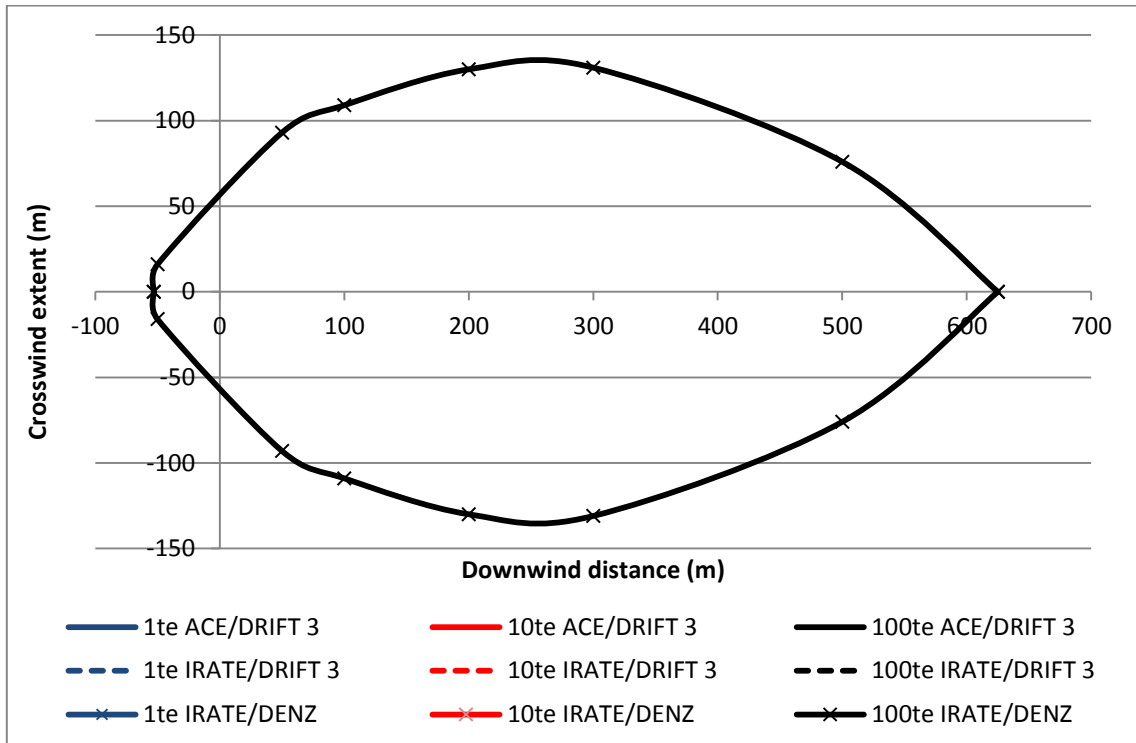


Figure 27 SLOT DTL isopleths obtained for instantaneous ammonia releases in D2.4 weather for an indoor recipient. The results show dispersion of the airborne puff.

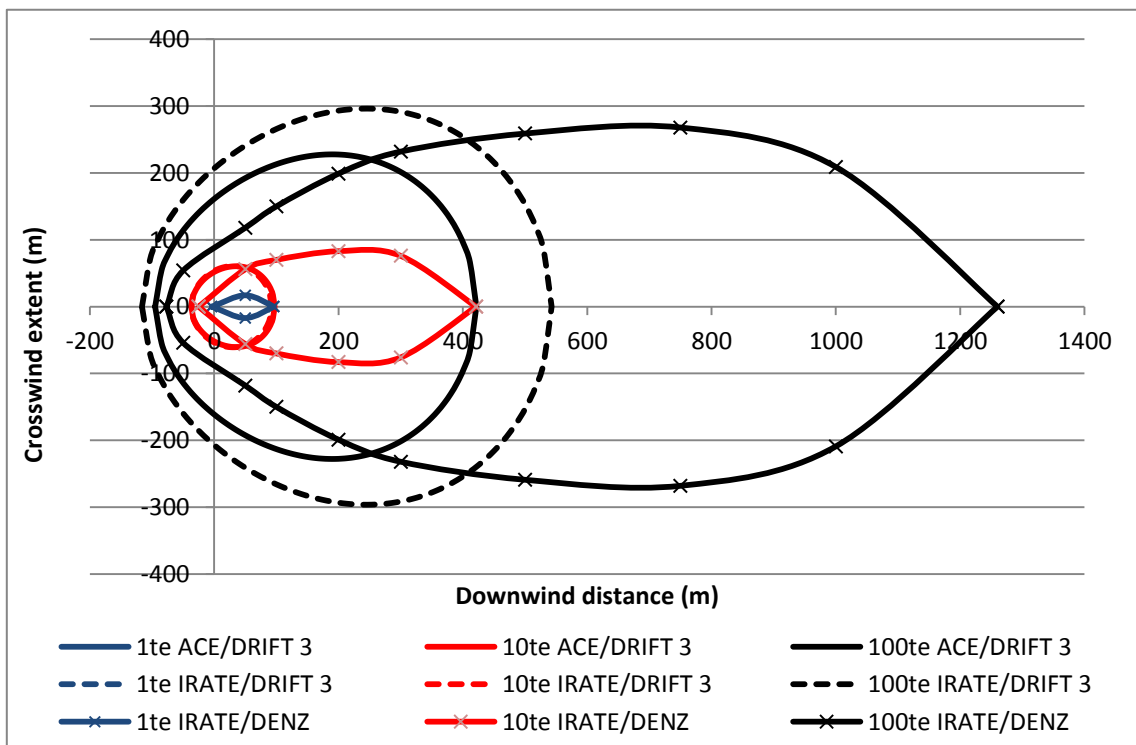


Figure 28 SLOT DTL isopleths obtained for instantaneous ammonia releases in D4.3 weather for an outdoor recipient. The results show dispersion of the airborne puff.

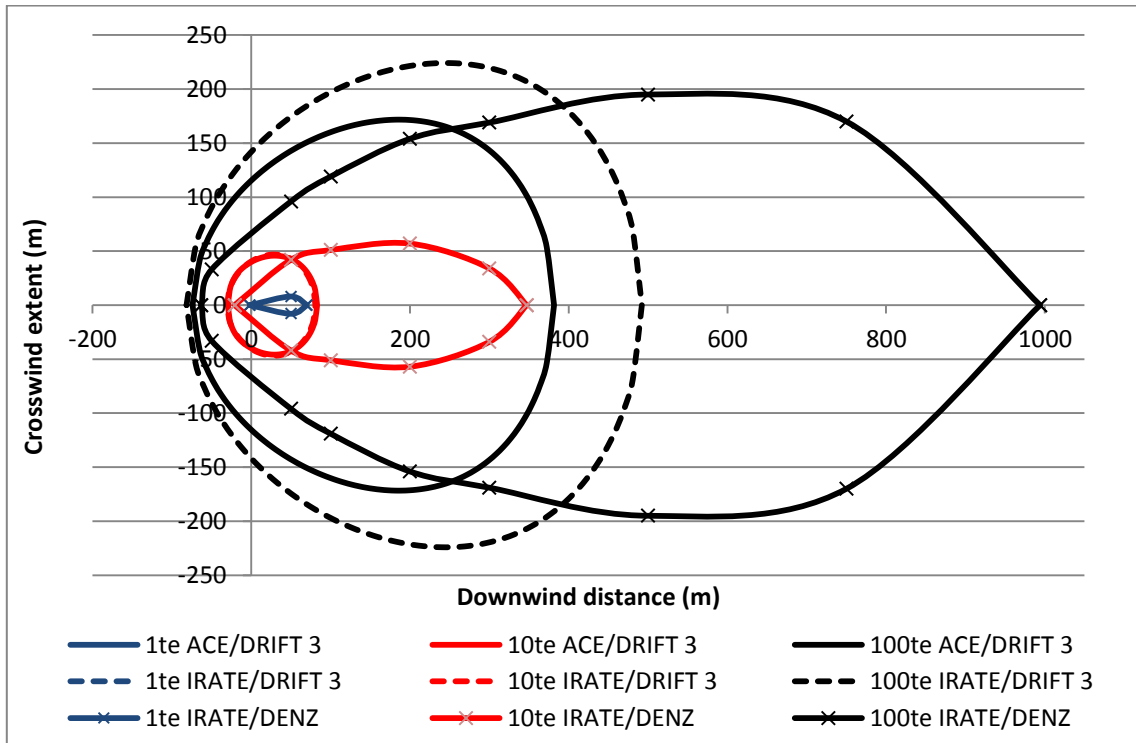


Figure 29 SLOT DTL isopleths obtained for instantaneous ammonia releases in D6.7 weather for an outdoor recipient. The results show dispersion of the airborne puff.

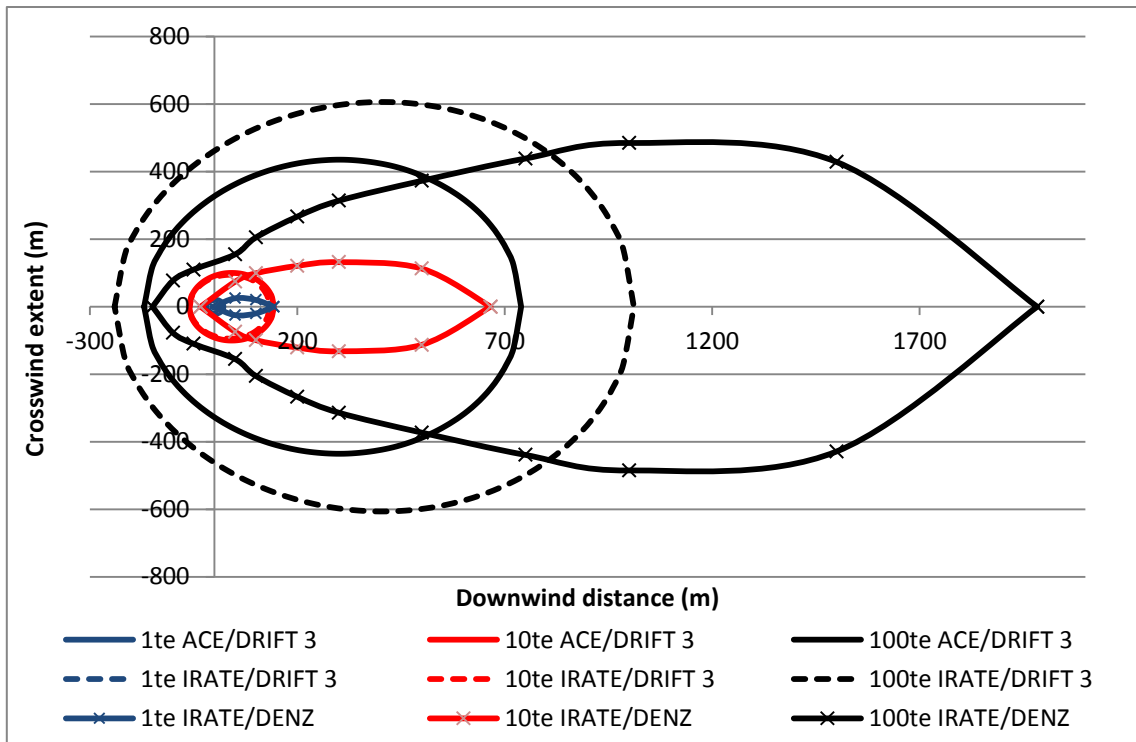


Figure 30 SLOT DTL isopleths obtained for instantaneous ammonia releases in F2.4 weather for an outdoor recipient. The results show dispersion of the airborne puff.

