

DRIFT Version 3 User Guide Issue 7 30th November 2022

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1.0 Introduction

DRIFT is an advanced gas dispersion model. DRIFT was originally developed to model dense gas dispersion from instantaneous or continuous releases. DRIFT Version 3 is a new computer implementation of the model containing a number of major model enhancements including:

- Buoyant lift-off and rise
- A fully integrated jet model
- Multi-component mixtures
- Finite duration and time-varying releases

Some of the above enhancements were driven by the requirements of modelling hydrogen fluoride dispersion in moist atmospheres under conditions where buoyant lift-off is predicted. Other enhancements were driven by the desire to cover a wider range of release scenarios within a single model.

Given the above enhancements to DRIFT, the original model acronym basis of 'Dense Releases Involving Flammables or Toxics' should perhaps be replaced by a more general one: 'Dispersion of Releases Involving Flammables or Toxics'.

This DRIFT User Guide is structured as follows:

- Installation instructions and an overview of the user interface are given in section 2.0.
- Model input is described in section 3.0.
- Running the model and extracting results is described in section 4.0.

2.0 Getting Started

2.1 Installation

Download the latest version of software using the supplied URL and password.

There is a choice of two installers: DRIFTSetup64.msi installs the 64-bit version of DRIFT and DRIFTSetup32.msi installs the 32-bit version. Either version can run on 64-bit Windows 10. The main consideration of which version to install is dependent upon whether DRIFT's Component Object Model (COM) interface is going to be used to automate running of DRIFT or obtaining results. DRIFT's COM interface can be used in suitable COM enabled software e.g., Microsoft Excel. To use DRIFT's COM interface, the bitness of the installed DRIFT must match that of the COM client. For example, if 32-bit Microsoft Office is installed then 32-bit DRIFT should be installed, conversely if 64-bit Microsoft Office is installed then 64-bit DRIFT should be installed. If the COM interface is not used, then it is recommended to install 64-bit DRIFT on 64-bit Windows. Administrator privileges will be required whilst installing DRIFT.

If an earlier version of DRIFT is already installed, then it is recommended that this is uninstalled first. Double click on DRIFTSetup64.msi or DRIFTSetup32.msi to install DRIFT.

DRIFT installs a shortcut on the Windows desktop as shown in Figure 2-1 below.



Figure 2-1 DRIFT desktop shortcut

DRIFT also installs on the Windows menu under ESR Technology. DRIFT can be run by clicking on either the Windows menu or the desktop shortcut.

When opening, DRIFT checks for the presence of a valid licence. If no valid licence is found, then a dialogue box as shown in Figure 2-2 is displayed. The installation ID is unique to the computer on which DRIFT is installed. Note that running on a different computer will generate a different installation ID and requires a new licence to be provided.

No valid licence found	?	×
A valid licence could not be found. Please contact <u>softwaresupport@esrtechnology.com</u> with the Installation ID to request a licence.	ne following	
Installation ID:		
023851B224		
Enter licence key	Close DF	RIFT

Figure 2-2 Dialogue box when no valid licence is found

To obtain a valid licence please email <u>softwaresupport@esrtechnology.com</u> with the installation ID. You can press the "Close DRIFT" button to close DRIFT whilst waiting for a valid licence. Subject to entitlement to a valid licence, a licence file will be emailed back to the sender. If you previously closed DRIFT, run DRIFT again and this time press the "Enter licence key" button on the 'No valid licence' dialogue box which presents the "Enter licence" dialogue box shown in Figure 2-3. Drag and drop the supplied licence file into the space provided and press the "Confirm" button.

Enter licence	?	×
Drag and drop the licence file below:		
C	onfirm	

Figure 2-3 Enter licence dialogue box

When a valid licence is detected, DRIFT's user interface will open as illustrated in Figure 2-4.



Figure 2-4 DRIFT user interface

2.2 Setting the Substance Properties Data Source

DRIFT can obtain substance properties data from three different sources:

- 1. The ESR substance properties database supplied with the model.
- 2. HSE Substance Property Information (SPI) files located in a specified folder.
- 3. From user input substance properties data entered and stored on a per run basis.

The ESR substance properties database is the default. This takes the form of a Microsoft Access .mdb file, which is installed in the same folder as the DRIFT executable (on 64-bit windows this is generally C:/Program Files/ESR Technology/DRIFT/ESRSubstance.mdb, on 32-bit Windows it is generally C:/Program Files (x86)/ESR Technology/DRIFT/ESRSubstance.mdb). Microsoft Access does *not* need to be installed for DRIFT to be able connect to this database. The ESR substance properties database is a port of the SRD Databank substance properties database always needs to be present since DRIFT. The ESR substance properties data from this for air and water, also it supports importing and running DRIFT from legacy (old DRIFT and EJECT) files.

HSE SPI Files are in a format specific to the UK Health and Safety Executive (HSE) and these are not generally available outside of HSE. To make use of HSE SPI files, all the .spi files must all be collated in one folder placed either locally on a user's machine or on a shared network drive.

Once DRIFT is open, the substance properties data source can be set via the **Settings->Substance Data Source...** menu item which displays the dialogue box shown in Figure 2-5.

🥔 Substance Properties Data Source	?	×
Data Source O <u>S</u> PI Files ESR Substance		
File Locations		
SPI <u>F</u> iles	Browse	
ESR Substance SR Technology/DRIFT/ESRSubstance.mdb	Browse	•
OK	Cance	el

Figure 2-5 Selecting the Substance Properties Data Source

Select either SPI Files or ESR Substance as the default data source. Generally, within HSE it is envisaged that SPI files shall be used, whereas elsewhere ESR Substance shall be used.

The file locations are specified below. In the case of SPI files this is the folder where the SPI files are located.

User input of substance properties data defined on a per run basis is described in Section 3.7.

2.3 Main Window

When DRIFT is first launched the user is presented with a main window containing a new DRIFT document ready for input. The main window is shown in Figure 2-6.



Figure 2-6 DRIFT Main Window.

Menu commands (actions) in DRIFT can be accessed via the menu bar located at the top of the window. The most commonly used actions can also be accessed through the toolbar, which is located just below the menu bar.

At the bottom of the window is a status bar that provides feedback on the program status (e.g. if the model is running or not). Hovering the mouse pointer over a menu button or field/ field heading will provide a brief description of the field.

The central portion of the main window is divided into three major sections as outlined below. Further information on each can be found in the sections referenced below.

• Scenario Input

Described in section 3.0, the input window is located at the left-hand side of the main window and is used to specify the inputs for the scenario to be modelled. The input window is arranged into tabbed pages. Most of the

inputs for a scenario can be entered using the controls on these tabbed pages. The tabbed pages are ordered so that when defining a new scenario, tabs are most conveniently filled in order from the left-most to the right-most tab. The right-most tab defines the toxic and flammable target levels that are required to be modelled.

• Graphical and Tabular Output

Described in section 4.3, graphical and tabular output is displayed on the right-hand side of the main window. Upon completion of a scenario run, DRIFT displays default plan view contour plots for the requested flammable and toxic target levels. Controls on these plots allow different views to be obtained, e.g., contour plots in plan view and elevation, centreline variation, hazard range summary and tabular results. Additionally custom centreline plots and tables can be created using the ***** button, or deleted using the **S** button. The outputs are cleared if any of the scenario inputs are changed.

Message Window

Below the graphs and tables is the message window. This window provides important feedback on how the model is running and any problems that the model encounters. Any messages that appear here during a run are saved with the document and can be viewed when the document is loaded at a later date.

2.4 Loading and Saving Documents

To save a document, use the **File** \rightarrow **Save** menu item, press Ctrl + S, or click on the interval toolbar button. If the document has been saved previously, then DRIFT will reuse this filename. Otherwise, if this is the first time that this document has been saved, DRIFT will show a standard save file dialog asking for a filename to save the document to. If the open document has a filename it is displayed in DRIFT's title bar. The scenario inputs, output specification, run-time messages, and results are all stored in a single file with a *.drift* extension. DRIFT documents contain all of the information necessary to modify or run a model at a later date, and they can be saved at any time, apart from when the scenario is being run.

An existing document can be loaded by using the File-Open... menu item, pressing

Ctrl + O, or by clicking on the is toolbar button. This will open a standard file dialog where you may select an existing file or cancel the operation. In addition to *.drift* files, DRIFT allows legacy file types from previous versions of DRIFT (*.din*) and files generated by Panache (*.pan*) to be loaded. Note, DRIFT only reads the input data from legacy files so that these scenarios may be re-run using the new version of DRIFT and, if desired, saved as a new *.drift* file. Also note that if DRIFT is given a *.din* file that specifies the *Isothermal* thermodynamic option (see DRIFT v2 documentation) with a user defined substance then the user may be required to manually enter the vapour specific heat capacity for the substance before the model will run. This is because the *Isothermal* thermodynamic option is incompatible with the use of atmospheric profiles in DRIFT and is accordingly not supported.

In the circumstance that the user wishes to simulate dispersion using the input data from an existing Panache (EJECT) jet run then only the Panache (*.pan*) file should be loaded rather than loading from the accompanying *.din* file.

DRIFT also supports a "recently used files" list that can be used to immediately open a recently used *.drift, .din* or *.pan* files. This list is updated each time a document is opened or saved and is accessed by the **File**→**Open Recent** menu item.

DRIFT supports long filenames throughout and, on a per user basis, it will remember the last directory that you accessed files from in between sessions, saving you having to navigate to the same directory each time.

.drift files are plain text XML (eXtensible Markup Language) documents that may be edited with any text editor. However, use of a text editor to edit DRIFT documents is not recommended as it requires a detailed knowledge of the keywords used the model and the dependencies between them. Also, editing files this way has the potential to corrupt the encoded output data which is also stored in the files.

2.5 Online Help

There are three options to obtaining online help whilst using DRIFT:

- 1. Tool-tips
- 2. What's this?
- 3. Online User Manual

2.5.1 Tool-tips

Tool-tips can be accessed either by hovering the mouse pointer over a user input name for a couple of seconds until a short description is displayed in a yellow text ribbon.

2.5.2 What's this?

What's this help is intended to provide a more detailed help than given by a tool-tip.

What's this help is obtained by either selecting the web button on the tool bar, **What's this?** from the **Help** menu, or Ctrl+F1. Clicking on the object of interest with the mouse pointer will display the What's this description.

2.5.3 Online User Manual

The online user manual is an electronic version of this User Guide. It is available through the **Help** \rightarrow **DRIFT User Manual...** menu item, pressing the \bigcirc button, or pressing F1.

2.5.4 About DRIFT

The **Help** \rightarrow **About DRIFT...** menu brings up an About dialogue box which displays the version number for DRIFT along with licensing and copyright information.

3.0 Scenario Input

The main scenario input for DRIFT is through the input tabs on the left-hand side of the main window. Optional scenario inputs relating to Ground Transfer, changing the default Termination Conditions and specifying Obstacles are located on the Scenario menu.

3.1 Description Tab

The description tab, shown in Figure 3-1, provides a means for assigning a reference number or title to a model for QA purposes in addition to the filename. There is also a text input box that may be used to store a longer description of the run and any other information that may be relevant to the model. Both the title/reference number and the entire description are included in the report when the document is printed or exported to HTML.

Description	Release	Geometry	Atmosphere	Flammable	Toxic
Heading					
Description					

Figure 3-1 Description Tab

3.2 Release Tab

The release tab, shown in Figure 3-2, is used to tell DRIFT about the conditions of the release, as well as any other associated information. The tab is split under a variety of subheadings which are described below.