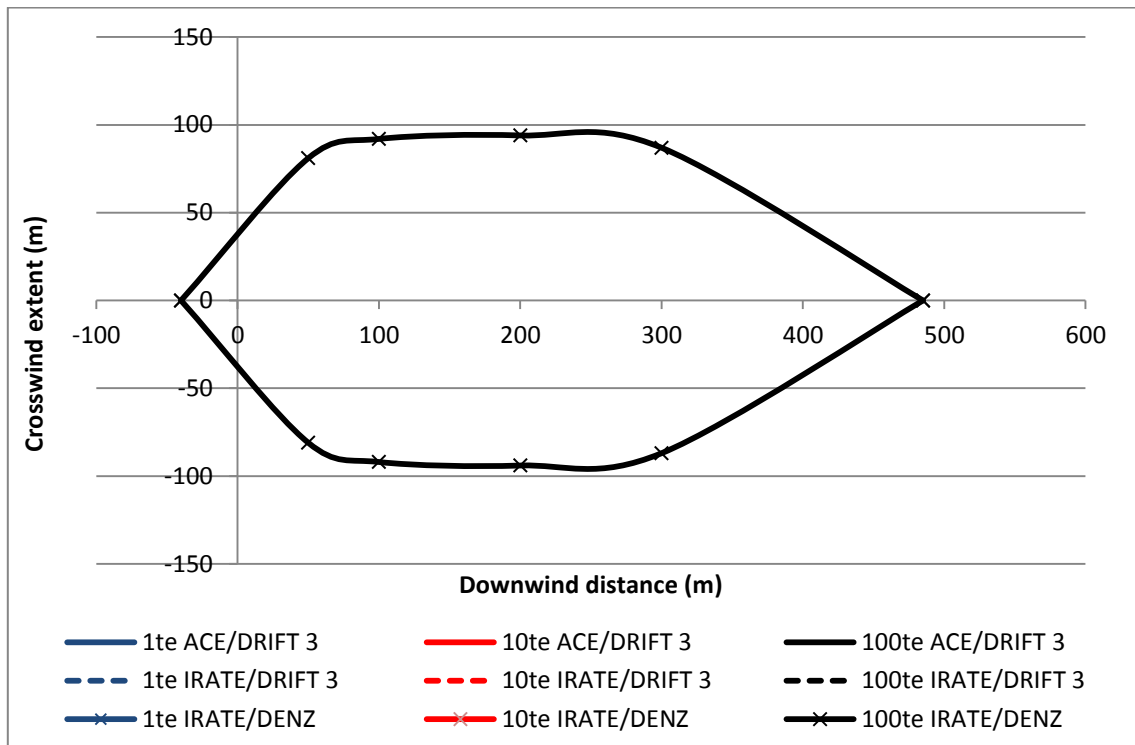


Figure 31 SLOT DTL isopleths obtained for instantaneous ammonia releases in F2.4 weather for an indoor recipient. The results show dispersion of the airborne puff.

For ammonia, Figures 26 to 31 show SLOT DTL isopleths are generally predicted for outdoor recipients where the release mass is 10 te or larger, for all the model combinations. For indoor recipients, isopleths are only produced for the 100 te release in low wind speeds using the IRATE/DENZ method. The isopleths generated using IRATE/DENZ generally have larger downwind and crosswind extents than the isopleths generated using ACE/DRIFT 3. The lack of results for indoor ammonia recipients could be due to the high SLOT DTL ($3.78 \times 10^8 \text{ ppm}^2 \cdot \text{min}$) value. When this value is used with the ventilation rates used by HSE for housing, then this leads to low concentrations and doses being modelled indoors, such that the toxicity criterion is never reached. Further discussion is given in the ammonia conclusions section, in Section 4.4.

The isopleth generated in IRATE and DENZ for an indoor recipient in D2.4 weather conditions (Figure 27) extends further downwind and to a greater crosswind extent than the isopleth generated for F2.4 weather conditions (Figure 31). This is counterintuitive because a cloud dispersing in a more stable atmosphere (i.e. the F2.4 weather) would normally be expected to dilute more slowly and generate a larger hazardous area than an identical cloud dispersing in less stable conditions (i.e. the D2.4 weather).

The reason for this behaviour in this case is the way that HSE has historically modified the DENZ outputs generated for D and F weather stability conditions, combined with the particular characteristics of the ammonia release modelled. The DENZ model outputs a 'top hat' concentration profile (i.e. the concentration is assumed to have a uniform 'flat-top' concentration and vertical 'sides') at downwind distances from the release source. HSE has historically converted the 'top hat' concentration profile to a Gaussian concentration profile. The Gaussian concentration profile is then used in conjunction with the cloud passage times output by DENZ at points downwind from the release to determine the maximum extent at which a user would receive the SLOT DTL from a release.

To distinguish between the different temperatures assumed for daytime and night-time conditions, HSE uses different modifiers in the 'top hat' to Gaussian conversion for D stability and F stability weather. It is assumed that D Pasquill stability weather represents day conditions and F Pasquill stability weather represents night conditions. The modifier used in the conversion for F weather results in a smaller peak

concentration in the Gaussian profile than that generated for an equivalent conversion for D weather conditions.

In most cases, the puff disperses more slowly in stable F Pasquill conditions than in neutral D Pasquill conditions. This usually leads to the SLOT DTL isopleths calculated for F weather being larger and wider than the isopleths calculated for D weather. In the scenario modelled to generate the isopleths in Figure 27 and Figure 31, however, similar ‘top hat’ concentration profiles and cloud passage times are obtained near to the release point for D and F Pasquill stabilities.

Near to the release point, the ‘top hat’ concentration in F weather conditions is therefore converted to a smaller Gaussian peak concentration than the ‘top hat’ concentration in D weather conditions. This particular scenario generates isopleths for indoor recipients that are relatively close to the source in both D and F weather conditions. The smaller Gaussian peak concentration in F weather conditions results in a smaller SLOT DTL isopleth being calculated for F weather conditions than for D weather conditions.

3.4.2 A comparison of results: ACE/DRIFT 3 and ACE/GASP/DRIFT 3

The source terms used for Figures 26 to 31 are based on the airborne component only. To estimate the importance of the contribution from the pool, GASP was used to calculate the pool evaporation rate for use in DRIFT 3. The pool properties, such as the pool radius and mass of liquid within the pool, were taken from the ACE output files and input to GASP. Figures 32 to 35 show the comparison between the airborne component (ACE/DRIFT 3) and the pool component (ACE/GASP/DRIFT 3) and indicate which source term is potentially the worst-case.

Figures 26 to 31 show similar patterns regardless of the weather and the location of the recipient. As there was little variation in the results obtained, a smaller set of GASP scenarios is shown in Figures 32 to 35. The legends in Figures 32 to 35 describe the scenarios that were modelled. Table 9 summarises what is shown in the figures and shows which scenarios could not be plotted because DRIFT 3 did not produce isopleths for the chosen harm criterion. The DRIFT 3 model predicted SLOT DTL isopleths for some scenarios when ACE was used as the source term, but more scenarios have predicted isopleths when the GASP source term is modelled in DRIFT 3. Where the GASP source term does not result in SLOT DTL isopleths, it is for small release masses and indoor recipients.

Table 9 Key for DRIFT 3 figures showing a comparison of the airborne and pool components for ammonia releases

<i>Figure #</i>	<i>Substance</i>	<i>Weather</i>	<i>Recipient location</i>	<i>Release masses where the dispersion model produces no isopleths for the SLOT DTL harm criterion</i>
32	NH ₃	D4.3	Outdoor	ACE/DRIFT 3: 1 te
33	NH ₃	D4.3	Indoor	ACE/DRIFT 3: 1 te, 10 te, 100 te; ACE/GASP/DRIFT 3: 1 te
34	NH ₃	F2.4	Outdoor	-
35	NH ₃	F2.4	Indoor	ACE/DRIFT 3: 1 te, 10 te, 100 te; ACE/GASP/DRIFT 3: 1 te

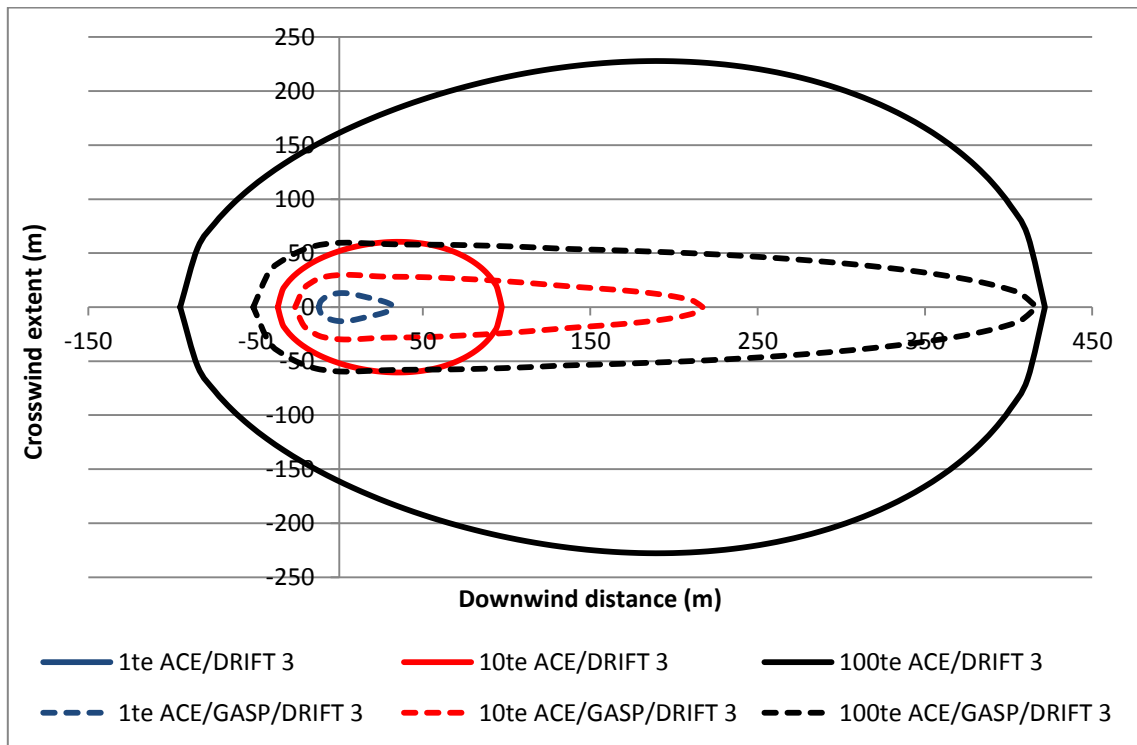


Figure 32 SLOT DTL isopleths obtained for instantaneous ammonia releases in D4.3 weather for an outdoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

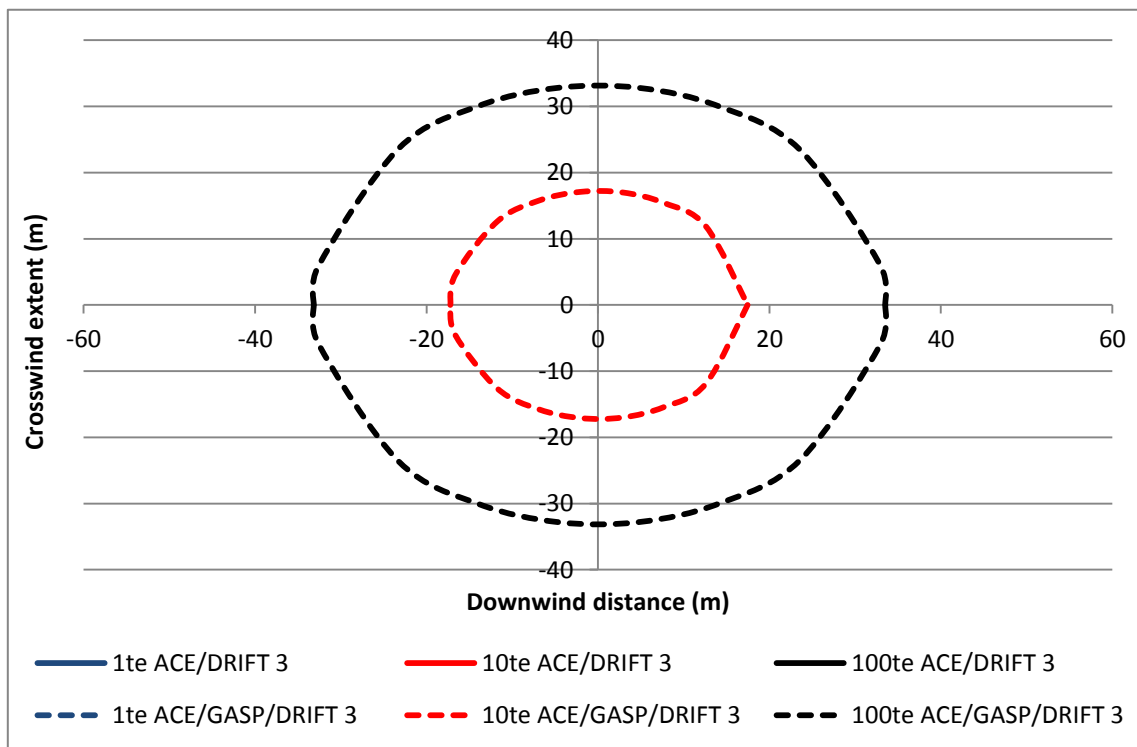


Figure 33 SLOT DTL isopleths obtained for instantaneous ammonia releases in D4.3 weather for an indoor recipient. The results show dispersion of the pool (ACE/GASP/DRIFT 3) component. No airborne puff results were obtained for this case.

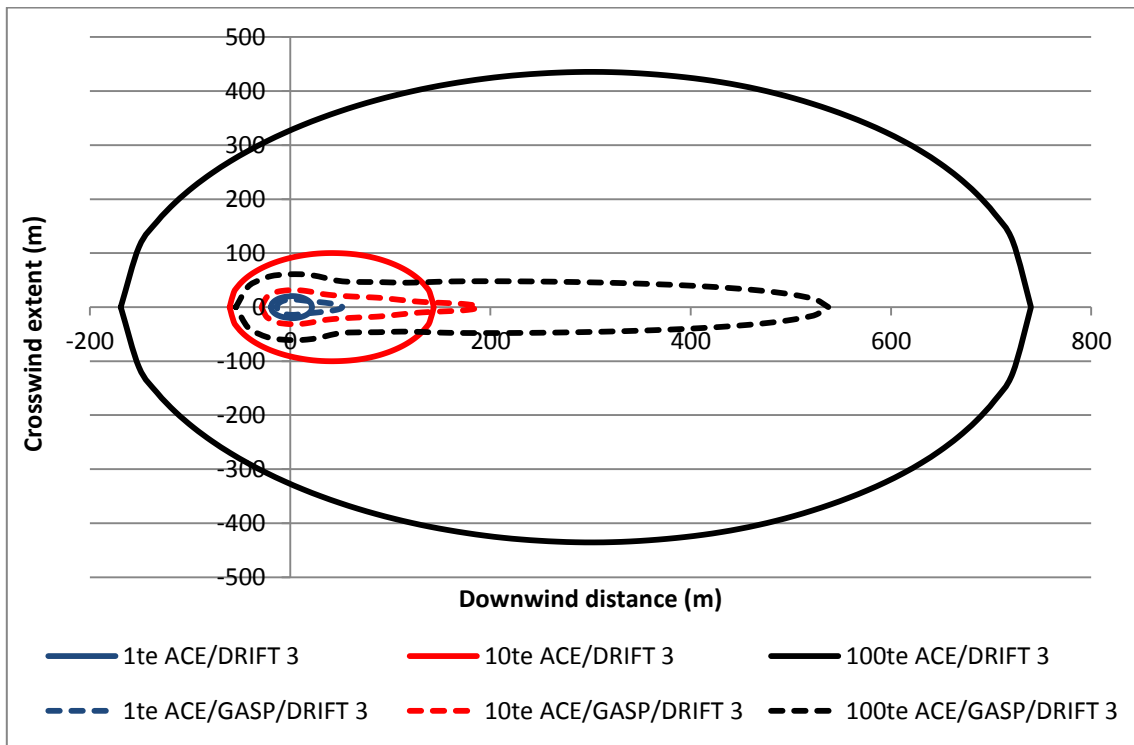


Figure 34 SLOT DTL isopleths obtained for instantaneous ammonia releases in F2.4 weather for an outdoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

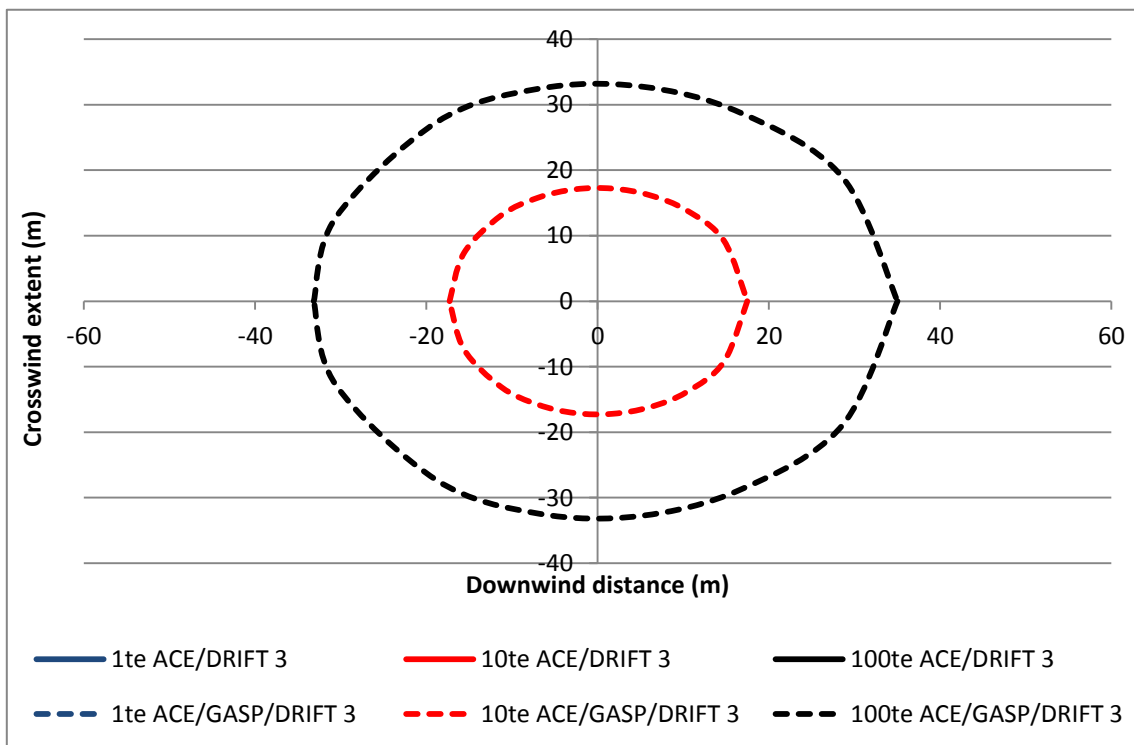


Figure 35 SLOT DTL isopleths obtained for instantaneous ammonia releases in F2.4 weather for an indoor recipient. The results show dispersion of the pool (ACE/GASP/DRIFT 3) component. No airborne puff results were obtained for this case.

Figures 33 and 35 show that only the pool component generates isopleths for an indoor recipient for the ammonia scenarios modelled. The isopleths generated in these cases are circular isopleths that

correspond to the pool source size that is output by ACE and used as an input in GASP and DRIFT 3. For example, ACE predicts a pool diameter of 66.3 m for the 100 te ammonia release. The circular isopleth diameters calculated by DRIFT 3 for this scenario are 67.1 m and 68.2 m for the D4.3 and F2.4 weather categories, respectively. For this scenario, only the region directly above the pool has a concentration profile with sufficient duration to lead to a person indoors receiving the SLOT DTL (the HSE Dangerous Dose). As the initial release is assumed to occur outdoors, then these results cannot realistically be of use in a hazard or risk assessment. As the pool diameters and subsequent dispersion isopleths are relatively small then the contribution from such a release is not likely to be significant in any risk assessment undertaken.

DRIFT 3 calculated no indoor isopleths for the airborne puff for the ammonia scenarios modelled. The DRIFT 3 model does not model the cloud from the start of an instantaneous release i.e. the catastrophic failure of the vessel. The initial phases of the release are modelled by the source term model ACE. If the early phases of the release modelled by ACE were included in the isopleth calculations then there is a possibility that the cloud would be of sufficient concentration to lead to a person indoors receiving the SLOT DTL. However, any isopleths calculated using such a method would be smaller in size than the cloud output by ACE and used as an input to GASP and DRIFT 3. For example, the diameter of the cloud output by ACE for the 100 te ammonia release is 66.3 m. This means that a more concentrated cloud calculated by ACE for the early phases of a release would be smaller than 66.3 m in diameter for this release scenario. This would be smaller than the isopleths generated for the pool dispersion component of the release and would not contribute significantly to any risk assessment undertaken for a site storing ammonia.

4 DISCUSSION OF RESULTS

This section presents a discussion of the DRIFT 3 results for the pressure-liquefied releases shown in Figures 2 to 35.

4.1 COMPARISON OF OLD AND NEW METHODOLOGIES

The new methodology (using the ACE and DRIFT 3 models) generates SLOT DTL (Specified Level Of Toxicity, Dangerous Toxic Load) isopleths that have shorter downwind extents than the isopleths obtained using the previous methodology (using the IRATE and DENZ models).

In some cases, the differences in the maximum downwind extents predicted by the old and new methodologies can be quite large. For example, the difference in the maximum downwind distance to the SLOT DTL in Figure 4 (chlorine release in D4.3 weather, for an outdoor recipient) is approximately 5 km. This difference is caused by changes to the modelling assumptions and differences in the source term models (IRATE and ACE) and the dispersion models (DENZ and DRIFT 3). Using DRIFT 3 with IRATE generated shorter SLOT DTL isopleths than when the same scenario was modelled using IRATE and DENZ.

Figure 36 shows the concentration versus distance profiles for the DENZ and DRIFT 3 models (using an IRATE source term). The transition from dense to passive dispersion for DENZ is marked by a visible discontinuity on the graph because once the criteria required by DENZ are met the transition occurs immediately, whereas for DRIFT 3 the transition is more gradual with downwind distance. For the initial stages of the release, the rate of reduction in concentration is comparable between the two models, but because the assumptions used to trigger the transition to passive dispersion are different, the concentrations predicted by the models diverge. The concentration predicted by DRIFT 3, as shown in Figure 36, is smaller than the concentration predicted by DENZ for the same downwind distance, which results in shorter DRIFT 3 isopleths in the downwind direction.

The predicted peak concentration at a given downwind distance has a significant effect on the size of the SLOT DTL isopleths for substances with a toxic exponent of two, such as chlorine, sulphur dioxide and ammonia. The dose to which a recipient is exposed is calculated using the following equation:

$$Dose = c^n t \quad \text{Equation 1}$$

where c is the concentration of the toxic substance (parts per million, ppm), t is the duration of the exposure (min), and n is the substance specific toxic exponent, values of which are given on the HSE website [25]. The form of Equation 1 means that the peak concentration has a greater influence on the dose for substances with a toxic exponent of two than for substances with a toxic exponent of one.

DENZ makes an abrupt transition from dense to passive behaviour when either the rate of gravity spread is less than the rate of passive spreading due to atmospheric turbulence, or the cloud density difference from air becomes small. In contrast, DRIFT models the transition from dense to passive behaviour smoothly as a function of the cloud Richardson number, a dimensionless number that measures the gravitational potential energy of the cloud relative to the turbulent kinetic energy. The dense gas limit occurs at a large Richardson number and the passive limit at a small Richardson number. The continuous transition in DRIFT is regarded as an improvement over that in DENZ, which can result in discontinuous changes that are not observed in real clouds. DRIFT's passive model is also more sophisticated than DENZ's since it includes the effect of shear on the cloud spread. This effect is recognised as being important and is included in most modern passive dispersion models.