Description	<u>R</u> elease	<u>G</u> eometry	<u>A</u> tmosphere	Flag	nmable	To <u>x</u> ic	
Туре			Phase				
Instant	aneous		Gaseo <u>u</u> s				
O Steady	<u>C</u> ontinuous		O Superheated Liguid / Two-Phase				
🔿 Finit <u>e</u> D	uration						
◯ Time <u>V</u> a	rying						
Su <u>b</u> stance		Propane	~		Define		
Temperatur	e	294] к	Sat Ten	n <u>p</u> .	
Pressure		101325		Pa	S <u>V</u> P		
Liquid Fract	ion	0					
Rainout Fra	cti <u>o</u> n	0		Po	ol Results	s	
Contaminan	t Fraction	1		kg/kg	g		
Contaminan	t <u>M</u> ass	1000		g			
Stationa	ary Initial Clou	<u>d</u>					

Figure 3-2 Release Tab

3.2.1 Type

The following release types are available:

• Instantaneous

An instantaneously released cloud, or cloud of very short release duration compared to the travel time to the target receptor location. Catastrophic failure of a pressure vessel containing gas or superheated liquid (i.e., stored above its normal boiling temperature) is an example of an instantaneous release.

• Steady Continuous

A plume formed from continuous release at a steady release rate. The steady continuous model neglects along-wind diffusion and a represents a release of duration much longer than the travel time to the target receptor. A release from a large inventory through a small hole is an example of a release that might be approximated as being steady continuous.

• Finite Duration

A steady release which stops after a finite time. The finite duration model includes along-wind diffusion. In the limit of a long duration, the finite duration model approximates the steady continuous case and for a short duration release it approximates the instantaneous case. Generally, this results in a finite duration release giving results similar to a steady continuous release in the near field and being capped by the release mass in the far field, which would otherwise be over-predicted by a steady continuous model. A steady release that is terminated e.g. by closing a valve is an example of a release that might be approximated as being finite duration.

• Time Varying

In the circumstance where the dispersing cloud cannot be considered to be steady over the release time, or instantaneously released, then time varying option may be selected. For the time varying option the release rate as a function of time must be provided by the user – the release rate at up to 100 steps may be entered. DRIFT approximates the input release rate profile into a generally smaller number of finite duration segments. When DRIFT is run, the results from the segments are combined to give a time varying dispersing cloud. The time varying model includes along wind-dispersion in each segment. A decaying release rate due to inventory depressurisation is an example of a scenario that might be approximated by the time varying model. The time varying model is also used by DRIFT when importing a vaporising pool source term from a GASP file – in this case the release rate profile is taken directly from the GASP results (see Section 3.11).

Some of the subsequent inputs differ depending on which release type is selected. The controls on the input tabs automatically change to reflect this dependency.

3.2.2 Phase

Here the user specifies the phase of the release material.

Gaseous

This option specifies that the released material is initially entirely in the vapour phase. Specifying this option does not preclude subsequent condensation of liquid in the cloud if DRIFT determines conditions imply this. Using this option DRIFT will always assume that the release is initially pure vapour, even in the circumstance that the release temperature is below the release substance boiling point. An example of a gaseous release is methane gas released from pressurised storage.

• Superheated Liquid / Two-Phase

This option allows liquid to be initially present in the release. If the liquid is superheated (i.e., above its normal boiling temperature) then at runtime DRIFT will perform a flash calculation to determine the conditions at atmospheric pressure. An example of a superheated liquid release is the release of pressure liquefied propane.

This option also covers the modelling of sub-cooled liquid (i.e., below it normal boiling point) as a spray. DRIFT assumes that liquid is present in the cloud as small drops at the same temperature as the vapour in the cloud. An example of a sub-cooled liquid spray is a pressurised release of toluene diisocyanate (TDI) at ambient temperature.

When modelling sub-cooled liquid releases and liquid releases with low superheat consideration should be given to removal of liquid by deposition, either directly near the source by specifying the Rainout Fraction or continuously during dispersion using the Scenario \rightarrow Ground Transfer \rightarrow Liquid Deposition menu Option.

When the Gaseous option is selected then only the substance, substance temperature, initial dilution and release rate can be changed by the user. If the Superheated Liquid / Two-phase option is selected then the Pressure, Liquid Fraction and the Rainout Fraction of the release material can also be entered by the user.

3.2.3 Substance

The Substance combo box allows the user to select the release substance they wish to model from a list of substances in the substance data source (either ESR Substance Database or HSE SPI Files). Alternatively, the user has the option of defining a new single-component release substance or specifying a multi-component mixture of substances by clicking on the Define button to the right of the combo box (see Section 3.7). All contaminant substances entered in this way are assumed to be immiscible with water – it is possible to enter a substance that is miscible (e.g. forms an ideal solution) with water by using the mixture editor (see Section 3.6.2).

3.2.4 Temperature

The stagnation temperature of the release in Kelvins.

In most cases the release temperature can be taken to be equal to the storage or reservoir temperature of the released fluid.

If the input temperature implies a superheated liquid release, then DRIFT will do a flash calculation to determine the conditions after flashing (neglecting air entrainment during this process).

If the input implies a sub-cooled liquid release (liquid spray) then DRIFT will run under the assumption that the release is broken up into a fine airborne spray. Efficient liquid break-up requires high pressure through a small/sharp edged orifice this is considered unlikely for an instantaneous release. In this circumstance DRIFT will not run but produce a warning message.

If the input implies a sub-cooled vapour (i.e., a condensable vapour below its saturation temperature) then DRIFT may condense some gas as liquid. However, this is based on the initial enthalpy of the release being that of the gas.

If source conditions have been estimated using another model, e.g., using a twophase release rate model then the input temperature should match the output from the model. For example, if the output is choked flow conditions (vapour fraction, temperature, pressure) at the exit then the temperature, pressure and liquid fraction should be entered to match. If the Superheated Liquid / Two Phase option is selected, then the Sat Temp. button becomes available. Pressing the Sat Temp. button sets the temperature to be the saturation temperature of the substance at the specified exit pressure (see Pressure).

3.2.5 Pressure

The absolute pressure of the release in Pascals.

The release pressure is not required as an input for gaseous releases since in this circumstance the pressure is calculated by the model.

The pressure to be input from DRIFT corresponds to the assumed pressure at the exit and is not necessarily equal to the storage or reservoir pressure. Guidance is given below:

In the case of unchoked flow the release pressure can be taken to be atmospheric pressure.

In the case of choked flow the release pressure can be taken to be the choke pressure.

In the case of a superheated liquid release through a hole in vessel wall then there may be insufficient time for flashing and the release may be approximated as an unchoked liquid release

If source conditions have been estimated using another model, e.g., using a twophase release rate model then the input pressure should match the output from the model. For example, if the output is choked flow conditions (vapour fraction, temperature, pressure) at the exit then the temperature, pressure and liquid fraction should be entered to match.

The main influence of pressure is in determining the momentum of jet releases.

Pressing the SVP button sets the exit pressure to be the saturated vapour pressure at the specified release temperature (see Temperature).

3.2.6 Liquid Fraction

Fraction of the release that is liquid at the exit. Strictly this input is a mole fraction. In the case of pure single component substance releases, the mole fraction equals the mass fraction. In the case of multi-component releases, the liquid fraction is input for each component in a separate dialogue box.

A liquid fraction of 1 indicates a pure liquid release and 0 a pure vapour release. DRIFT will do a flash calculation for superheated liquid releases. DRIFT will model sub-cooled liquid releases as an airborne spray (except for a sub-cooled instantaneous liquid release in which case complete break-up to small drops is less likely)

If source conditions have been estimated using another model, e.g., using a twophase release rate model then the input liquid fraction should match the output from the model. For example, if the output is choked flow conditions (vapour fraction, temperature, pressure) at the exit then the temperature, pressure and liquid fraction should be entered to match.

3.2.7 Rainout Fraction

The fraction of the release liquid mass after flashing that is assumed to rainout as liquid drops at the source. The rainout liquid is assumed to be directly deposited on the ground at the source and does not contribute further to the atmospheric dispersion, i.e., no vaporisation of rained out material is accounted for in the model. In addition to immediate rainout, it is possible to specify continuous liquid deposition based upon drop size (see Section 3.8).

3.2.8 Contaminant Mass Fraction

The mass fraction of contaminant at the source. A value of 1 specifies that the release is 'pure contaminant' i.e., consists only of the specified release substance. When the value is less than 1, the remaining fraction of the release is made up of ambient moist air. In the circumstance that another model has been run prior to DRIFT to predict dilution due to the source term, e.g., dilution during catastrophic failure of a pressure vessel, then the mass fraction implied by this dilution should be input.

3.2.9 Contaminant Mass [Instantaneous]

The initial mass of contaminant (in kilograms) in the instantaneously released cloud. Note this mass excludes any moist air that is specified using a contaminant mass fraction less than 1.

3.2.10 Stationary Initial Cloud [Instantaneous]

The default for an instantaneous release which initially has no moist air mixed in (contaminant mass fraction equal one) is that the cloud centroid starts from rest. Alternatively, if the cloud initially consists of a mixture of contaminant and moist air (contaminant mass fraction less than one) then a non-zero velocity is calculated associated with entraining momentum from the air that is initially present. This is intended to represent the conditions after entrainment of air from the atmosphere, e.g., due to momentum driven turbulent growth after catastrophic failure of a pressure vessel. To force the cloud to initially be at rest check the Stationary Initial Cloud checkbox to ensure that starts from rest – useful for validation (e.g., Thorney Island instantaneous trials).

3.2.11 Release Rate [Steady Continuous, Finite Duration]

The release rate of contaminant in kilograms per second. Note this rate excludes any moist air that is specified using a contaminant mass fraction less than 1.

3.2.12 Release Duration [Steady Continuous, Finite Duration]

The duration of the release in seconds. In the case of a steady continuous release this simply determines the exposure duration for the release. The exposure duration may also be capped by the maximum exposure duration on the targets tab (see Section 3.5.1). For a finite duration release this also affects the rate of dilution due to the inclusion of along-wind diffusion at the front and back of the cloud.

3.2.13 Time Varying Release Rate Profile [Time Varying]

When the Time Varying release type is selected the Release Tab changes to that shown in Figure 3-3. This gives the user the option to enter a time varying release rate profile in up to 100 rows. The first column is the time (in seconds) from start of the release and the second column is the release rate at that time (in kilograms per second). The release rate profile should be ordered with increasing time and the release rate should be single valued in time (i.e., not have multiple values at the same time).

Stantaneous eady Continuous Superheated Liguid / Two-Phase Superheated Liguid / Two-Phase Superheated Liguid / Two-Phase Superheated Liguid / Two-Phase Define reverting Teraction Define Pa SVP Fraction 0 Pool Results ninant Eraction 1 Kate (kg/s) Time (s) Rate (kg/s)
eady <u>C</u> ontinuous ○ Superheated Liguid / Two-Phase itg_Duration ● nce Propane ○ Define rature 294 K Sat Temp. re 101325 Pa SVP Fraction 0 ● t Fractign 0 ● Pool Results ninant Eraction 1 kg/kg Varying Release Rate Profile Time (s) Rate (kg/s) ^
ite Duration ne Varying nce Propane ✓ Define rature 294 K Sat Temp. re 101325 Pa SVP Fraction 0 t Fraction 0 t Fraction 1 kg/kg Varying Release Rate Profile Time (s) Rate (kg/s) ↑
nce Propane Define rature 294 K Sat Temp. re 101325 Pa SVP Fraction 0 tt Fractign 0 Pool Results ninant Eraction 1 kg/kg Varying Release Rate Profile Time (s) Rate (kg/s)
nce Propane Define rature 294 K Sat Temp. re 101325 Pa SVP Fraction 0 t Fractign 0 Pool Results ninant Eraction 1 kg/kg Varying Release Rate Profile Time (s) Rate (kg/s)
nce Propane Define rature 294 K Sat Temp. re 101325 Pa SVP Fraction 0 t Fraction 0 ninant Eraction 1 kg/kg Varying Release Rate Profile Time (s) Rate (kg/s)
rature 294 K Sat Temp. re 101325 Pa SVP Fraction 0 t Fractign 0 Pool Results ninant Eraction 1 kg/kg Varying Release Rate Profile
re 101325 Pa SVP
Traction
t Fractign 0 Pool Results ninant Eraction 1 kg/kg Varying Release Rate Profile Time (s) Rate (kg/s)
ninant <u>F</u> raction 1 kg/kg Varying Release Rate Profile Time (s) Rate (kg/s)
Varying Release Rate Profile

Figure 3-3 Release Tab for Time Varying Release

Pressing the Recalculate button (re-)calculates the total mass released from the input release rate profile.