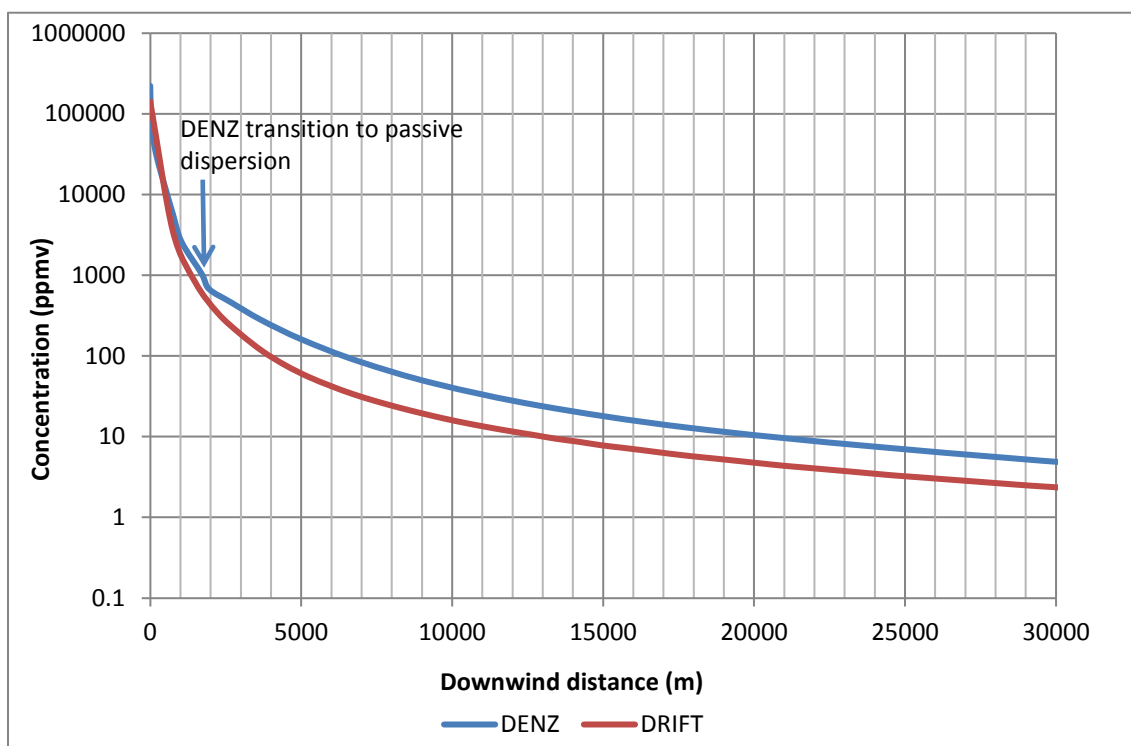


Figure 36 Transition from dense to passive dispersion for DENZ and DRIFT 3. The scenario is a 100 te release of chlorine in D4.3 weather for an outdoor recipient.

4.2 CHLORINE RELEASES

For chlorine releases, the airborne component (ACE/DRIFT 3) and the pool component (ACE/GASP/DRIFT 3) result in isopleths of similar length; this pattern is produced for most of the scenarios modelled, including those with low masses. For all the scenarios considered in this study, the airborne component produces isopleths that are significantly wider than those produced by the pool component.

GASP predicts that the peak vaporisation rate for a pool release will be greater than twice the mean vaporisation rate over the release duration for all of the modelled chlorine releases. Cruse et al. [21] describe a methodology for modelling releases of this type (referred to as ‘peaky’ releases by HSE), which involves modifying the vaporisation rate and release duration to better account for the peak in the vaporisation curve. The modified vaporisation rate and release duration are used as inputs for DRIFT 3. This methodology was followed in the modelling of these scenarios and resulted in relatively high vaporisation rates with very short durations, as shown in Table 10.

Table 10 Results from ACE and GASP for a chlorine release in D4.3 weather

<i>Release mass (te)</i>	<i>Airborne CM (vapour and aerosol) as output by ACE (te)</i>	<i>Mass of air entrained in cloud as output by ACE (te)</i>	<i>CMF as output by ACE</i>	<i>Pool CM as output by ACE (te)</i>	<i>‘Peaky’ evaporation rate derived from GASP output (kg/s)</i>	<i>Modified pool release duration derived from GASP output (s)</i>	<i>CMF as output by GASP</i>
1	0.73	13.2	0.19	0.27	191	1.38	0.954
10	7.3	17.1	0.30	2.7	240	11.02	0.818
100	73	163	0.31	27	521	42.63	0.716

CM: contaminant mass; CMF: contaminant mass fraction

The GASP results suggest almost instantaneous vaporisation of the pool occurs. The instantaneously released airborne puff component (ACE/DRIFT 3) in Figures 10 to 13 is therefore being compared against another instantaneous puff from the pool. For the airborne component, the initial expansion entrains a considerable amount of air into the cloud causing rapid dilution. The pool component does not experience the same expansion, and consequently the air entrainment in the vicinity of the pool is considerably less; it is behaving as a rapidly evaporating pool. Even though the mass of contaminant in the pool is smaller than the mass of contaminant in the airborne component, the lower dilution of the pool source produces isopleths that are similar in length to those obtained from the more dilute puff source. The rapid expansion of the airborne puff (ACE/DRIFT 3) release, however, causes wider isopleths to be generated for the airborne component than those produced for the pool component (ACE/GASP/DRIFT 3).

For the 100 te release in Table 10, ACE predicts that 73 te of the total mass becomes airborne and that the remainder, 27 te, forms a pool. ACE predicts that 163 te of air is entrained into the 73 te cloud, giving a contaminant mass fraction (CMF) of 0.31. The contaminant mass fraction is calculated using Equation 2:

$$CMF = \frac{CM}{CM + M_{air}} \quad \text{Equation 2}$$

where CMF is the contaminant mass fraction, CM is the contaminant mass of the airborne fraction (te), and M_{air} is the mass of air entrained (te).

For the 100 te release in Table 10, the 'peaky' evaporation rate predicted by GASP is 521 kg/s and lasts for 43 s. This is representative of a near-instantaneous vaporisation of approximately 22.4 te. The remaining 4.6 te released does not vaporise and remains on the ground to form the pool. The contaminant mass fraction is calculated by GASP based upon saturation at the pool surface and in this case is 0.716. Using a rearranged version of Equation 2, and setting the contaminant mass to the mass vaporised from the pool (22.4 te), the mass of air associated with the pool source is calculated to be 8.9 te. This difference in the dilution characteristics could explain why the maximum downwind extents of the isopleths are similar when the masses entering each of the puffs are dissimilar.

The chlorine results show that DRIFT 3 predicts isopleths of similar length for the pool and puff components for many of the scenarios modelled. For pool scenarios where material is released almost instantaneously (as in the chlorine results shown in this report), the time scales of this scenario and the airborne puff scenario are broadly similar i.e. both are short duration events. Any static receptor downwind is exposed to two puffs.

Ideally, the contributions from the airborne puff and the pool should be recombined and modelled together in DRIFT 3, but this is not currently possible. In most cases, the preferred approach is to model the puff and pool components separately and use the larger of the two sets of SLOT DTL isopleths for Hazardous Substances Consent assessment purposes. However, for the chlorine scenarios considered here, this may not be a cautious approach because any downwind receptor is exposed to two puffs that occur very close together, and these should be modelled concurrently.

When considering the risk from a release, the arc subtended by the isopleth at a specific distance from the release point is used to determine the probability of a person receiving the HSE Dangerous Dose at that distance from the release. The variation of the width of the isopleth with downwind distance, therefore, has a direct impact on the risk calculated from a release. The isopleth width is an important element to consider for any risk assessment undertaken.

The chlorine results show that much wider isopleths are produced for the airborne puff component, even for cases where the maximum downwind extent is less than that predicted for the pool component. This suggests that for the scenarios considered here, the results from the airborne puff modelling should be

used in preference to the pool dispersion results. Care would be required if the pool dispersion gave much larger downwind extents than the dispersion of the airborne puff.

4.3 SULPHUR DIOXIDE RELEASES

For the sulphur dioxide releases considered here, the airborne component (ACE/DRIFT 3) produces longer and wider isopleths than the pool component (ACE/GASP/DRIFT 3) for outdoor recipients in D4.3 weather conditions. Although not shown here, the same trend is observed for outdoor recipients in D2.4 and D6.7 weather. As shown in Table 11, the vaporisation rates for sulphur dioxide are relatively small (when compared to those for chlorine), which subsequently affects the size of the vapour cloud that is produced from the evaporating pool. A neutral atmosphere (Pasquill category D) enhances turbulence and causes rapid dilution of the sulphur dioxide vaporising from the pool, and even though most of the sulphur dioxide enters the pool (as shown in Table 11), smaller isopleths are produced from the pool than from the airborne puff. The airborne component is predicted to entrain larger amounts of air at the source than the pool component, but despite this, SLOT DTL isopleths with larger downwind extents are predicted for the airborne component than for the pool component.

Table 11 Results from ACE and GASP for a sulphur dioxide release in D4.3 weather

<i>Release mass (te)</i>	<i>Airborne CM (vapour and aerosol) as output by ACE (te)</i>	<i>Mass of air entrained in cloud as output by ACE (te)</i>	<i>CMF as output by ACE</i>	<i>Pool CM as output by ACE (te)</i>	<i>'Peaky' evaporation rate derived from GASP output (kg/s)</i>	<i>Modified pool release duration derived from GASP output (s)</i>	<i>CMF as output by GASP</i>
1	0.44	2.39	0.15	0.563	11	52.29	0.611
10	4.4	13.3	0.25	5.63	10	388.9	0.561
100	44	102	0.30	56.3	35	647.43	0.573

CM: contaminant mass; CMF: contaminant mass fraction

The pool component produces slightly longer isopleths than the airborne component for outdoor recipients in F2.4 weather. A combination of a stable atmosphere (Pasquill category F) and less turbulence in the release mechanism for the pool allows the vaporising sulphur dioxide from the pool to disperse farther downwind to the SLOT DTL compared to the airborne puff. For the airborne component, the air entrainment from the turbulent release mechanism sufficiently dilutes the cloud such that it does not disperse as far downwind as the vapour from the pool.

For indoor recipients, the airborne component (ACE/DRIFT 3) produces SLOT DTL isopleths for all but the 1 te release masses. The pool component (ACE/GASP/DRIFT 3) produces isopleths for all of the indoor cases. It is likely that the lack of indoor isopleths calculated for the airborne component of the 1 te releases is due to a combination of air entrainment, and the large SLOT DTL (4.655×10^6 ppm².min) of sulphur dioxide. For the small airborne puff released in this case, the air entrainment reduces the concentration of the cloud rapidly, so that in many cases, the toxicity criterion is never reached. The housing ventilation rates used by HSE (2 air changes per hour for this case) lead to low concentrations and doses indoors, and taking into account a cloud that has already been significantly diluted, no SLOT DTL isopleths are predicted for these cases. The pool scenarios modelled (ACE/GASP/DRIFT 3) do not experience the same rapid dilution and indoor recipient results are produced for all these cases.

For the airborne puff scenario, the toxic response is calculated based on a puff of material moving downwind. Any static receptor standing downwind will only receive a short duration exposure as the puff moves over the receptor. For the pool scenario, material is released at a steady rate over a longer release duration than the puff scenario, resulting in a longer exposure duration. Any static receptor will be exposed until the release ends and the remaining cloud passes over the receptor. For the same static person standing downwind, the timescales for the puff exposure and pool exposure are different. For

these scenarios, using the larger of the SLOT DTL isopleths in subsequent risk calculations seems appropriate, but this means that the static person is only exposed to material released from one scenario rather than the two. The exposure from either the puff or the pool is neglected from the dose calculation.

Combining the contributions from the puff and pool components of a single release is an area under development in DRIFT and will be made available in future versions of the model.

4.4 AMMONIA RELEASES

For the ammonia releases considered here, the pool component (ACE/GASP/DRIFT 3) produces isopleths for most cases except for the 1 te release masses for indoor recipients. However, the indoor isopleths calculated from modelling the dispersion of the pool are circular in shape with the same dimensions as the pool source. This indicates that to receive the ammonia SLOT DTL, an indoor recipient would have to be located within or directly above the pool.

The airborne component (ACE/DRIFT 3) produces SLOT DTL isopleths for outdoor recipients for all the ammonia releases considered here, apart from the 1 te release in D4.3 weather. No isopleths were generated for indoor recipients from any of the airborne component dispersion modelling in DRIFT 3. If the initial phases of the instantaneous release modelled by ACE were included in the isopleth calculation then there is a possibility that isopleths could be generated for these cases. However, any isopleth generated using ACE would be small (less than the puff/pool size output by ACE).

Table 12 shows that, of the three sets of pressure-liquefied releases examined (chlorine, sulphur dioxide and ammonia), the ammonia releases entrain the most air. When measured at the saturation temperature, ammonia has a larger latent heat of vaporisation (1337 kJ/kg) than sulphur dioxide (402 kJ/kg) and chlorine (286 kJ/kg); this means ammonia requires a much larger amount of energy to convert from liquid droplets to vapour.