Pressing the plot button displays the release rate profile for the release as shown in Figure 3-4. The black line shows the user input for release rate profile and the dotted grey lines display the segmentation of the release that DRIFT will use to approximate the time-vary release as a series of finite-duration segments. The segmentation of the release rate profile is controlled by two parameters - *Release Segment Tolerance* and *Minimum Segment Duration* these can be adjusted from their default values

using the Preferences dialogue box available from the **Settings** \rightarrow **Preferences** menu (see Section 5.0).



Figure 3-4 Time Varying Release Profile Plot

3.2.14 Pool Results... button

The Pool Results... button allows a pool source from a GASP run to be added to the specified release. See Case 2 of Section 3.11 for more details.

3.3 Geometry Tab

The Geometry Tab contains inputs relating to the source geometry (location, size and orientation). The input controls displayed on the Geometry Tab depend upon the release type selected under the Release Tab.

The geometry tab for an instantaneous release is shown in Figure 3-5.

Description Releas	se <u>G</u> eor	metry	<u>A</u> tmosphere	Flam	nable	To <u>x</u> ic
Location						
<u>×</u> 0	m					
У 0	m					
<u>z</u> 0	m					
✓ Assume Unit Asp Initial Cloud Radius	ect Ratio (H	leight =	Radius)		m	

Figure 3-5 Instantaneous Release Geometry Tab

The geometry tab for a continuous or time varying release is shown in Figure 3-6

Description Release	<u>G</u> eometry	<u>A</u> tmosphere Fla <u>m</u> mable To <u>x</u> ic
Location <u>x</u> 0 m <u>y</u> 0 m <u>z</u> 2 m		Source Type Momentum Jet Low Momentum Area Source
Orifice Diameter	0.05	m
Discharge <u>C</u> oefficient	0.8	
Angle from Hor <u>i</u> zontal	0	•
Angle from North	90	•

Figure 3-6 Continuous or Time Varying Release Geometry Tab

3.3.1 Location

Co-ordinate System Definition

For the purpose of defining release and wind angles, DRIFT treats East as being in the positive x-direction, North as being in the positive y-direction. These labels do not necessarily imply alignment with True North or Plant North and the definition of these directions is merely a matter of convenience.

The z-axis is directed upwards with z = 0m corresponding to ground-level.

The (x,y) origin can be chosen to suit the user.

In some cases, e.g., dispersion of a downwind directed release, it may be simplest to define the coordinate system relative to the wind with the source at x=0, y=0, such that x is the downwind direction and y the crosswind direction. In other cases, e.g. when modelling dispersion in the presence of buildings, defining axes based on a geographic co-ordinate system may be desirable.

Source Location

Use the location inputs to specify the (x, y, z) location of the central point of the release source.

z = 0 m specifies a ground-level source. For an elevated stack release specify z equal to the stack height, reduced if appropriate to account for stack down-wash (see below). Instantaneous and low momentum area sources are always at ground-level.

Stack downwash

DRIFT does *not* model downwash for stack releases. Stack downwash affects releases with relatively small upward momentum - it reduces plume rise due to the turbulent wake around the stack. In circumstances where the vertical release velocity is less than approximately 1.5 times the wind speed at the stack height, consideration should be given to reducing the stack height by an amount indicated by accepted stack downwash algorithms.

3.3.2 Initial Cloud Radius [Instantaneous]

The initial instantaneous cloud is taken to be cylindrical, and the initial radius of the cloud can be entered in the text box. Use the unit aspect ratio check box to tell DRIFT to take the height of the cylinder to be the same as its radius. – in this case DRIFT calculates the initial cloud radius at runtime.

A unit aspect ratio cloud might be considered an appropriate approximation for a pressurised catastrophic failure where a hemi-spherical cloud is expected to initially form. In the case of a release from a pool it may be more appropriate to input the pool radius as the initial cloud radius.

3.3.3 Source Type [Steady Continuous, Finite Duration, Time Varying]

The following source types are available for steady continuous, finite duration and time varying sources:

• Momentum Jet

The momentum jet option should be selected for modelling directed dispersion resulting from a pressurised release through an orifice.

• Low Momentum Area Source

The low momentum area source should be selected when DRIFT is being used to model dispersion from a low momentum source, such as vapour evolution from an evaporating pool. The low momentum model does not apply exclusively to a pool however, although this does seem like the most likely use.

Generally, for a pool the release rate would be the vaporisation rate; the release temperature would be the temperature of vapour evolving from the pool (which for most pool models is the same as the pool, or, if different, the pool surface temperature); and the pressure would be atmospheric.

Specifying a liquid/two-phase option would be equivalent to having a low momentum aerosol release spread over the source area. It is unclear in what practical circumstance this would apply (possibly a two-phase release through a cyclone device). The liquid option is not intended to be a source from a pool. If the liquid/two-phase option were used, then the rainout fraction would specify the fraction of post-flash liquid that rains out (rained out liquid does not contribute to the cloud). The input pressure is the pressure at the exit. For jet releases this is used to calculate the initial momentum; for low momentum sources it is probably best to set the pressure to atmospheric to be consistent with the source having low momentum.

3.3.4 Orifice Diameter [Momentum Jet, Low Momentum Area Source]

The diameter of the release orifice for a momentum jet.

The diameter of area source (e.g., pool radius) for a low area momentum source.

DRIFT assumes that the release occurs through a circular orifice or hole. In the case of a non-circular source, a diameter should be input which has an equivalent area. However, this may be a poor approximation in the near field for releases through slits where the along slit dimension is much larger than the across slit dimension.

3.3.5 Include Dilution Over Source [Low Momentum Area Source]

When this is selected [the default] DRIFT will include dilution due to mixing with air over the area source and, if predicted, upwind spreading for a dense source.

DRIFT's model for dilution and spreading over the source attempts to find a steady state solution where the material released from the source moves downwind at a rate equal to the rate of release from the source. In some circumstances (low wind and

large release rate) DRIFT may predict that in the steady state, the cloud has diluted (on average) below the level of concern – this is indicated by a runtime warning message.

When calculating initial dilution DRIFT runs a modified version of the instantaneous model (with a source rate feeding into the cloud) until an appropriate steady source window can be set up. In the case of the steady continuous model this initial upfront instantaneous run is discarded once a source window has been established; in the case of the finite duration and time varying models the instantaneous run is included in the time-history of the concentration profiles. Note that occasionally the transient concentration contours can be bigger than the steady state contours around the source, meaning that the finite duration model predicts a larger cloud footprint than the steady continuous model.

3.3.6 Discharge Coefficient [Momentum Jet]

The entered discharge coefficient should match that used for the discharge rate calculation. Generally different values are used for liquid and gases.

DRIFT default inputs are: 0.61 for liquids and 0.80 for gases.

DRIFT uses the discharge coefficient to calculate the exit velocity corresponding to the supplied release rate. The release rate itself is unchanged from the input value.

3.3.7 Release Direction [Momentum Jet]

The initial release direction for a momentum jet is set by specifying two angles:

• Angle from Horizontal

The angle in degrees between the initial jet direction and the horizontal plane. A positive angle represents a jet initially tilted upwards from the horizontal, a negative angle an initially downward tilted jet and zero an initially horizontal jet. Valid input range: +90° to -90°.

• Angle from North

The bearing angle (in degrees) clockwise from the North (y-axis) in which the momentum jet is initially pointing. The default, 90°, corresponds to a release directed along the x-axis. Valid input range: 0° to 360°, except for time varying jets which must be directed within 60° of the downwind direction (e.g., 30° to 150° if the wind blows along the x-axis).

Depending on the trajectory of the jet, DRIFT may encounter modelling difficulties (returning one of the solver related errors in Section 6.0) for certain combination of release and wind angle – generally these correspond to conditions where there is predicted to be a reversal of the flow, e.g. a jet directed into the wind, or a dense jet that is initially vertical upwards. In such circumstances, it may be possible to run the scenario by adjusting the release direction and/or the wind direction.

3.4 Atmosphere Tab

The Atmosphere Tab, shown in specifies the atmospheric conditions to apply to the dispersion scenario.

Description Release	Geometry	<u>A</u> tmosphere	Flam	nable	To <u>x</u> ic
Scheme					
easquill					
🔘 H <u>o</u> ltslag					
🔘 Monin-Obukhov					
Inversion					
Input Inversion Heig	iht				
Inversi <u>o</u> n Height	800			m	
Temperature	294			К	
Relative H <u>u</u> midity	70			%	
Referen <u>c</u> e Height	10			m	
Roughness <u>L</u> ength	0.1			m	
Wind Angle from <u>N</u> orth	270			۰	
Pasquill Stability	D		*		
Wind Speed	5			m/s	

Figure 3-7 Atmosphere Tab

3.4.1 Weather Scheme

DRIFT supports the following schemes for input of atmospheric conditions:

- Pasquill
- Holtslag
- Monin-Obukhov

The user only needs to enter information for one of the three schemes. DRIFT converts, at runtime, the input from either the Pasquill or the Holtslag scheme into an equivalent Monin-Obukhov scheme and uses this for the calculation of atmospheric dispersion.

3.4.2 Inversion Height

DRIFT models dispersion only within the atmospheric boundary layer (also called the atmospheric mixing layer). DRIFT conservatively assumes that all released material

remains trapped within the atmospheric boundary layer. The top of this layer is defined by the inversion height.

User input of inversion height is only required for the Monin-Obukhov scheme. For the other weather schemes the inversion height is either calculated (Holtslag) or determined from a look-up table (Pasquill). Optionally, the user may input an inversion height for any scheme by checking the input inversion height check box.

3.4.3 Temperature

The air temperature in Kelvins at the Reference Height.

3.4.4 Relative Humidity

Relative humidity is a measure of the water content of moist air relative to saturated conditions.

Valid range: 0% - 107%

Relative humidity may affect dispersion behaviour through latent heat released/absorbed when condensing/evaporating water drops in the cloud (this can affect the predicted behaviour of dispersion of a cold LNG cloud). Relative humidity may also influence the dispersion behaviour of released substances which strongly interact with water releasing heat. DRIFT includes specific water interaction models for ammonia and hydrogen fluoride.

DRIFT defaults to the specific humidity being constant with height (apart from in the Holtslag scheme, see below). This can be altered by specifying the *Inverse Bowen Ratio* on the **Preferences** dialogue box accessed via the Settings→Preferences menu (see Section 5.0), in which case relative humidity varies with height and the input relative humidity should be at the *Reference Height*. In the Holtslag scheme the Bowen Ratio is calculated automatically by the model.