Ammonia has a large SLOT DTL (3.78×10^8 ppm².min), so that in some cases, the toxicity criterion is never reached and isopleths are not produced. This, together with the large latent heat of vaporisation of ammonia, explains why no significant SLOT DTL isopleths are produced for indoor recipients for the ammonia scenarios modelled here.

Table 12 Results from ACE and GASP for an ammonia release in D4.3 weather

<i>Release mass (te)</i>	<i>Airborne CM (vapour and aerosol) as output by ACE (te)</i>	<i>Mass of air entrained in cloud as output by ACE (te)</i>	<i>CMF as output by ACE</i>	<i>Pool CM as output by ACE (te)</i>	<i>'Peaky' evaporation rate derived from GASP output (kg/s)</i>	<i>Modified pool release duration derived from GASP output (s)</i>	<i>CMF as output by GASP</i>
1	0.72	17.3	0.04	0.281	89	3.14	0.578
10	7.2	111	0.06	2.81	115	24.26	0.325
100	72	755	0.09	28.1	140	99.33	0.299

CM: contaminant mass; CMF: contaminant mass fraction

For outdoor recipients, DRIFT 3 predicts much wider SLOT DTL isopleths for the airborne puff than for the pool component of an ammonia release. For the 100 te release, DRIFT 3 also predicts that the SLOT DTL isopleths for the airborne puff will have a larger downwind extent than the isopleths generated for the pool component. For the 10 te release, however, the SLOT DTL isopleths for the pool component are predicted to extend further downwind than the SLOT DTL isopleths for the puff component. For example, in D4.3 weather conditions, Figure 32 shows that the pool component of the 10 te release generates an isopleth that extends 217 m downwind; the puff component isopleth extends 97 m downwind.

In this case, there could be an underestimation of the risk from the release in the far field if the puff results are used in subsequent risk calculations because the harmful effects of the pool component extend further downwind than those from the puff component. Using the pool component results in the risk calculations could lead to an underestimation of the risk in the near field since, close to the source, the harmful effects of the pool component do not extend as wide as those from the puff component.

Combining the maximum isopleth dimensions of the two release components, i.e. using the maximum width from the puff and the maximum downwind extent from the pool, could provide an interim solution for these small number of cases until a more robust method of combining the puff and pool components is developed in the DRIFT model. The use of a combined isopleth for the risk calculation would give a reasonable estimation of the risk in the near field and may be slightly cautious in some parts of the far field.

5 HEATED RELEASES

In process vessels and reactors, liquids are actively heated to above their normal boiling point temperature, but may remain in the liquid state due to the pressure. DRIFT 3 has been shown to handle pressure-liquefied gases well, and the set of scenarios presented in this section shows how it handles substances that are heated.

The substances given in Table 13 are liquid at standard atmospheric temperature and pressure. To represent process vessel or reactor failures, the materials are assumed to be stored at a temperature that gives a saturation vapour pressure of 4 barg (bar gauge pressure). The gauge pressure is the pressure above atmospheric and can also be written as 5 bar absolute, which is equivalent to a pressure of 5×10^4 Pa.

Table 13 Heated release scenarios at 5×10^4 Pa

<i>Substance</i>	<i>Storage temperature (K)</i>	<i>Normal boiling point (K)</i>	<i>Vapour pressure at 293 K (Pa)</i>	<i>SLOT DTL (ppm.min)</i>
Methyl chloroformate	398	343	11318	1320
Propionitrile	434	370	4772	4900
2-chloroethanol	458	402	700	1920

Similar input conditions to the pressure-liquefied gas scenarios were used: release masses of 1 te, 10 te and 100 te were chosen and the same weather conditions (D2.4, D4.3, D6.7 and F2.4) were used. Only results for D4.3 weather for an outdoor recipient and F2.4 weather for an indoor recipient are plotted for the heated releases in the following sections.

The substances in Table 13 were chosen based on their volatility and toxicity. Liquids with low volatility have a lower vapour pressure and a higher normal boiling point than those with high volatility. For example, 2-chloroethanol is a substance with low volatility and propionitrile is one with moderate volatility. There are substances, such as methyl chloride, which have much larger vapour pressures than methyl chloroformate. However, prior to 2015 when CHIP (Chemical (Hazard Information and Packaging)) classification [35] was still in use for Hazardous Substances Consent, methyl chloroformate was used frequently as an exemplar for very toxic liquids, and has therefore been chosen to represent substances with high volatility here. Under CHIP classification, propionitrile was a toxic liquid and methyl chloroformate and 2-chloroethanol were very toxic liquids [35]. Since 2015, HSE has reviewed the exemplars used due to changes in the classification categories in the Planning (Hazardous Substances) Regulations 2015 [3]. These regulations also include the implementation of the CLP (Classification, Labelling and Packaging) harmonised classification [36], which removes the Toxic and Very Toxic categories and introduces exposure route categories, such as inhalation, and health hazard categories, such as carcinogenicity. Although the exemplars have changed, this does not affect the conclusions of this work.

All the substances chosen in Table 13 have low SLOT DTL values (i.e. a relatively low concentration/exposure combination that leads to a person receiving the HSE Dangerous Dose), which could potentially result in very large isopleths. The use of these substances illustrates the behaviour of the DRIFT 3 model in the very far field. All the substances in Table 13 have a toxic exponent of $n = 1$ [25]. The pool evaporation methodology used by HSE [21] was followed for the pool formation scenarios.

This section presents a small selection of representative results for the substances in Table 13. The figures show results for both the airborne puff component (modelled using ACE and DRIFT 3) and the pool

component (modelled using ACE, GASP and DRIFT 3) to illustrate how DRIFT 3 handles heated releases. The ACE outputs for these scenarios are presented in Appendix 3.

5.1 METHYL CHLOROFORMATE

Figures 37 and 38 show example DRIFT 3 isopleths for instantaneous releases of methyl chloroformate. For these scenarios, SLOT DTL isopleths were produced for both the pool (modelled using ACE, GASP and DRIFT 3) and the airborne puff (modelled using ACE and DRIFT 3) components.

For methyl chloroformate, the SLOT DTL isopleths predicted for the airborne puff are significantly larger than those predicted for the pool component.

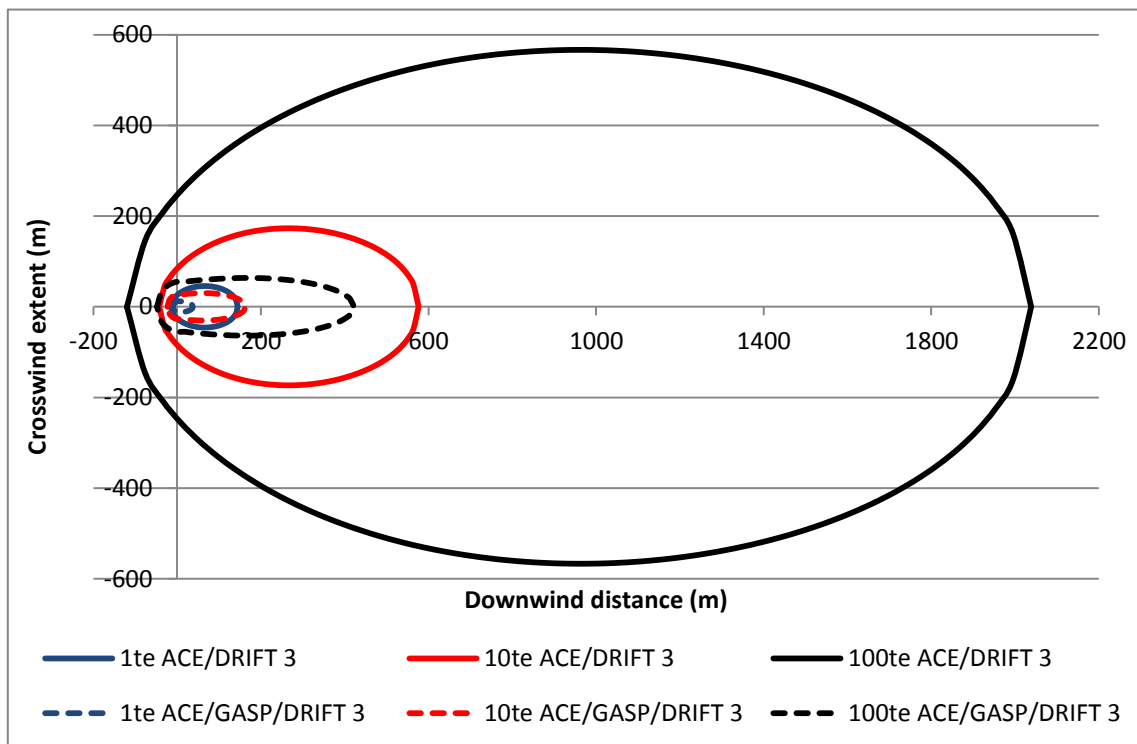


Figure 37 SLOT DTL isopleths obtained for instantaneous methyl chloroformate releases in D4.3 weather for an outdoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

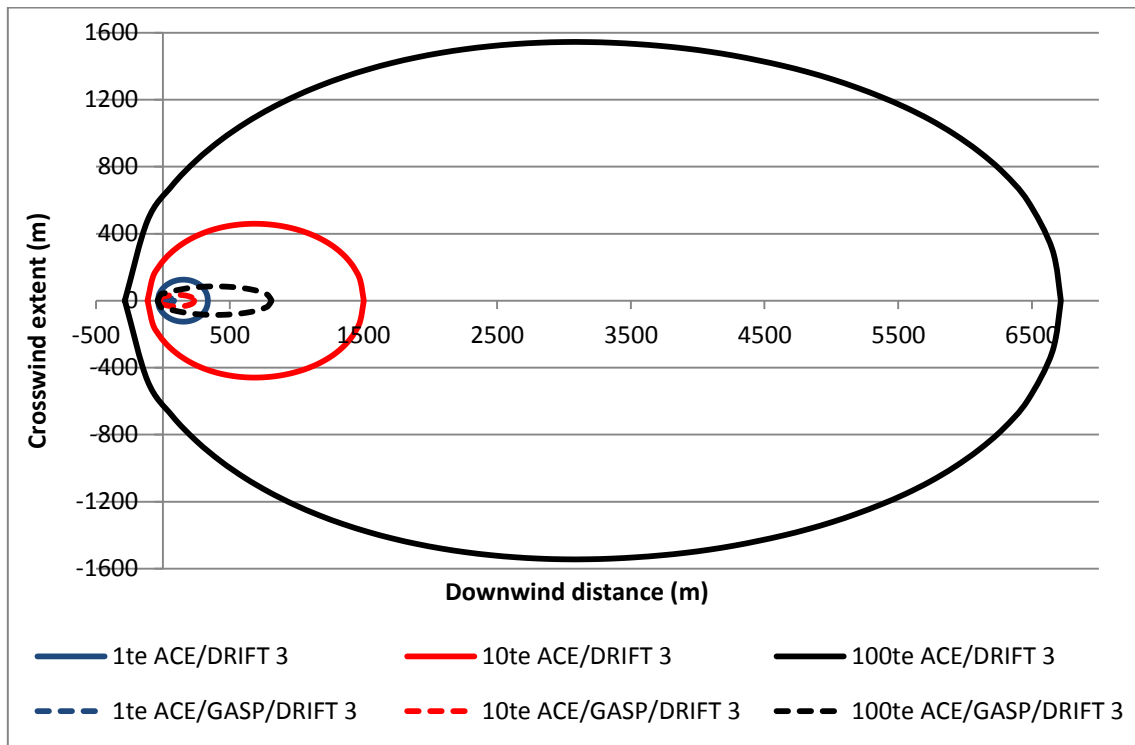


Figure 38 SLOT DTL isopleths obtained for instantaneous methyl chloroformate releases in F2.4 weather for an indoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

5.2 PROPIONITRILE

Figures 39 and 40 show example DRIFT 3 isopleths for instantaneous releases of propionitrile. For these scenarios, the models produced SLOT DTL isopleths for all the source terms except for the 1 te ACE generated source term in D4.3 weather.

ACE predicts that only a small fraction of the released material (approximately 6%) will enter the pool, but because propionitrile is moderately volatile, sufficient material is evaporated to give small SLOT DTL isopleths for the pool component.

In general, releases of propionitrile are best represented by the initial puff component (modelled using ACE and DRIFT 3) because it produces the larger isopleths when measured to the SLOT DTL harm criterion. However, the GASP source term may be appropriate for representing small release masses where the ACE source term does not produce isopleths for the SLOT DTL (e.g. the 1 te release in D4.3 weather).