3.4.5 Reference Height

This is the height above the ground at which the input wind speed, air temperature and relative humidity (in the case of varying relative humidity with height) apply.

3.4.6 Roughness Length

The roughness length (z_0) is a characteristic of the roughness of the terrain over which the dispersion occurs. Roughness length, together with Monin-Obukhov length and friction velocity are scaling parameters for the atmospheric boundary layer.

Roughness length may be estimated simply based upon land-use type or using more sophisticated methods. Guidance on estimating roughness length is given Hanna and Britter's CCPS book 'Vapor Cloud Dispersion at Industrial and Urban Sites', ISBN: 0-8169-0863-X.

In general, higher roughness length gives rise to more cloud dilution and short hazard ranges.

Note: The Pasquill weather scheme is strictly only valid for roughness lengths between 0.0001 m and 0.5 m. Values outside this range are permitted by DRIFT, but should be used with caution.

3.4.7 Wind Angle from North

Specifies the direction **from** which the wind is blowing. The angle is measured in degrees clockwise from North (y-axis).

For example, a wind angle of 270° [the default] corresponds to the wind blowing towards the positive x-direction from the west (negative x-direction).

Note: The wind direction convention used here differs from that in DRIFT version 2, but matches standard meteorological convention. DRIFT automatically corrects for this when reading a legacy DRIFT input file.

Valid input range: 0° to 360°

Depending on the trajectory of the cloud, DRIFT may encounter modelling difficulties (returning one of the solver related errors in Section 6.0) for certain combination of release and wind angle – generally these correspond to conditions where there is predicted to be a reversal of the flow, e.g. a jet directed into the wind. In such circumstances, it may be possible to run the scenario by adjusting the release direction and/or the wind direction.

3.4.8 Wind Speed [Pasquill, Holtslag]

The wind speed (measued in metres per second) at the specified reference height.

Note: DRIFT cannot model dispersion in zero wind speed.

3.4.9 Pasquill Stability [Pasquill]

This is the categorisation of the atmospheric stability. The Pasquill categories are defined as follows:

- A: very unstable
- B: unstable
- C: slightly unstable
- D: neutral
- E: slightly stable
- F: stable

	Day- Inco	oming Solar F	Night		
10m wind speed	Strong	Moderate	Slight	Thinly Overcast or >4/8 Low Cloud	Clear or <3/8 Low Cloud
< 2	А	A-B	В		
2-3	A-B	В	С	E	F
3-5	В	B-C	С	D	E
5-6	С	C-D	D	D	D
> 6	С	D	D	D	D

Table 3-1 A guide to Pasquill categories (Panofski and Dutton (1984))

Pasquill category A indicates strong convection (and large vertical dispersion). D represents purely mechanical turbulence, and F implies stable air in which mechanical turbulence is strongly damped by stratification. The neutral category, D, should be assumed for overcast conditions during day or night. No Pasquill category is defined for clear night or light wind, where vertical turbulence is eliminated - in this circumstance F stability is a pragmatic choice.

3.4.10 Cloud Cover [Holtslag]

The Holtslag weather scheme uses the cloud cover, together with the latitude, longitude, date and time, to calculate the net solar radiation. The net solar radiation is an input to calculating the Monin-Obukhov length and inversion height.

Valid range: 0%-100%

3.4.11 Latitude, Longitude, Date & Time [Holtslag]

The Holtslag weather scheme uses the latitude and longitude of the site, together with the date and time (GMT 24 hour clock) and cloud cover, to calculate the net solar radiation. The net solar radiation is an input to calculating the Monin-Obukhov length and inversion height.

Valid range for Latitude: +90° to -90° Valid Range for Longitude +180° to -180°

3.4.12 Inverse Monin-Obukhov Length [Monin-Obukhov]

The Monin-Obukhov length, L_a, is a fundamental scaling length for the atmospheric boundary layer. For the Pasquill and Holtslag weather schemes, the Monin-Obukhov length is calculated/looked-up by DRIFT from the supplied inputs.

To avoid singularities under neutral stability conditions, the Monin-Obukhov length is directly input via its inverse i.e. $1/L_a$.

The inverse Monin-Obukhov length is zero for neutral stability, positive for stable stratifications and negative for unstable stratifications.

3.4.13 Friction Velocity [Monin-Obukhov]

The friction velocity is a characteristic scaling velocity for the lower parts of the atmospheric boundary layer. For the Pasquill and Holtslag weather schemes, the friction velocity is determined from the input wind speed, roughness length and reference height. For the Monin-Obukhov weather scheme the friction velocity is a direct input.

Note: DRIFT cannot model dispersion in zero friction velocity (corresponding to zero wind)

3.5 Toxic Tab

When the toxic target type is selected, the targets tab is shown in Figure 3-8. The tab is split under a variety of subheadings which are described below.

Description Re	lease <u>G</u> e	ometry	<u>A</u> tmosphere	Flammable	To <u>x</u> ic			
Plume Meander:								
✓ Use Time Averaging								
Lateral Meander A <u>v</u> eraging Time 1800								
Maximum E <u>x</u> posu	Maximum Exposure Duration 1800							
Substance	Toxic Expo	nent						
1 Propane	2							
Method of evalua	ating toxic do	se fraction	:: 💿 # <u>1</u>	○ # <u>2</u>				
Target Indoor Pa	rameters							
Ventilation Rate	2.5			ACPH				
Indoors <u>L</u> ag Time	600			s				
clevels of Interest								
Concentration	~		00	tdoors 🔉				
Outdoor Concentration Level 1								
Substance	Level (ppm)						
1 Propane	21000							

Figure 3-8 Toxic Targets Tab

3.5.1 Time Averaging

If the Use Time Averaging checkbox is checked then DRIFT will account for lateral and vertical meander of the plume induced by fluctuations in wind direction.

The lateral meander model in DRIFT uses a fluctuation model based on the EU COFIN project. This takes the *averaging time* as an input, which is the period in seconds over which to average the toxic concentration and dose predictions. In general, the longer the averaging time the more the effective the dilution due to plume meander. For toxic exposure it is usual for the averaging time to match the assumed toxic exposure duration, or release duration if shorter. This is the default in DRIFT.

DRIFT also has a vertical meander model to account for the effects of updraughts and downdraughts, but this only applies in unstable atmospheric conditions. The averaging time has no effect on the vertical meander.

Time averaging has no effect on the predicted dilution of instantaneously released clouds.

IMPORTANT NOTE: Only the output displayed in the toxic and general results windows and in the toxic results section of the DRIFT report (printed or HTML) include the effect of time averaging. All flammable results are based on short (near-instantaneous) average values. All custom plots and tables are also based on short (near-instantaneous) average values.

3.5.2 Toxic Dose

In this group box the following inputs are specified:

Maximum Exposure Duration

The maximum exposure duration in seconds is used to limit the time over which toxic dose is accumulated.

Where the maximum exposure duration is shorter than the passage time of the cloud, DRIFT reports the toxic dose corresponding to the maximum exposure duration (plus the *Indoors Lag Time* for an indoors target) for the worst case (highest dose) time interval during the passage of the cloud.

The default in DRIFT is for the maximum exposure duration to be set equal to the release duration.

Toxic Exponent, n

The toxic exponent, *n*, is the power to which the concentration (in parts per million) is raised when integrating over time to calculate the toxic dose.

Enter a toxic exponent for each component substance by clicking on the number displayed next to the substance name and entering the value. A value of zero may be used to indicate that a component does not contribute any toxic dose.

DRIFT reads the toxic exponent from HSE SPI files (when present) which include toxicity information. In this case the toxic exponent read from the SPI file is displayed but cannot be changed in DRIFT.

Toxic exponents can be found from a variety of sources such as the HSE website. The recommended values are updated from time to time so users are advised to check for the latest values.

3.5.3 Target Indoor Parameters

DRIFT uses a simple indoor ventilation model to calculate the toxic concentration and dose for indoors targets. The required inputs are:

Ventilation Rate

Indoor ventilation rate is specified in air changes per hour. Higher ventilation rate will lead to greater indoor concentrations and dose. In general natural ventilation will be wind speed dependent, with higher wind speeds leading to higher ventilation rates.

• Indoors Lag Time

Indoors Lag Time is the time in seconds that people are assumed to remain indoors after the toxic cloud has passed. The default lag time in DRIFT is 600 seconds. The Indoors Lag Time is added to the Maximum Exposure Duration to determine the worst case indoors toxic dose.

3.5.4 Levels of Interest

This subsection allows the user to define specific toxic doses or toxic concentrations of interest for DRIFT to calculate the hazard ranges for and plot concentration/ dose contours.

• Adding Levels of Interest

To add a level of interest the user should select if the level is indoors or outdoors from the right-hand drop-down list and from the left hand drop down list either a concentration or a dose of interest should be selected. The level

of interest can then be added by clicking on the T button.

The substance(s) will now become available within the Substance-Level text box and the user can add either a concentration level of interest (in ppm) or a dosage level of interest (in ppmⁿ.min, where n is the toxic exponent).

Additional indoor and outdoor levels of interest can be added by the same method and they can be switched between by using the drop down list. To

remove a level of interest, select it in this fashion and then click onto the $\overleftarrow{\mathsf{A}}$ next to the drop-down list.

Where there is toxicity information in the HSE SPI file, DRIFT will automatically load the 1% fatality level (SLOT DTL) as indoor and outdoor levels of interest. These particular levels cannot be edited with DRIFT, although new levels may be added.

Note that the averaging time, maximum exposure duration and toxic exponents always need to be entered, even if no toxic levels of interest are added, because they are used when computing dose results for the general tab.

3.5.5 Method of Evaluating Toxic Dose Fraction

DRIFT offers two alternative methods for combining the results for multi-component toxic releases:

Method 1

This involves adding the fractions of the target level concentration and doses. For each stored level of interest DRIFT outputs results corresponding to the sum over the component fraction of target levels equalling 1. This may be represented by

$$z_{toxic} = \sum_{i \in \mathbf{T}} \frac{z_i}{C_i}$$

where C_i is the specified level of harm for component i corresponding to the concentration or dose, z_i is the predicted concentration or dose and $i \in T$ signifies the sum only applies to those components that are toxic.

This approach assumes that each added level of interest, C_i corresponds to same level of harm (e.g., a specified level of toxicity). In this approach each toxic component is assumed to be 'independent'. This has the merit that when a single component dominates the composition, the predicted toxic fractions match tends to those for that component.

Method 2

An alternative method of combining toxic dose (method 1 is always employed for toxic concentration) for components is:

$$z_{toxic} = \sum_{i \in \mathcal{T}} \left[\frac{z_i}{C_i} \right]^{1/n_i}$$

where n_i is the toxic exponent for component *i*. This alternative approach has the merit that for multiple components with similar or the same toxicity (same or similar target dose levels C_i and toxic exponents n_i) then similar or the same results would be found using a single component with the same toxicity. This would only be the case in Method 1 if $n_i = 1$ and for other circumstances, e.g., with $n_i = 2$ then Method 1 might be considered non-cautious.

It is recognised that combining toxicity for multi-component mixtures in either of the above ways is at best uncertain. Should mixture specific toxicity be available it would be preferable to apply this more directly (e.g., by inputting this as a toxic dose equivalent for a single component)

3.6 Flammable Targets

When the flammable target tab is selected, the targets tab shown in Figure 3-9is shown. The tab is split under a variety of subheadings which are described below.

Description	Release	Geometry	<u>A</u> tmosphere	Fla <u>m</u> mable	To <u>x</u> ic				
Flammable Limits									
User Input Flammability Limits									
Lower Flar	– mmable Limit	2.1		%					
Upper Hammable Limit		10.1		70					
CLevels of Interest									
	Fraction of L	FL							
Level 1	1.0								
				-	×				

Figure 3-9 Flammable Targets Tab

3.6.1 Flammable Limits

By default, DRIFT extracts the *Lower Flammability Limit* (LFL) and *Upper Flammability Limit* (UFL) for the released substance from the substance property data source (set via **Settings→Substance Data Source**, see Section 2.2). In the case of multi-component releases, DRIFT calculates the flammable limits from those of the components using Le Chatelier's empirical mixing rule.

The Lower and Upper Flammability Limits are displayed and input as %mol/mol values. It should be noted that these limits relate to the flammable components of the mixture only. This means that the mixture of a flammable component (e.g., methane) with a non-flammable component (e.g. air) will have flammability limits the same as that of the pure flammable component.

Check the User Input Flammability Limits box to manually enter the Lower Flammability Limit (LFL) and Upper Flammability Limit (UFL) of the release.

Values for user defined substances can often be found on material safety data sheets (MSDS).

3.6.2 Levels of Interest

Levels of interest to various fractions of the LFL can be added by clicking on the green cross underneath the text box. The fraction can be greater than unity. To delete a level of interest select it by clicking on the level and then clicking the red cross button.
3.7 Defining New Release Substances

Pressing the Define button on the Release Tab displays the dialog box shown in Figure 3-10.



Figure 3-10 Define Substance Dialogue Box

Selecting single component allows the user to specify a new substance and selecting multi-component allows the properties of a mixture of substance to be defined.

3.7.1 Defining a New Single Component Substance

If the user selects **Single component** in the Define Substance dialogue box, the User Defined Substance Properties dialogue box shown in Figure 3-11 is displayed. The input data in this window is initially populated using data for the initially selected database substance. The user can edit/enter new substance property data appropriate for the new substance to be modelled.

🥔 User Defined Substanc	e Properties	? ×
Substance <u>N</u> ame	User Defined Propane]
Molecular <u>W</u> eight	44.097	g mol ⁻¹
Vapour Heat Capacity	1326.06	J kg^1 K -1
Binary <u>D</u> iffusion Coeff in Air	7.00915e-06	m ² s ⁻¹
Is <u>C</u> ondensible?		
Critical Temperature	369.8	к
Liquid <u>D</u> ensity	584.153	kg m ⁻³
Liquid Heat Capacity	2218.98	J kg-1 K -1
Antoine <u>A</u>	15.726	In(mmHg)
Antoine <u>B</u>	1872.46	ln(mmHg) K
Antoine <u>C</u>	-25.16	κ
Heat of Vaporisation at NBP	425900	J kg-1
Heat of Vaporisation <u>I</u> ndex	0.38]
Is <u>F</u> lammable?		
Lower Flammable Limit	2.1	% mol
Upper Flammable Limit	10.1	% mol
	OK	Cancel

Figure 3-11 User Defined Substance Dialogue Box

Required substance property data are:

Substance Name	Name of the substance
Molecular Weight	Molecular weight of the substance in g/mol
Is Condensible	Determines whether the substance can condense as liquid in the cloud. If this is set to false then several of the other inputs below do not need to be input and will be greyed out appropriately.
Critical Temperature	The critical temperature, T _c , in Kelvins.
Liquid Density	The liquid density, assumed to be constant, in kg/m ³ .
Vapour Heat Capacity	Heat capacity of vapour, assumed to be constant, in J/(kg K)
Liquid Heat Capacity	Heat capacity of liquid, assumed to be constant, in J/(kg K).

Antoine Coefficients for Vapour Pressure

The Antoine correlation used by DRIFT is

$$P_{v} = P_{ref} \exp\left(A - \frac{B}{T+C}\right)$$

where P_{v} is the vapour pressure in Pascals, *T* is the temperature in Kelvins, P_{ref} is a conversion factor (=133.322) from millimetres of mercury (mmHg) to Pascals and A, B and C are the Antoine coefficients. The units of A, B and C as used by DRIFT are ln(mmHg), ln(mmHg) K and K respectively.

Note on Antoine coefficients:

A number of different forms of the Antoine correlation are published, some simply involving different units, some using a different base e.g. log_{10} of the vapour pressure instead of the natural logarithm In. It is important to correctly convert from these to the form and units used by DRIFT. For example, if a reference gives Antoine coefficients for Bromine of A = 9.2239 ln(bar), B = 2582.32 ln(bar) K and C = -51.56 K based upon P_{v} being in bar and *T* in Kelvins and an Antoine correlation of the form:

$$\ln(P_{\nu}) = A - \frac{B}{T+C}$$

To convert the above coefficients to the units required by DRIFT we need to adjust the coefficient A by first adding $ln(10^5)$ to convert from ln(bar) to ln(Pascals) and then subtracting ln(133.322) to convert from ln(Pascals) to ln(mmHg). Thus the user would input to DRIFT A = 15.844, with B and C unchanged. A useful check that the Antoine coefficients are correctly entered is, once the User Defined Substance Properties dialogue is accepted, to set the **pressure** on the Release Tab to equal ambient pressure (101325 Pascals) and to press the **Sat Temp.** button. This should set the **temperature** equal the normal boiling temperature in Kelvins. Remember to reset the temperature and pressure to the correct release values after this check.

Heat of Vaporisation

DRIFT determines the heat of vaporisation as a function of temperature, *T* using Watson's formula:

$$\Delta H_{v} = \Delta H_{b} \left(\frac{1 - T / T_{c}}{1 - T_{b} / T_{c}} \right)^{\prime}$$

where ΔH_b is the heat of vaporisation (J/kg) at the normal boiling point T_b (referred to as the latent heat reference value), T_c is the critical temperature and n is an index to parameterise the temperature dependence (n is referred to as the latent heat of vaporisation index).

Guidance: Reid, Prausnitz and Poling (1987) suggest that n is typically 0.38. Where the temperature dependence is not known the user may input the known latent heat with a value of n set to zero.

Binary Diffusion Coeff in Air

The binary diffusion coefficient (in m²/s) of the substance in air is used by DRIFT for calculating vapour deposition to the ground. Vapour deposition is enabled by selecting Deposition to the ground using the Ground Transfer menu option (see Section 3.7). Methods of estimating binary diffusion coefficients are given in for example: Reid, Prausnitz and Poling (1987) "The Properties of Gases and Liquids", ISBN: 0070517991.

Is Flammable, Lower Flammability Limit, Upper Flammability Limit

Checking the isFlammable box specifies that the substance is flammable. When this box is checked the user should enter the lower and upper flammable limits in % by mol.

3.7.2 Defining a Multi-Component Mixture

If the user selects **Multi-component** in the Define Substance Properties dialogue box then Mixture Editor dialogue box shown in Figure 3-12 is displayed.

The Mixture Editor dialogue box allows the user to name a mixture and define its composition.

7	Mixture Editor			? ×
/lixt	ture <u>N</u> ame User Def	ined Mixture		
	Substance Name	Vapour Composition	Liquid Composition	Liquid Phase
1	Air	0	-	-
2	Water	0	0	Miscible
C	omposition defined by	y:	Acrylonitrile	✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓✓<
C	omposition defined by Moles O Mass	y:	Acrylonitrile .iquid Phase 1	✓✓

Figure 3-12 Mixture Editor Dialogue Box

The Mixture Editor allows a wide range of multi-component mixtures to be specified, ranging from simple mixtures of vapour components to multi-component two-phase mixtures. Liquid phases may be specified as either being miscible with water, or as being in a separate distinct liquid phase (immiscible). DRIFT supports there being

multiple distinct liquid phases referred to as 'Liquid Phase 1', 'Liquid Phase 2', etc. Each distinct liquid phase can consist of multiple substance components that are assumed to mix ideally (i.e., obey Raoult's Law) within that phase. 'Miscible with Water' is a special phase reserved for substances that form an ideal solution with water. DRIFT also contains non-ideal mixing models for the hydrogen fluoride-water and ammonia-water interactions.

The user can add mixture components by selecting the substance from the upper drop down menu and specify if the substance is 'Miscible with Water' or add an additional Liquid Phase by using the lower drop down menu. For each additional substance added, a separate phase level can be added for the substance, or it can be added to an existing Liquid Phase.

Example

To model a mixture of water, isobutane and n-butane the user is advised to use Liquid Phase 1 for both isobutane and n-butane as they are both miscible with each other but essentially immiscible with water. If an additional substance was to be modelled which is immiscible with water, isobutene and n-butane then the user would add this substance in the now available Liquid Phase 2.

To add the substance the user selects the name from the drop down list and the liquid phase and clicks the reduction. To delete a substance click on the substances name in the table and then click on the button which becomes available. Note that the air and water options cannot be deleted; however leaving their vapour and liquid compositions as zero will exclude them from the mixture.

The mixture composition can be specified either on a molar or a mass basis depending on the Moles and Mass radio buttons in the 'Composition Defined By' group box.

To input the mixture vapour and liquid composition select the composition to be changed by double clicking on the number and inputting the required value. The input values do not need to add to 1.0, but should result in the correct proportioning between phases and the correct composition within each phase.

At the start of the run DRIFT does a flash calculation to determine the phase content of the initial cloud - consistent with the initial enthalpy, the overall mole fractions (irrespective of phase) and phase equilibrium (if liquid is predicted to be present). In the circumstance that the flash calculation indicates the phase remains all vapour then the mole fractions and temperature will remain unchanged. In the circumstance that there is predicted to be liquid present then the model will determine the partitioning between phases based upon the flash calculation - this will differ from the input phase composition if the initial input conditions are not consistent with phase equilibrium. The flashing is assumed to be instantaneous - therefore the change shows at time t = 0 seconds.

3.8 Ground Transfer

By default, DRIFT neglects heat and mass transfer between the cloud to the ground. However, heat and mass transfer can be modelled as an option.

Selecting the ground transfer option under the main menu bar, **Scenario** \rightarrow **Ground Transfer...** displays the ground transfer window shown in Figure 3-13. Use this option to specify the Heat and Mass Transfer to the ground.

area Ground Transfer	? ×
Heat Transfer to Ground	
Surface Temperature 288.15	к
Deposition to Ground	
Use Fixed Vapour Deposition Velocit	у
Deposition Velocity	m/s
Surface Resistance 1000	s/m
Leaf Area Index 1	
Max Dry Deposition 0.005	kg/m ³
Mean Drop Diameter 5e-5	m
Evaluate only (no removal from cloud)
ОК	Cancel

Figure 3-13 Ground Transfer Dialogue Box

• Heat Transfer to Ground

To calculate the forced/convective heat transfer from the ground requires the ground surface temperature to be input in Kelvin. The default is to neglect heat transfer from the ground.

Deposition to Ground

When the Deposition to Ground tick box is checked, DRIFT will calculate mass transfer (vapour and liquid deposition) from the cloud to the ground when they are in contact. If this option is not selected DRIFT will assume there is no mass transfer from the cloud to the ground.

Optionally a fixed vapour (dry) deposition velocity can be specified by checking the 'Use Fixed Deposition Velocity' checkbox and entering a value for the deposition velocity in m/s.

Alternatively, DRIFT calculates the deposition of vapour based upon the calculated atmospheric resistance. The surface resistance relates to the

resistance at the surface which is likely to be dependent upon the nature of the surface and reactivity of the deposited substance. Zero surface resistance corresponds to all material transported to the surface being absorbed. The leaf area index is a multiplier of the surface area to account for the area of leaves absorbing the material being higher than the planar area of the ground surface.

Max Dry Deposition velocity is for future use only. Currently changing its value has no effect.