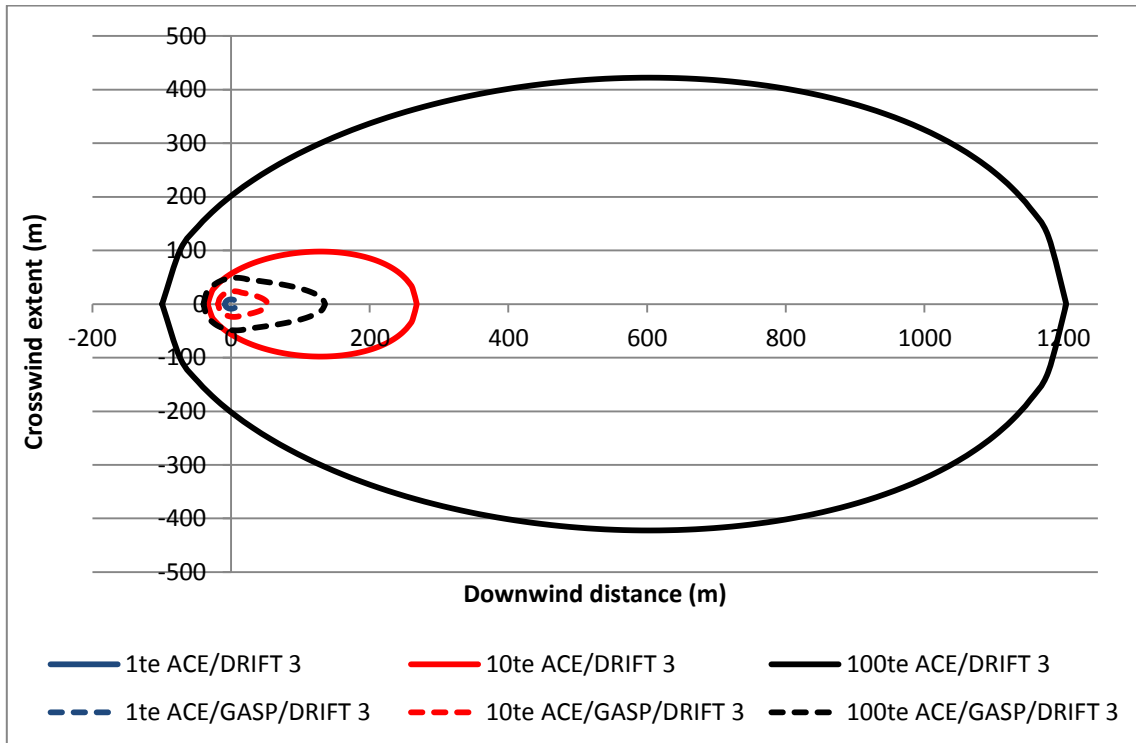


Figure 39 SLOT DTL isopleths obtained for instantaneous propionitrile releases in D4.3 weather for an outdoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

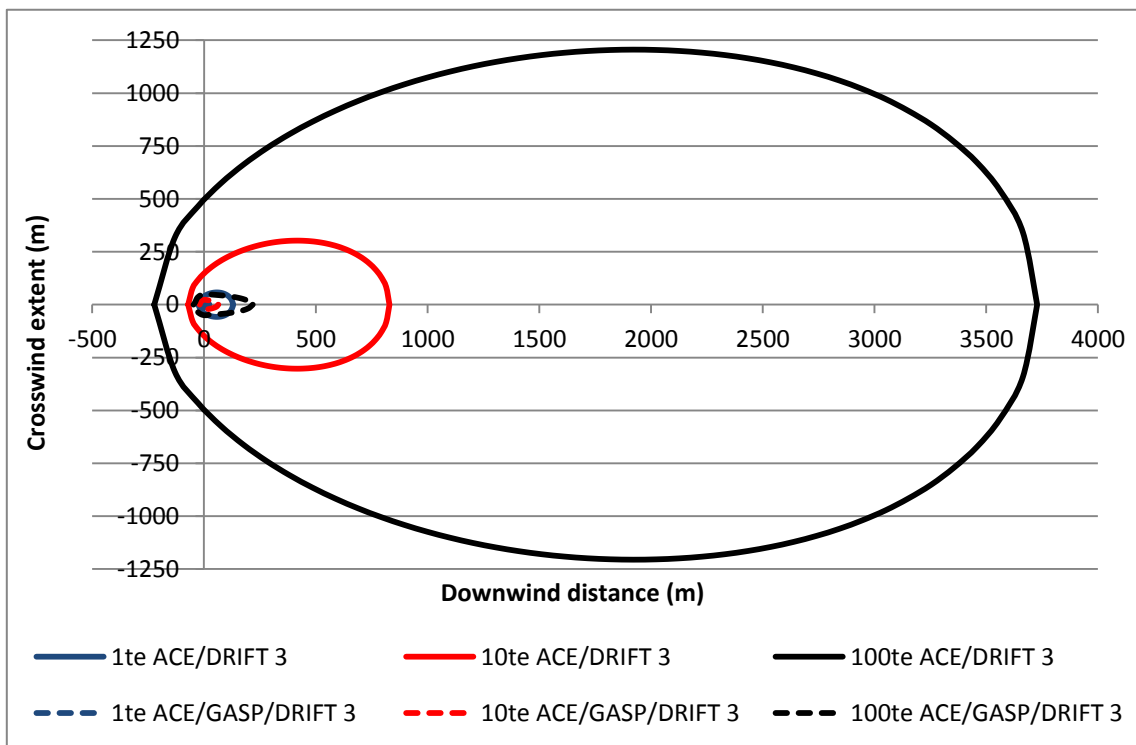


Figure 40 SLOT DTL isopleths obtained for instantaneous propionitrile releases in F2.4 weather for an indoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

5.3 2-CHLOROETHANOL

Figures 41 and 42 show DRIFT 3 isopleths for instantaneous releases of 2-chloroethanol. For these scenarios, SLOT DTL isopleths were produced for all of the GASP and ACE generated source terms, although this is difficult to see on the figures due to the scale. The initial airborne component (modelled using ACE and DRIFT 3) produces significantly larger isopleths than the pool component (modelled using ACE, GASP and DRIFT 3).

For the 2-chloroethanol releases, ACE predicts that the majority of the released material (approximately 80%) will enter the airborne puff; it mostly consists of vapour because there is minimal aerosol present. For the material that enters the pool, DRIFT 3 produces small isopleths because 2-chloroethanol has low volatility.

For 2-chloroethanol, an ACE generated source term is of more significance than the pool generated source term calculated by GASP.

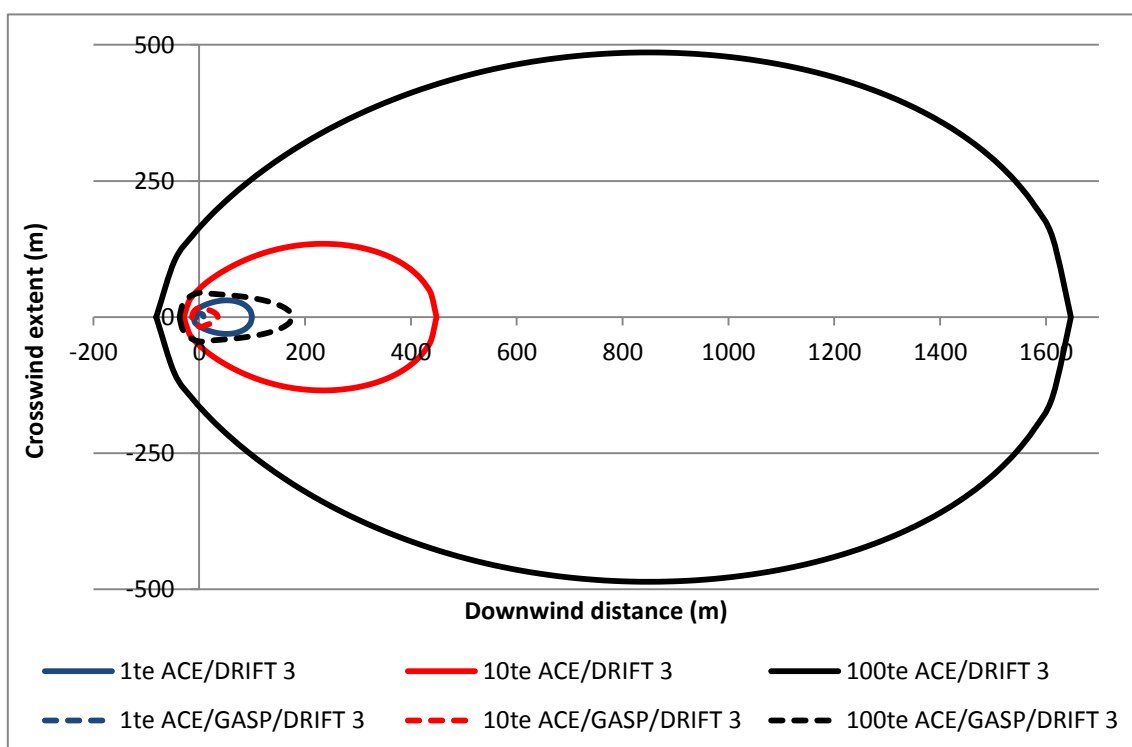


Figure 41 SLOT DTL isopleths obtained for instantaneous 2-chloroethanol releases in D4.3 weather for an outdoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

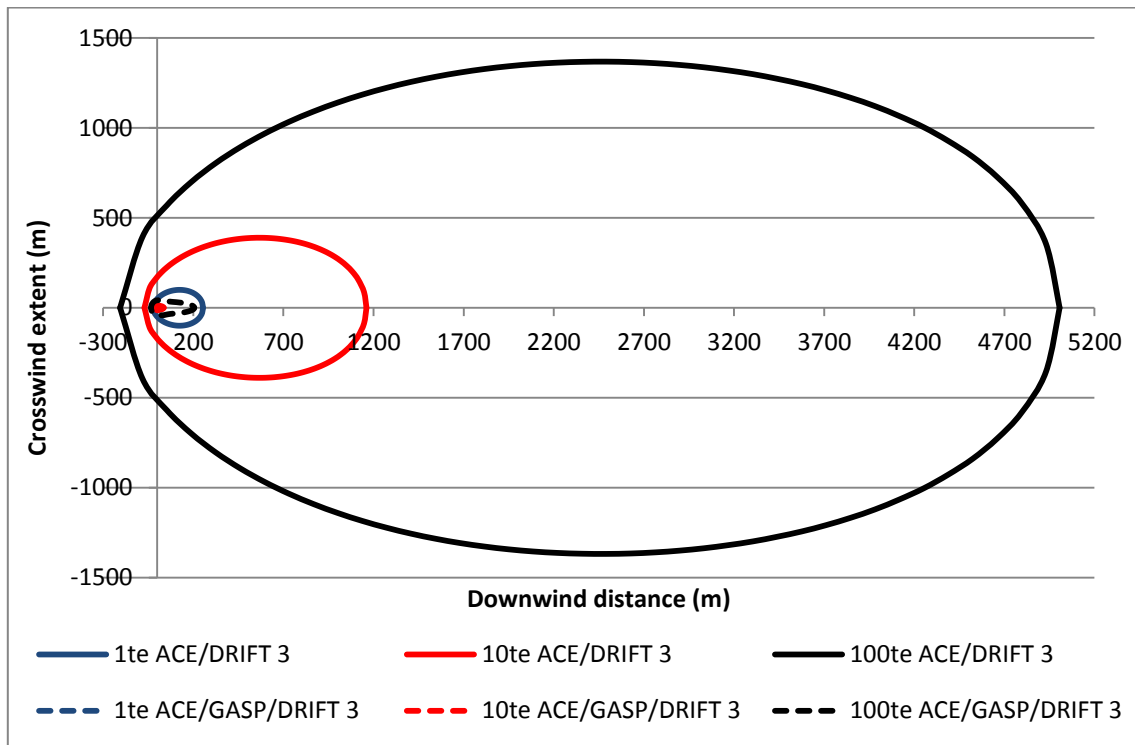


Figure 42 SLOT DTL isopleths obtained for instantaneous 2-chloroethanol releases in F2.4 weather for an indoor recipient. The results show dispersion of the airborne puff (ACE/DRIFT 3) and pool (ACE/GASP/DRIFT 3) components.