Calculation of liquid deposition requires the input of a non-zero mean drop diameter – this is the initial mean drop size after liquid break-up and immediate rainout (specified using *rainout fraction* on the Release Tab -see Section 3.2.7). DRIFT will shrink the mean drop size based upon the evaporation rate calculated by the Homogeneous Equilibrium thermodynamic model. Liquid deposition continuously removes liquid from the cloud base until no liquid remains. Liquid deposited in this way is permanently removed from the cloud and will not re-vaporise.

3.9 Termination Criteria

Selecting the Termination Criteria option under the main menu bar,

Scenario→Termination... displays the Termination Criteria dialogue box shown in either Figure 3-14 or Figure 3-15. If not already terminated due to exceeding the distance to the requested levels of interest, DRIFT will run the dispersion model until one of the Termination Criteria is exceeded.

a Termination Criteria		?	×
			_
Dilution Factor	1e-12		
Minimum Concentration	0.1		ppm
Maximum Travel Distance	100000] m
Maximum Computing Time	18000		s
			_
Maximum <u>T</u> ravel Time	3e+06		s
Maximum Downwind Extent	10000] m
Maximum Crosswind Extent	10000] m
	ОК	Can	ncel

Figure 3-14 Termination Criteria Dialogue Box for Instantaneous Release

Dilution Eactor		1
Maximum Travel Distance 100000] m
Maximum Computing Time 18000] s
		L
Maximum Plume Width 10000] m
OK	Car	vcel



• Dilution Factor

Terminate when the cloud concentration divided by the initial cloud concentration falls below this value.

• Minimum Concentration

Terminate when the cloud concentration in parts per million falls below this value.

• Maximum Travel Distance

This is the maximum distance for the containment cloud to travel in metres. Note that when this distance is very short (e.g. <10m) it may be desirable to decrease the minimum slice separation on the preferences dialog (see Section 5.0) so that the required level of accuracy is maintained.

• Maximum Computing Time

This is the maximum time for DRIFT to run (compute) a release scenario in seconds.

• Maximum Travel Time

This is the maximum time for the cloud to travel, in seconds, before the model terminates.

• Maximum Downwind Extent

This is the maximum downwind spread of the cloud before the model terminates.

• Maximum Crosswind Extent / Maximum Plume Width

This is the maximum crosswind spread of the cloud before the model terminates.

3.10 Obstacles

DRIFT incorporates sub-models for the interaction of dispersing clouds with simple obstacles such as cuboid buildings and linear fences. Interaction with such obstacles can induce extra mixing and spreading of the cloud. Interaction of dispersing clouds with obstacles such as buildings and fences is in reality very complex, the obstacle interaction models in DRIFT are intended only to give an indication of overall bulk effects on the cloud and not a detailed representation of the changes to the concentration in the immediate vicinity of obstacles. DRIFT's obstacle models cover dense and passive releases only (i.e., they are not applicable to momentum jets or buoyant clouds). The user is referred to the EU FLADIS Report (AEA Technology AEA/CS/FLADIS/1994 Vol 2 Issue 1) for the scope and validation of the obstacle models in DRIFT. It should be noted that the obstacle models are not valid in the circumstance that the obstacle lies within the low momentum area source and dilution over the source is being calculated.

Obstacles are specified via the **Scenario** \rightarrow **Obstacles**... menu which displays the Add Obstacles dialogue box shown in Figure 3-16.

Add obstacles	· · ·			?	×
Obstacle collection:	Create a new <u>b</u> uilding				
	Create a new <u>f</u> ence				
	<u>R</u> emove this obstacle from collection				
	<u>C</u> lear all obstacles				
			ОК	Cance	el 🛛

Figure 3-16 Add Obstacles Dialogue Box

Obstacles can either be specified as buildings or fences. Fences can be specified as either an infinite fence a specified distance from the release source or as a finite fence

3.10.1 Buildings

Pressing the 'Create a new building' button causes the Add Obstacles dialogue box to display the inputs shown in Figure 3-17.

Buildings are input as rectangular obstacles inserted at a central coordinate and angle from North of the longest side. The building length, width and angle definitions are illustrated in Figure 3-18.

add obstacles			?	×
Obstacle collection:			- 41	1
Building		Name	Building]
	Create a new	<u>H</u> eight	5] m
	building	<u>W</u> idth	5] m
		<u>L</u> ength	10] m
	Create a new	Angle from north	0	•
	<u>f</u> ence	Centre <u>x</u> -location	50] m
		Centre <u>v</u> -location	0	m
	Remove this obstacle from collection			
		Inserts a cuboidal building angle is taken clockwise f the building.	g at the specified location. Th rom north to the longest edge	e e of
	<u>C</u> lear all obstacles			
			OK Car	ncel

Figure 3-17 Adding a New Building



Figure 3-18 Building Definitions

3.10.2 Fences

Pressing the 'Create a new fence' button causes the Add Obstacles dialogue box to display the inputs shown in Figure 3-19.

		Name	Fence	
Building Fence	Create a new	 Height	2	m
	building	Distance from source	5	m
		Angle from north	0	٥
	Create a new	Centre <u>x</u> -location	50	m
	<u>f</u> ence	Centre <u>v</u> -location	0	m
		<u>L</u> ength	10	m
	Remove this obstacle from collection	The fence is assumed to 60 and 90 degrees to th is being modelled, the je wind direction.	Infinite extend indefinitely and li e wind direction. If a mor t direction should coincide	e Fence ie betwee mentum je e with the

Figure 3-19 Adding a New Fence

Fences can be specified as either an infinite fence a specified distance from the release source or as a finite fence. An infinite fence is always assumed to be perpendicular to the direction of cloud travel at the specified. The geometry (location, length and orientation) of finite fences is defined in the same way as for buildings, except that fences do not require a width.

3.11 Importing Pool Vaporisation Results from GASP

Results from a pool vaporisation calculation using GASP can be directly imported into DRIFT for defining a dispersion scenario. DRIFT requires that the GASP run has been saved as a GASP Version 4 file with file extension *.gasp*.

There are two ways of using GASP results:

- 1. The only source is vaporisation from the pool
- 2. Add the pool source term to a user specified instantaneous, steady continuous, finite duration or time varying release

Case 1: Only source is from Pool Vaporisation

To import the results from a GASP run go to File→Import Gasp Results... on

DRIFT's menu and browse to the .*gasp* file (or click on the sicon on the tool bar). Once the file is imported DRIFT displays graphs of the vaporisation rate, pool radius and pool temperature in tabs in the right-hand window as shown in Figure 3-20. The dotted lines on these graphs show the default segmentation that shall be applied by DRIFT for the run. As for Time Varying releases, the segmentation of the release rate profile is controlled by two parameters - *Release Segment Tolerance* and *Minimum Segment Duration* these can be adjusted from their default values using the Preferences dialogue box available from the **Settings**—**Preferences** menu (see Section 5.0).

DRIFT - D:/Projects/GASP example.gasp					-	Х
Elle Scenario Settings Help						
Description Release Geometry Atmosphere Flammable Toxic	Gasp Vaporisation Rate	Gasp Pool Radius	Gasp Pool Temperature	Gasp Vapour Fraction		ω
Description Belease Geometry Atmosphere Flagmable Togic Type Instantaneous © Gaseous © Gaseous © Gaseous © Finitg Duration © Time Yarying © Gaseous © Competended Liguid / Two-Phase Substance Methane Define, Teggerature Teggerature N/A K Sat Temp. Pressure 101325 Pa Syp Liquid Fraction 0 Pool Results Contaminant Eraction Contaminant Eraction 1 kg/kg Compute Release Segments	Gasp Vaporisation Rate	Gasp Pool Radus	Gasp Pool Temperature	Gasp Vapour Fraction	1,500	2,000

Figure 3-20 Imported GASP Run

In addition to importing time varying source conditions from the GASP file, DRIFT also reads the Atmosphere inputs from the GASP file. Certain inputs on the Release

and Geometry Tabs are not applicable when a GASP run is imported and are disabled (shown as grey).

Targets may be set on the Targets Tab as for other types of release and DRIFT run as described in Section 4.0.

Case 2: Add the pool source term to a user specified instantaneous, steady continuous, finite duration or time varying release

In this case set up the release conditions for the non-pool source. This defines the 'direct' source or primary source which might be the release minus liquid rained out into the pool. Then import the pool source by pressing the 'Pool Results...' button on the Release Tab. DRIFT will run the dispersion from the 'direct' source and pool as separately cloud segments and add together the concentrations from each of these to give an approximation for the combined effect.



Figure 3-21 Example of combined flammable results from a pool and gas jet

Note: DRIFT can sometimes struggle to contour the output from the added segments and the combined results should be inspected carefully before being accepted. In some cases overlapping segments can give unphysical spikes in the concentrationtime history.

4.0 Running the Model and Viewing Output

4.1 Running DRIFT

Once the input model parameters are entered, including setting of target levels,

DRIFT is run by clicking on the **Run Model** v button ,or using the 'Ctrl + R' keyboard shortcut.

DRIFT will then immediately begin calculating your results. Most simulations run very quickly on modern hardware (of the order of a few seconds). Any information or error messages about the calculations will be output to the message window at the bottom of the main window. Once the calculation has terminated, assuming that there were no critical errors, a set of summary graphs and a summary table are displayed in the main window. By default, the displayed graphs for flammable (toxic) targets are the plan and elevation view of the flammable (toxic) hazard ranges and the centre line concentration. The displayed tables include the flammable (toxic) hazard ranges and the tabulated values of centre line concentration. A set of general results showing graphs and tables of centre line (along the curvilinear trajectory) outdoor concentration/dose is also displayed. It is possible to switch between the general, flammable and toxic results by selecting the corresponding tab at the top of the graphs and tables window. Each of the graphs can be selected by clicking on combo box at the bottom left of the graphs and tables window and selecting the graph or table of interest. In the case of a continuous release the flammable centre line results (on the flammable tab) are for zero time-averaging and may differ from those shown on the general and toxic tabs, which include time-averaging.

The default view of the automatically displayed graphs is to show the maximum extent of the hazard ranges over the duration of the release. However the user can examine the hazard ranges at a particular time after the onset of the release by unticking the 'Maximum Over Time' check box and entering a time of interest in the adjacent text box. An example of the main window after a successful simulation is shown in Figure 4-1.

To add grid lines to the graphs for ease of interpretation the user can select the Show Gridlines check box at the top left of the graphs and tables window.

For particular graphs users will be able to select either axis to be logarithmically or linearly scaled for ease of interpretation of results. This is achieved by using the corresponding toggles available on appropriate graphs.

Any changes to the input parameters will automatically invalidate the results, causing the graphs and tabular data to be erased. Therefore the user should save DRIFT run

on completion by clicking on the toolbar button and entering an appropriate run name. There is no need to re-run a model to look at the results as all of the result data is stored along with the input parameters when you save the file to disk. Loading a DRIFT file from disk will automatically display any saved results. DRIFT files are stored on disk with a *.drift* file extension.



Figure 4-1 Main Window after a competed run

The combo box in the bottom left-hand corner of the output window allows the views to be changed between the following:

• Plan view contours

This displays a plan view (XY plane) contour plot of the levels of interest. The default is for the contours to be a *Maximum Over Time* and to *Use Centreline Height*² – these settings ensure that the worst-case contour extents are displayed. Alternatively, the user may specify results at a fixed receiver height by unchecking the *Use Centreline Height* box an entering a height above ground in the *Receiver Height* field. Also, the user may view contours at a specified time for finite duration and time varying releases by unchecking the Maximum Over Time box and entering the required output time in the *Time* box.