5.4 CONCLUSIONS FOR HEATED RELEASES

Figures 37 to 42 show that the source term models, ACE and GASP, and the dispersion model DRIFT 3 are suitable for use when modelling superheated liquid releases.

The airborne component (ACE/DRIFT 3) produces larger (length and width) SLOT DTL isopleths than the pool component (ACE/GASP/DRIFT 3) for all the presented scenarios. This is because the substances are stored above their normal boiling point temperatures in the form of a saturated liquid. On release, the substances rapidly flash to vapour leaving minimal liquid material available to form a pool.

6 CONCLUSIONS

The DRIFT dispersion model was developed for HSE by ESR Technology. DRIFT version 3 (DRIFT 3) has recently been released [6] and contains many additions and modelling enhancements over DRIFT 2.31, the version previously used by HSE.

HSE will use DRIFT 3 in its assessment of the hazards and risks posed by toxic and flammable substances stored at major hazards sites. To ensure that DRIFT 3 is fit for purpose, a programme of work is being undertaken at HSE. This includes an evaluation of the dispersion modelling capabilities of DRIFT 3 and an assessment of the performance of DRIFT 3 for modelling the types of release scenario typically considered by HSE for Hazardous Substances Consent assessments.

This report presents an assessment of the use of DRIFT 3.6.14 for modelling the dispersion of flashing instantaneous releases of toxic pressure-liquefied gases such as chlorine, sulphur dioxide and ammonia. Releases of superheated liquids from heated process vessels and reactors have also been considered.

The proposed methodology for modelling releases from catastrophic failures of vessels storing toxic pressure-liquefied gases using DRIFT 3 has been described. The modelling recommendations were made in consultation with the developers of the model and experts within HSE.

The purpose of this study was to compare the previous HSE methodology for modelling flashing instantaneous releases (using the in-house IRATE source term model with the DENZ dispersion model [8]) with the new methodology that has been proposed in this report (using the ACE source term model [30] with the DRIFT 3 dispersion model). SLOT DTL isopleths produced using the two methodologies were compared, to assess the impact of adopting ACE and DRIFT 3 on HSE's land-use-planning advice.

An intermediate step between the previous and new methods was also reviewed. The effect of using the same source term model (IRATE) but changing the dispersion model from DENZ (IRATE/DENZ) to DRIFT 3 (IRATE/DRIFT 3) was examined. The purpose of this was to observe how the model outputs are affected when only the dispersion model is changed. The results from IRATE/DRIFT 3 were also compared to the results from the new methodology (ACE/DRIFT 3), to illustrate the effect of changing the source term model.

The ACE source term model can account for rainout and subsequent pool formation. The spreading and vaporisation of the pool predicted by ACE can be modelling using GASP [15], which can generate a source term for use in DRIFT 3. Comparisons have been made between the SLOT DTL isopleths predicted by DRIFT 3 for the initial airborne puff (modelled in ACE and DRIFT 3) and for the pool component of the release (modelled in ACE, GASP and DRIFT 3).

The test scenarios were based on substances available in DENZ: chlorine, sulphur dioxide and ammonia. The mass of substance released was based on the size of vessels present at small- and large-scale chlorine facilities.

In process vessels and reactors, liquids are actively heated to above their normal boiling point temperature, but may remain in the liquid state due to elevated pressure. Heated releases of methyl chloroformate, propionitrile and 2-chloroethanol were modelled in DRIFT 3, to test the performance of the model when considering releases of superheated liquids. The SLOT DTL isopleths obtained for the airborne component (modelled using ACE and DRIFT 3) and the pool component (modelled using ACE, GASP and DRIFT 3) of each heated release were compared. The same release masses and weather conditions were assumed as for the releases of pressure-liquefied gases.

Considering all the results presented in this report, the following conclusions can be made:

- ACE has been identified as a suitable source term model to replace IRATE.
- For the releases of chlorine, sulphur dioxide and ammonia considered in this study, the SLOT DTL isopleths generated using ACE and DRIFT 3 have smaller maximum downwind extents than the SLOT DTL isopleths generated using IRATE and DENZ. Close agreement between the predicted isopleths should not necessarily be expected because there are significant differences between the modelling assumptions used in the two methodologies. DRIFT 3 contains a more sophisticated passive dispersion model than DENZ, and the smooth transition from dense to passive behaviour in DRIFT 3 is an improvement on the abrupt transition in DENZ.
- For many of the chlorine, sulphur dioxide and ammonia releases presented here, the initial airborne component (modelled in ACE and DRIFT 3) and the pool component (modelled in ACE, GASP and DRIFT 3) produce SLOT DTL isopleths that are similar in length. However, for most scenarios, the isopleths for the airborne component are significantly wider than the isopleths generated for the pool component.
- For ammonia, no significant SLOT DTL isopleths were produced for indoor recipients when using DRIFT 3.
- ACE, GASP and DRIFT 3 are suitable for modelling flashing heated instantaneous releases, as well as pressure-liquefied instantaneous releases.
- For all the presented heated scenarios, the airborne component (modelled in ACE and DRIFT 3) produces longer and wider SLOT DTL isopleths than the pool component (modelled in ACE, GASP and DRIFT 3).

6.1 COMPARISON OF THE AIRBORNE AND POOL COMPONENTS

There is currently no option within the DRIFT 3 tool that allows the pool and puff components of a release to be combined in a single run to produce a combined set of SLOT DTL isopleths. This option is under development and will be made available in future versions of DRIFT. Until this option becomes available, a judgement must be made about which set of SLOT DTL isopleths (puff or pool) should be used in subsequent risk calculations. In most cases, the preferred approach is to use the larger of the two sets of SLOT DTL isopleths for Hazardous Substances Consent assessment purposes, noting that this may not give a cautious estimate of the overall risk if the isopleths are similar in size.

For many of the scenarios modelled, the SLOT DTL isopleths generated from the initial airborne puff have a similar maximum downwind extent to those generated from the pool component of the release. In all cases, however, the isopleths generated for the airborne puff are much wider than those generated for the pool component. The width of the isopleth at a downwind distance determines the proportion of an area within which a person at that distance would receive harm from a release and is directly used in the calculation of the risk levels. This suggests that the SLOT DTL isopleths from the airborne puff should be used in the subsequent risk calculations for the scenarios modelled in this study.

Care is required, however, if the isopleths for the pool component have a significantly longer downwind extent than the isopleths generated for the airborne puff, as is the case for some of the ammonia scenarios considered in this report. In such cases, combining the maximum isopleth dimensions of the two release components, i.e. using the maximum width from the puff and the maximum downwind extent from the pool, could provide an interim solution until a more robust method of combining the puff and pool components is developed in the DRIFT model. The use of a combined isopleth for the risk calculation would give a reasonable estimation of the risk in the near field and may be slightly cautious in some parts of the far field.

Other considerations related to the use of a combined isopleth include:

- As the HSE Dangerous Dose criterion is for a person receiving the SLOT DTL, or greater, then once a person has received the SLOT DTL then they cannot 'receive' this dose again at the same location. This means that care has to be taken to avoid double counting the effects of a release.
- There are areas where a person will not receive the SLOT DTL from either the puff or the pool component but might receive this criterion dose if the doses from the puff and pool components are combined.
- Any consideration of the impact of the different durations of the puff component and the longer-duration pool component would require a review of current assumptions on indoor and outdoor occupancy and evacuation times from buildings.

Combining the contributions from the puff and pool components of a single release is an area under development in DRIFT and will be made available in future versions of the model.

6.2 OUTCOMES

As a result of this work, ACE and DRIFT 3.6.14 have now been adopted by HSE to model flashing instantaneous releases of toxic substances. ACE and DRIFT 3.6.14 have therefore replaced IRATE, DENZ and DRIFT 2.31 for use in Hazardous Substances Consent assessments relating to such substances.

For flashing instantaneous releases, both the initial airborne component of the release (consisting of vapour and entrained liquid droplets) and the component that rains out to form a pool may contribute to the overall risk posed by the release. For the purposes of Hazardous Substances Consent assessment, the contribution from the pool component is modelled in ACE, GASP and DRIFT 3.6.14.

DRIFT 3.6.14 does not have the capability to combine the puff and pool components of a release into a single run to produce a combined set of SLOT DTL isopleths. Therefore, for the purposes of Hazardous Substances Consent assessment, the preferred approach is to use the larger of the two sets of SLOT DTL isopleths in the subsequent risk calculations. For ammonia scenarios which produce short, wide isopleths for the puff component and long, narrow isopleths for the pool component, an alternative option is to combine the maximum isopleth dimensions of the two release components i.e. to use the maximum isopleth width from the puff component and the maximum downwind extent from the pool component in the risk calculations.

ACE, GASP and DRIFT 3.6.14 have also been adopted by HSE for modelling superheated liquid releases of toxic substances.

7 APPENDICES

7.1 APPENDIX 1 – ACE SOURCE TERM FLOWCHART

Figure 43 is a flowchart that describes the method that should be used to calculate the source term and subsequent dispersion of flashing instantaneous releases when using the ACE, GASP and DRIFT 3 models. ACE version 3.15 was used for this work. ACE creates a text file that contains the inputs used and the outputs that are generated (a .ACE file). ACE also outputs DRIFT 2 and DRIFT 3 compatible input files.

DRIFT 2 input files are text files that contain input information associated with DRIFT 2 keywords (.DIN files). DRIFT 3 input files are Markup Language format files that contain the input information in a structured format (.DRIFT files). The GASP model can write outputs generated in a DRIFT 2 (.DIN) input file format. DRIFT 3 can read legacy DRIFT 2 (.DIN) input files.

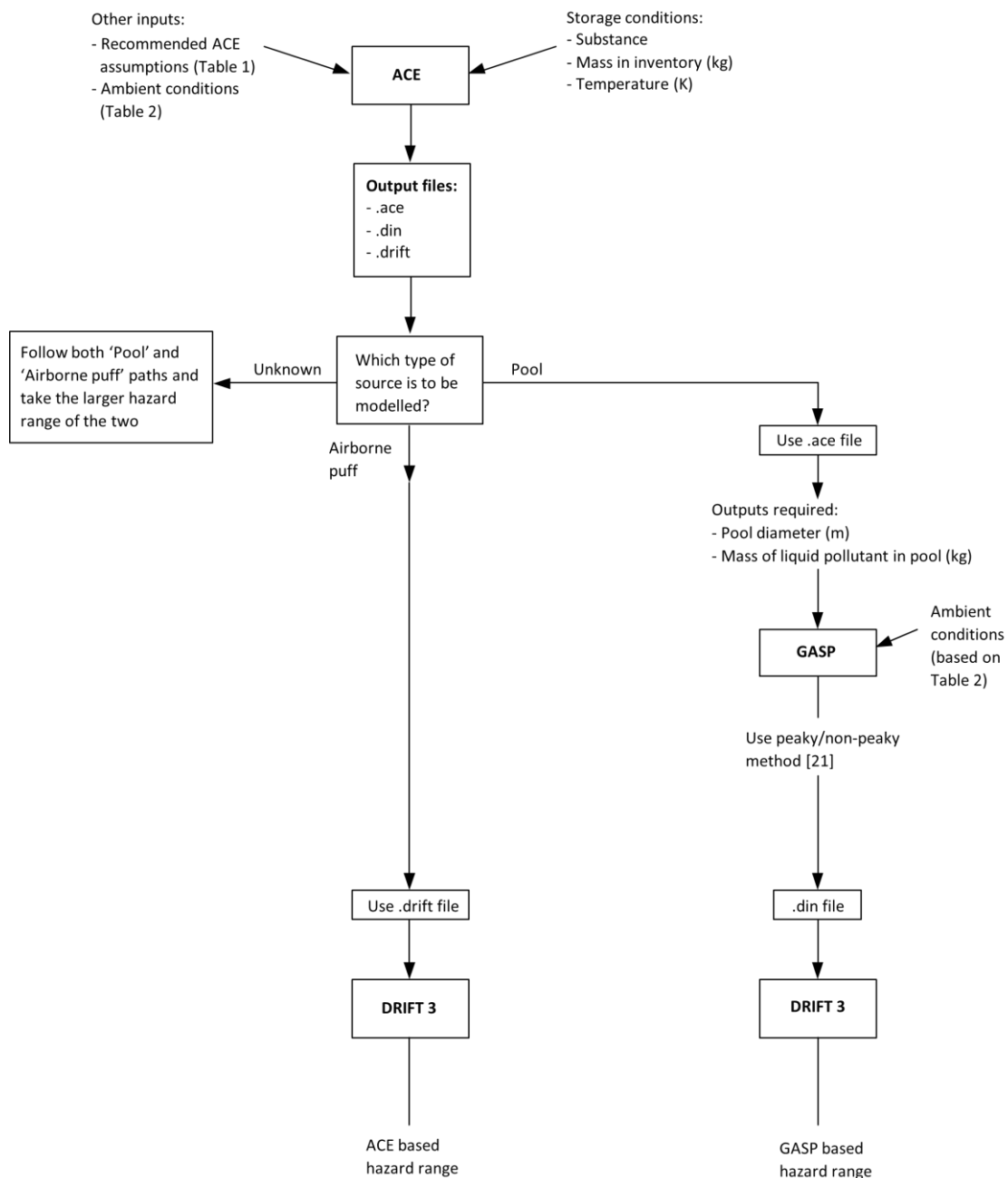


Figure 43 Method flowchart for modelling flashing instantaneous releases

7.2 APPENDIX 2 – GASP INPUTS

Table 14 shows example GASP inputs for 100 te releases of chlorine, sulphur dioxide and ammonia in D4.3 weather. GASP inputs for 100 te releases of heated substances in D4.3 weather are shown in Table 15. The remaining GASP inputs can be set to the same values as the recommended DRIFT 3 inputs given in Table 2.