• Elevation contours

This displays elevation (XZ plane) view contour plot of the levels of interest. The user may specify output at a particular time as for the plan view contours. The receiver height has no effect on the elevation contour plot.

The contour plotting output from DRIFT is intended to give an approximate graphical indication of the predicted extents of the cloud. In some circumstances, e.g. where there is a rapid bending of the cloud trajectory, then the contour plot may show overlapping cloud sections or omit to show some parts of the contours. It is usually obvious when this occurs and often one view (side elevation or plan) gives a better representation of the contours.

² Use Centreline Height corresponds to the contouring at a height following the centreline trajectory – for an elevated cloud this height will be above ground-level and will change according to the cloud trajectory.

• Centreline graph

This displays the centreline variation of the centreline concentration/dose expressed as either a fraction of the lower flammable limit (LFL) for flammables or for toxics as a fraction of the input levels of interest (concentration or dose). The downstream distance on this plot is the travel distance along the trajectory of the cloud. The user may specify output at a particular time as for the plan view contours. Specifying a receiver height returns the maximum values for the receiver height.

• Tabular Results

For flammables this displays in tabular form: the fraction of LFL at the centreline of maximum concentration, and the horizontal half-width distance (from centreline) to the specified flammable levels of concern. For toxics this displays the centreline fractions of the target criteria and the half-widths to these. The user may specify output at a particular time as for the plan view contours. Specifying a receiver height returns the maximum values for the receiver height.

• Hazard Ranges

This displays a summary of the upstream/downstream distances (*measured along the curvilinear centreline trajectory*) and maximum half-widths to the specified levels of interest. In the case of flammables, additional output is given for the *Flammable Volume* and the *Flammable Mass*. The Flammable Volume is the maximum volume occupied by the flammable mixture plus air which is enclosed by the LFL contour. The Flammable Mass is the maximum mass of flammable contaminant, excluding air, which is enclosed by the LFL contour. The time at which the flammable volume and flammable mass are at their maximum values is displayed in the Worst Case Time fields. By default, the flammable volume and flammable mass calculations include the region of the cloud where the concentration exceeds UFL – optionally this region can be excluded by checking the *Exclude region within UFL* check boxes.

Section 4.3.1 gives information on changing the displayed graphs and tabulated results for user customised results in DRIFT.

4.2 Warning and Error Messages

Any error and warning messages generated during the run are displayed in the message window below the output window. Warning and error messages are listed in Section 6.0

4.3 Output and Reporting

DRIFT provides the facility to customise the output displayed after a calculation has been performed. The user is able to choose which graphs to plot and which variables should be listed in the tabular output display.

The currently defined table and graphs are displayed in the main window immediately after a model run has been completed.

IMPORTANT NOTE: Only the output displayed in the toxic results window and in the toxic results section of the DRIFT report (printed or HTML) include the effect of time averaging. All flammable results are based on short (nearinstantaneous) average values. All custom plots and tables are also based on short (near-instantaneous) average values.

In addition to displaying results within the DRIFT program, it is also possible to obtain a printed hard copy or to export an HTML file of the model specification and a summary of the results. These options are described in more detail in section 4.3.2.

4.3.1 Customising the Output

By default DRIFT is configured to display graphs of the plan and elevation view of the contours to levels of interest, the centreline concentration of the cloud, and tabulated values for the concentration and the maximum hazard ranges. These default values are mirrored for both Toxicity and Flammability targets and can be accessed via the corresponding tabs at the top of the graphs and tables window.

If the default output does not meet your requirements then the output can easily be customised. To open up the dialogue box used to adjust the output, shown in Figure 4-2, click on the 🚔 button on the left of the row of output tabs:

DRIFT - Configure Output View		?	
ne:		Output Type	<u>T</u> abl
Horizontal Axis Variable		Vertical Axis Variable	
	^		^
Ambient Density (kg/m3)		Ambient Density (kg/m3)	
Ambient Pressure (Pa)		Ambient Pressure (Pa)	
Ambient Temperature (K)		Ambient Temperature (K)	
Ambient Vertical Diffusivity (m2/s)		Ambient Vertical Diffusivity (m2/s)	
Ambient Wind Speed (m/s)		Ambient Wind Speed (m/s)	
Cloud Bulk Speed (m/s)		Cloud Bulk Speed (m/s)	
Cloud Bulk Velocity X (m/s)		Cloud Bulk Velocity X (m/s)	
Cloud Bulk Velocity Y (m/s)		Cloud Bulk Velocity Y (m/s)	
Cloud Bulk Velocity Z (m/s)		Cloud Bulk Velocity Z (m/s)	
Cloud Centreline Velocity X (m/s)		Cloud Centreline Velocity X (m/s)	
Cloud Centreline Velocity Y (m/s)		Cloud Centreline Velocity Y (m/s)	
Cloud Centreline Velocity Z (m/s)		Cloud Centreline Velocity Z (m/s)	
Cloud Centroid X (m)		Cloud Centroid X (m)	
Cloud Centroid Y (m)		Cloud Centroid Y (m)	
Cloud Centroid Z (m)		Cloud Centroid Z (m)	
Cloud Density (kg/m3)		Cloud Density (kg/m3)	
Cloud Dimensionless Meander Parameter, kappa	¥	Cloud Dimensionless Meander Parameter, kappa	¥
Linear O Logarithmic		Linear C Logarithmic	
		ОК Са	nc

Figure 4-2 Configure Output View Dialogue Box- Graph

This dialogue box allows the user to select between graphical and tabular results. If the graphical option is selected, then DRIFT displays a list of possible graphs to choose from. When OK is selected, the appropriate graph will appear in a new tab on the output window. In addition, by filling in the *name* field on the output configuration window, the user can give this tab a unique name for ease of reference. A complete list of Axis Variables can be found in the tables in Appendix 1.

If the table option is checked, then the output configuration dialogue box changes to that shown in Figure 4-3.

a DRIFT - Configure Output View				? ×
Name:				Output Type
Available Global Variables:			Selected Variables:	
Ambient Density (kg/m3) Ambient Pressure (Pa) Ambient Temperature (K) Ambient Vertical Diffusivity (m2/s) Ambient Wind Speed (m/s) Cloud Bulk Speed (m/s) Cloud Bulk Velocity X (m/s) Cloud Bulk Velocity Y (m/s) Cloud Bulk Velocity Z (m/s) <	^ >	Add	Cloud Travel Distance (m)	Move Up Move Down
Available Component Variables: Component Liquid Molar Flux (mol/s) Drop Radius (m) Liquid Fraction Liquid Molar Flux (mol/s) Liquid Mole Fraction Molar Flux (mol/s) Mole Fraction Number Flux of Drops (/s) Phase Balance	•	Add		
				OK Cancel

Figure 4-3 Configure Output View Dialogue Box - Table

From this dialogue box the user can add any selection of output variables into a custom table. The upper list of variables refers to general properties of the cloud as a whole; the lower list of variables refers to properties of the individual cloud components. The user's choice of variable can be added to the table by clicking on its name and pressing the appropriate "add" button (the upper button relates to the upper list of variables; the lower button relates to the lower list of variables). Once the table is populated with variables, the columns themselves can be reordered, or removed altogether, by clicking on the name of the variable in question and using the "move up", "move down" and "remove" buttons.

To remove an output graph or table, simply select the tab in question and click on the small 💿 icon that is positioned at the end of the row of output tabs.

4.3.2 Reporting

DRIFT provides the capability to produce simple reports about a model run. The reports produced by DRIFT are either sent to the printer to obtain a hard copy or exported to an HTML file for online viewing. In both report types, DRIFT outputs a complete listing of the input parameters, a log of any error or information messages that were output during the model run, and a graph of the dispersion distances to the flammable and toxic limits at a worst-case time.

To print out a copy of a report from DRIFT, run your model as normal and then select the **File**→**Print Report...** menu item, click on the → toolbar button or press the 'Ctrl

+ P' keyboard shortcut. This will display a standard print dialog from which you can choose the printer to use and any other print options.

To produce an HTML report, select the **File→Export to HTML...** menu item or click

on the solution. This will display a file selection dialog which may be used to decide where to save the HTML report to. DRIFT will automatically suggest a report name that has the same name as your *.drift* file but with an *.html* extension (if you have saved one that is). Once you click OK in the file dialog, DRIFT will save your report. As a part of this process DRIFT will also create an image file that contains the flammable plan view graph. This file will be saved in the same directory as the HTML report and will be called *"<basename>_gflammablePlanView.png"* where <basename> is the name that you selected for your HTML report. If you move your HTML report to another location at a later date, it is important to remember to move the .png file too; otherwise you will not see the graph when you open the report in a browser.

4.3.3 Printing graphs

DRIFT also allows users to print out individual graphs as a hard copy or to export graphs as graphics files (.png files) so that they may be included into other documents (e.g. MS Word or Excel). To output a graph, simply select the graph that you wish to save in the main window by clicking on the corresponding tab, and then choose either the **File→Print Selected Graph** or **File→Export Current Graph** menu item. Then proceed as for a printed report or an exported HTML report as describe above.

5.0 Preference Settings

Preferences settings may be accessed and changed via the **Settings** \rightarrow **Preferences** menu which displays the Preferences dialogue box shown in Figure 5-1.

Preferences	?	×
Distance Precision	0.05	m
Time Precision	0.25	s
Release Segmentor Tolerance	0.3	
Mininum Segment Duration	1	s
Number Of Points on Contour Plots	50	
Minimum Slice Separation (Continuous)	0.25	m
Minimum Slice Separation (Instantaneous)	0.25	s
Maximum Slice Separation (Continuous)	1e+10	m
Maximum Slice Separation (Instantaneous)	100	s
Tabular Output Decimal Precision	6	sf
Inverse <u>B</u> owen Ratio	0	
Sol <u>v</u> er Tolerance	1e-05	
Finite Duration Model Time Series Precision	0.1	
Finite Duration Model Time Series Extent	3	
	OK Ca	ancel

Figure 5-1 Preferences Dialogue Box

• Distance Precision

The precision in metres with which to solve for distances to concentration and dose.

Time Precision

The precision in seconds when solving for the time of a particular event, e.g. for determining the time of maximum concentration or maximum flammable volume.

• Release Segmentor Tolerance

The tolerance that DRIFT uses for converting a time varying release into discrete segments. This specifies the maximum fractional change allowed in release rate between consecutive segments. In general a smaller value produces a greater number segments.

Minimum Segment Duration

The minimum duration that DRIFT uses for converting a time varying release into discrete segments. This specifies the minimum time duration of a segment.

• Number of Points on Contour Plots

The number of points that are used for plotting each contour. Increase this number to produces greater detail or smoother plots. A higher number of points will require a longer time to generate the contour plots.

• Minimum Slice Separation (Continuous)

DRIFT's continuous model stores output by writing results to a number of discrete 'slices' with each slice corresponding to results at a particular downstream distance. The minimum slice separation specifies the minimum downstream distance step in metres between output slices. Note that for dispersion runs that occur over very short distances this parameter may need to be decreased to maintain the required level of accuracy and smoothness.

• Minimum Slice Separation (Instantaneous)

DRIFT's instantaneous model stores output by writing results to a number of discrete 'slices' with each slice corresponding to results at a particular time after release. The minimum slice separation specifies the minimum time step in seconds between output slices. Note that for dispersion runs that terminate very quickly this parameter may need to be decreased to maintain the required level of accuracy and smoothness.

• Maximum Slice Separation (Continuous)

DRIFT's continuous model stores output by writing results to a number of discrete 'slices' with each slice corresponding to results at a particular downstream distance. The maximum slice separation specifies the maximum downstream distance step in metres between output slices.