For each scenario where pool generated source terms are required, ACE outputs the pool diameter and the pool mass (shown in Tables 16 to 18 in Appendix 3), which are used as inputs to GASP. ACE does not output the pool temperature, so the release temperature in GASP is set to just below the substance boiling point temperature.

The GASP inputs for the remaining release masses (1 te, 7.5 te, 10 te, 15 te and 50 te) and weather conditions (D2.4, D6.7 and F2.4) are not shown here but are set up using similar assumptions.

A description of the GASP methodology can be found in Cruse et al. [21]. The DRIFT input (.DIN) file output by GASP can be opened within DRIFT 3 and used to generate isopleth results. If the release meets the HSE ‘peaky’ criteria, then the DRIFT input (.DIN) file output by GASP needs to be amended by the user to include the calculated ‘peaky’ vaporisation rates prior to being input to DRIFT 3 [21].

Table 14 GASP inputs for flashing instantaneous releases of pressure-liquefied substances. Applicable for a release mass of 100 te and D4.3 weather.

<i>Input</i>	<i>Chlorine</i>	<i>Sulphur dioxide</i>	<i>Ammonia</i>
Bund radius (m)	50	50	50
Puddle depth (m)	0.0082	0.011	0.011
Release type	Instantaneous	Instantaneous	Instantaneous
Pool mass (kg)	26700	56300	28100
Pool radius (m)	20.16	17.25	33.14
Release temperature (K)	238.4	261.9	239.4
Release constraints	Pool vaporisation time limited to 1800 s	Pool vaporisation time limited to 1800 s	Pool vaporisation time limited to 1800 s

Table 15 GASP inputs for instantaneous releases of heated substances. Applicable for a release mass of 100 te and D4.3 weather.

<i>Input</i>	<i>Methyl chloroformate</i>	<i>Propionitrile</i>	<i>2-chloroethanol</i>
Bund radius (m)	50	50	50
Puddle depth (m)	0.0057	0.0061	0.0082
Release type	Instantaneous	Instantaneous	Instantaneous
Pool mass (kg)	7630	6140	22000
Pool radius (m)	23.81	29.77	23.71
Release temperature (K)	343.64	370.24	400.85
Release constraints	Pool vaporisation time limited to 1800 s	Pool vaporisation time limited to 1800 s	Pool vaporisation time limited to 1800 s

7.3 APPENDIX 3 – ACE OUTPUTS

ACE was set up according to the recommendations in Section 2 and the scenarios specified in Table 3.

Tables 16 to 18 show the ACE outputs for releases of chlorine, sulphur dioxide and ammonia. They are applicable to scenarios in D4.3 weather conditions with a storage temperature and ambient temperature of 288.15 K. The ACE outputs for scenarios in D2.4, D6.7 and F2.4 weather conditions are not shown here.

Tables 19 to 21 show the ACE outputs for heated releases of methyl chloroformate, propionitrile and 2-chloroethanol. As before, these results are applicable to D4.3 scenarios; the D2.4, D6.7 and F2.4 scenarios are not shown here.

Referring to Figure 43 in Appendix 1, the DRIFT input (.DRIFT) file created by ACE can be opened directly within DRIFT 3 and run for airborne releases. Where prediction of the pool component is required, the relevant ACE outputs are used as inputs to GASP; Appendix 2 provides further information on the modelling of the pool in GASP.

Table 16 ACE outputs for flashing instantaneous releases of chlorine in D4.3 weather

<i>Amount released (te)</i>	1	7.5	10	15	50	100
<i>Vapour mass (kg)</i>	493	2020	2140	2660	8870	17,700
<i>Cloud radius (m) and pool diameter (m)</i>	10.61	17.58	18.95	21.43	32	40.32
<i>Cloud temperature (K)</i>	259.76	272.13	279.53	285.15	285.19	285.2
<i>Aerosol fraction (kg/kg)</i>	0.061	0.18	0.21	0.24	0.24	0.24
<i>Aerosol mass (kg)</i>	240	3491	5194	8319	27,730	55,696
<i>Airborne mass (kg)</i>	3930	19,500	24,500	35,400	118,000	236,000
<i>Mass of liquid pollutant in pool (kg)</i>	267	2000	2670	4000	13,300	26,700
<i>Initial flash fraction</i>	0.17	0.17	0.17	0.17	0.17	0.17
<i>Mass of air entrained into cloud (kg)</i>	3200	14,000	17,100	24,400	81,400	163,000
<i>Droplet mass (kg)</i>	240	3480	5200	8330	27,800	55,600

Table 17 ACE outputs for flashing instantaneous releases of sulphur dioxide in D4.3 weather

Amount released (te)	1	7.5	10	15	50	100
Vapour mass (kg)	173	1000	1240	1620	4500	9000
Cloud radius (m) and pool diameter (m)	9.71	16.16	17.32	19.05	27.37	34.48
Cloud temperature (K)	274.26	275.68	277.27	280.97	286.56	286.57
Aerosol fraction (kg/kg)	0.094	0.16	0.18	0.21	0.24	0.24
Aerosol mass (kg)	265	2286	3133	4920	17,399	34,894
Airborne mass (kg)	2830	14,200	17,700	24,000	72,800	146,000
Mass of liquid pollutant in pool (kg)	563	4220	5630	8440	28,100	56,300
Initial flash fraction	0.09	0.09	0.09	0.09	0.09	0.09
Mass of air entrained into cloud (kg)	2390	10,900	13,300	17,500	50,900	102,000
Droplet mass (kg)	265	2280	3130	4940	17,400	34,700

Table 18 ACE outputs for flashing instantaneous releases of ammonia in D4.3 weather

Amount released (te)	1	7.5	10	15	50	100
Vapour mass (kg)	494	3290	4250	6040	16,100	27,300
Cloud radius (m) and pool diameter (m)	18.62	31.93	34.49	38.49	53.94	66.27
Cloud temperature (K)	263.11	257.79	257.63	257.9	263.03	268.65
Aerosol fraction (kg/kg)	0.013	0.023	0.025	0.029	0.044	0.054
Aerosol mass (kg)	225	2106	2950	4740	19,890	44,658
Airborne mass (kg)	18,000	93,200	118,000	164,000	450,000	827,000
Mass of liquid pollutant in pool (kg)	281	2110	2810	4210	14,000	28,100
Initial flash fraction	0.17	0.17	0.17	0.17	0.17	0.17
Mass of air entrained into cloud (kg)	17,300	87,800	111,000	153,000	414,000	755,000
Droplet mass (kg)	225	2100	2940	4750	19,900	44,600

Table 19 ACE outputs for flashing instantaneous releases of heated methyl chloroformate in D4.3 weather

<i>Amount released (te)</i>	1	10	100
<i>Vapour mass (kg)</i>	763	4620	27,000
<i>Cloud radius (m) and pool diameter (m)</i>	12.86	23.03	47.61
<i>Cloud temperature (K)</i>	268.47	276.68	292.55
<i>Aerosol fraction (kg/kg)</i>	0.025	0.11	0.18
<i>Aerosol mass (kg)</i>	161	4617	65,331
<i>Airborne mass (kg)</i>	6550	40,500	357,000
<i>Mass of liquid pollutant in pool (kg)</i>	76.3	763	7630
<i>Initial flash fraction</i>	0.27	0.27	0.27
<i>Mass of air entrained into cloud (kg)</i>	5630	31,200	265,000
<i>Droplet mass (kg)</i>	161	4610	65,300

Table 20 ACE outputs for flashing instantaneous releases of heated propionitrile in D4.3 weather

<i>Amount released (te)</i>	1	10	100
<i>Vapour mass (kg)</i>	892	7980	32,900
<i>Cloud radius (m) and pool diameter (m)</i>	17.27	31.41	59.53
<i>Cloud temperature (K)</i>	273.08	268.54	290.78
<i>Aerosol fraction (kg/kg)</i>	0.0032	0.016	0.1
<i>Aerosol mass (kg)</i>	47	1403	60,932
<i>Airborne mass (kg)</i>	14,400	90,500	613,000
<i>Mass of liquid pollutant in pool (kg)</i>	61.4	614	6140
<i>Initial flash fraction</i>	0.28	0.28	0.28
<i>Mass of air entrained into cloud (kg)</i>	13,500	81,100	519,000
<i>Droplet mass (kg)</i>	46.6	1400	60,900

Table 21 ACE outputs for flashing instantaneous releases of heated 2-chloroethanol in D4.3 weather

<i>Amount released (te)</i>	1	10	100
<i>Vapour mass (kg)</i>	609	4360	19,500
<i>Cloud radius (m) and pool diameter (m)</i>	13.16	23.81	47.42
<i>Cloud temperature (K)</i>	269.56	272.53	296.84
<i>Aerosol fraction (kg/kg)</i>	0.025	0.08	0.17
<i>Aerosol mass (kg)</i>	171	3436	58,638
<i>Airborne mass (kg)</i>	6820	42,900	337,000
<i>Mass of liquid pollutant in pool (kg)</i>	220	2200	22,000
<i>Initial flash fraction</i>	0.19	0.19	0.19
<i>Mass of air entrained into cloud (kg)</i>	6040	35,100	259,000
<i>Droplet mass (kg)</i>	171	3440	58,500

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HSE uses gas dispersion modelling in its assessment of the hazards and risks posed by toxic and flammable substances stored at major hazards sites. To update its dispersion modelling capability, HSE commissioned ESR Technology to develop a new version of the gas dispersion model DRIFT. The new version, DRIFT 3, includes a significant number of modelling enhancements over the version previously used within HSE (DRIFT 2.31). These include the extension of the model to treat buoyant plumes and time varying releases. Before DRIFT 3 is adopted for use by HSE, it must undergo thorough evaluation and assessment for a range of release scenarios. The initial phases of the DRIFT 3 testing programme used DRIFT 3.6.4 and are described in reports RR1100 and RR1101. Further testing is described in four reports including this one: RR1165, RR1166, RR1167 and RR1168. The four reports cover the evaluation of the model and assessment for a range of scenarios using the enhanced version DRIFT 3.6.14.

This report describes an assessment of the performance of DRIFT 3.6.14 for modelling the dispersion of flashing instantaneous releases of toxic substances. Releases of toxic pressure-liquefied gases such as chlorine, sulphur dioxide and ammonia are considered, together with flashing heated releases from pressure vessels. These scenarios are typically used by HSE to assess Hazardous Substances Consent applications and set Land Use Planning zones around major hazards sites. This report describes sensitivity tests which show that DRIFT 3.6.14 works reliably for these scenarios. As a result of this assessment and accompanying model evaluation (see RR1165), DRIFT 3.6.14 has been adopted by HSE to model instantaneous releases of toxic pressure-liquefied gases.