Maximum Slice Separation (Instantaneous) DRIET's instantaneous model stores output by w

DRIFT's instantaneous model stores output by writing results to a number of discrete 'slices' with each slice corresponding to results at a particular time after release. The maximum slice separation specifies the maximum time step in seconds between output slices.

Tabular Output Decimal Precision

Specify the number of significant figures to be included in tabular output

Inverse Bowen Ratio

The Bowen ratio, B_0 , is the ratio of the sensible heat flux from/to the ground surface to the latent heat flux due to evaporation/condensation of water at the ground surface. In the case of zero evaporative flux at the surface the Bowen ratio is infinite, therefore it is more convenient to work with the inverse Bowen ratio $1/B_0$. $1/B_0$ is dependent upon the nature of the ground surface. If the humidity and air temperature are known at two heights, then $1/B_0$ can be determined (see e.g. Panofsky and Dutton, 1984, Atmospheric Turbulence, ISBN 0-471-05714-2). For daytime conditions $1/B_0$ is positive ranging from 10 for water bodies to 1 for temperate grasslands and 0.1 for deserts. At night-time $1/B_0$ may take either sign and is difficult to determine using simple weather schemes. The default in DRIFT is for $1/B_0=0$ which implies a constant specific humidity with height.

Solver Tolerance

The solver tolerance determines the accuracy to which DRIFT will solve its equation set. The lower the tolerance the more accurate the solution; the higher the tolerance the faster the model will run. Occasionally the solver may run into difficulties when the equation set enters a new regime - increasing the tolerance may alleviate this.

• Finite Duration Model Time Series Precision

Determines the accuracy to which DRIFT calculates the dose received in the finite duration and time-varying models. The smaller the value the more accurate the results, but the longer the model will take to run.

Finite Duration Model Time Series Extent

This parameter is used in the calculation of dose in the finite duration and time-varying models. It controls how far into the tails of the dose distribution to calculate the concentration time series. The number entered is internally multiplied by a typical timescale taken for the cloud to pass through the particular point of interest. Larger values of this parameter lead to more accurate results. The default value is 3.

6.0 List of Warning and Error Messages

Warning and error messages output by DRIFT are given in the following table.

Warning Message	Additional Explanation/Guidance
All of the release is liquid and has rained-out. Terminating model	Complete liquid deposition has occurred for a sub-cooled liquid source. Check that the release conditions do correspond to a sub-cooled liquid and
	that appropriate values have been used for rainout fraction (Section 3.2.7) and liquid deposition drop size (Section 3.8).
A steady source window could not be established during the duration of the release.	This message implies that the release has not yet reached state conditions by the time that the release (or release segment) ends - applies only when calculating dilution over a low momentum area source or from a GASP pool vaporisation run. For finite duration, time varying and GASP pool options this message is for information only – the model will attempt to model the transient cloud. For the 'steady continuous' release try re-running using the finite duration option. This message should not result from an instantaneous release.
At xx m downstream from the source At t = xx s	Information regarding changes occurring at a particular downstream distance or cloud travel time.
the cloud centreline has started to lift-off from the ground	
the cloud centreline has reached ground-level	
the cloud has fallen below the top of the atmospheric boundary layer	
the cloud has hit the top of the atmospheric boundary layer (assumed to be impervious)	
liquid is now present in the cloud in phase z	Liquid phases are referred to by number 0: represents a phase that is
there is no liquid remaining in the cloud in phase z	phase etc
At xx s the cloud has diluted below the level of interest	This message may be given when calculating dilution over the source. It

Warning Message	Additional Explanation/Guidance
before a steady source window could be established.	indicates that the cloud is predicted to have diluted below the lowest level of interest before steady state conditions are established.
The results shown are from the transient model.	In the circumstance of a finite duration, time varying or GASP pool options DRIFT automatically uses its transient model and no further user intervention should be required.
To see the time-dependent output from the transient cloud please re-run the model with the finite-duration option selected.	In the circumstance that the user is running the steady continuous model it is necessary to re-run using the finite duration model
At a downstream distance of xx m and a centroid height of hh m the cloud has left the xxxx layer and has now entered the yyyy layer	Here xxxx and yyyy refer to named layers in the atmosphere (see Mathematical Model Description for details)
At a time of xx s and a centroid height of hh m the cloud has left the xxxx layer and has now entered the yyyy layer	Here xxxx and yyyy refer to named layers in the atmosphere (see Mathematical Model Description for details)
AtmosphericBoundaryLayer::computeStrata: Numerical routine has failed to find a solution.	This message indicates a problem initialising the layers in atmosphere model. Please check input data. If the problem persists contact DRIFT support.
AtmosphericBoundaryLayer::getVerticalDiffusivity: The input height is above the AtmosphericBoundaryLayer	This message indicates that the model is attempting to determine conditions outside the atmospheric boundary layer. Please check input data – in particular the source height and inversion height. If the problem persists contact DRIFT support.
AtmosphericBoundaryLayer::getVerticalDiffusivityDerivative: The input height is above the AtmosphericBoundaryLayer	This message indicates that the model is attempting to determine conditions outside the atmospheric boundary layer. Please check input data - in particular the source height and inversion height. If the problem persists contact DRIFT support.
AtmosphericBoundaryLayer::getVerticalDiffusivityIndex: Error. Diffusivity not well defined at this height.	This message indicates that the model is attempting to determine conditions outside the atmospheric boundary layer. Please check input data - in particular the source height and inversion height. If the problem persists contact DRIFT support.
AtmosphericBoundaryLayer::update: The roughness height is higher than the surface layer.	The roughness height is required to be less than 0.1 times the boundary layer height. Please specify a lower roughness height or increase the inversion height.
Calculating initial cloud dilution using the transient	For information only.

Warning Message	Additional Explanation/Guidance
model	•
Could not load results for time-varying model:	Indicates a problem loading the results from a time-varying model run.
inconsistency between inputs and stored results.	Please check the input data and try rerunning. If the problem persists
	contact DRIFT support.
DRIFTCloudODEModel::interpolateSlice. No results available.	This indicates an attempt by the model to interpolate between results slices
	when no results are available. This may indicate another problem that has
	caused the model not to run. Please check input data. If the problem
	persists contact DRIFT support.
DRIFTContinuousModel::initialise has failed.	This message indicates a problem initialising the continuous model. Please
	check input data. If the problem persists contact DRIFT support.
DRIFTContinuousModel::initialise::solve: No solution could	This message indicates a problem initialising the continuous model. Please
be found	check input data. If the problem persists contact DRIFT support.
DRIFTInstantaneousGeometryInitialisor::solve: No solution	This message indicates a problem initialising the instantaneous model.
could be found.	Please check input data. If the problem persists contact DRIFT support.
DRIFTContinuousProfile::update_3() Exception thrown when	This indicates a problem with the numerical solution. Please check input
evaluating profile functions.	data. If the problem persists contact DRIFT support.
DRIFTVerticalProfile::F_tilde_v: The profile index 's' is	This indicates a problem with the numerical solution. Please check input
equal to zero.	data. If the problem persists contact DRIFT support.
DRIFTVerticalProfile::F_tilde_v() Exception thrown when	This indicates a problem with the numerical solution. Please check input
evaluating vertical profile function.	data. If the problem persists contact DRIFT support.
DRIFTVerticalProfile::H_tilde: The profile index 's' is	This indicates a problem with the numerical solution. Please check input
equal to zero.	data. If the problem persists contact DRIFT support.
<pre>ExpandedGasousJetSource::ExpandedGaseousJetSource()</pre>	Please check the vapour heat capacity data and units for the released
ratioOfSpecificHeats=1	substance.
For the given inputs the atmospheric boundary layer is	A warning message indicating that the atmospheric conditions in this very
predicted to be a pure Intermittency Layer. The physics of	stable regime where there is no reliable model - dispersion in surface layer
this regime is not well-understood and so DRIFT will	conditions is assumed.
instead assume that the cloud remains within the surface	
layer for the duration of this run. If this is problematic,	
try either reducing the mixing height or selecting a less	
stable atmosphere.	
GaspData::GaspData: Unable to load Gasp run.	Please check the location of the GASP file and that this is a valid Gasp 4.0
	run, it necessary by re-running Gasp Version 4 and resaving.
HydrogenFluorideMixture::initialise: No solution could be	Problem initialising a hydrogen fluoride-water mixture. Please check input

Warning Message	Additional Explanation/Guidance
found	data. If the problem persists contact DRIFT support.
No solution could be found to the flashing equations.	This indicates a problem in finding a solution to the flashing equations for the
	release. Please check input data. If the problem persists contact DRIFT
No solution to the flashing equations could be found. Run	support.
terminated.	
Obstacle related messages:	Information messages relating to building and fence obstacles. More
	information about the obstacles model and the Britter Criteria can be found
Low area momentum source in near wake <i>obstacle</i> of editing	in section IVa of the FLADIS report ("Complex Features in Dense Gas
source accordingly.	Dispersion Modelling", D.M. Webber, December 1994, AEA contract
Prittor critoria violated for obstacle Terminating	research report).
calculation	
Ignoring <i>obstacle</i> for upstream calculation: source is not	
in near wake.	
Ignoring upstream <i>obstacle</i> : only taken into account for a	
low momentum area source.	
Ignoring <i>obstacle</i> for upstream calculation: only taken into	
account for a low momentum area source.	
Source is too close to <i>obstacle</i> and just upstream of it.	
Terminating calculation.	
Ignoring obstagle for timewarking model	
ignoring obstacle for timevarying model.	
Pasquill Stability x is unlikely to occur for wind speeds \geq	A warning message indicating that the input Pasquill stability class is unlikely
v m/s	to occur with such a high wind speed. Please check your input data.
Plume velocity is zero. Terminating run.	Check input release rate is not zero and that rainout is less than 100%. If
	the problem persists contact DRIFT support.
Run terminated after xx s / xx m.	Information on the reasons that the model run terminated.
Maximum computing time exceeded.	

Warning Message	Additional Explanation/Guidance
Specified maximum downstream distance exceeded.	
Specified maximum plume width exceeded.	
Specified maximum cloud time exceeded.	
Specified minimum concentration level reached.	
Dilution factor has dropped below specified value.	
Steady source window established after xx s. Proceeding to	Information message when calculating dilution over a low momentum area
run continuous model.	source.
Strata::getAtmosphericLayer: Error. Height is negative.	This message indicates that the model is attempting to determine conditions outside the atmospheric boundary layer. Please check input data. If the problem persists contact DRIFT support.
SubstanceDataSourceSPI::substance() No entry found for	Indicates missing substance property data from the substance SPI file
Antoine coefficients	
boiling point	
critical pressure	
critical temperature	
enthalphy of vaporisation	
flammability	
liquid density	
liquid specific heat	
molecular weight	
vapour specific heat	
Incomplete flammability information	Upper and lower flammability limits must be entered if the substance is specified as being flammable
SubstanceMixture::calcRatioOfSpecificHeats. Cv=0.0	Check the vapour heat capacity data and units for the released substance.
SubstancePropertiesDB: Unable to find substance of this	Check that the correct path is entered for the ESRSubstance and where
name.	applicable SPI file data sources. See Section 2.2.
The cloud centroid is initially within the xxxx Layer	This message is for information only – indicating that the cloud centroid is so
	elevated that it is initially within the named layer of the atmosphere. No
	message is given if the cloud centroid is in the surface layer (lowest layer of
	atmosphere). Please check that the input source elevation and the

Warning Message	Additional Explanation/Guidance
	predicted initial cloud height are both reasonable for your scenario.
The file is not a DRIFT file.	This message results from attempting read a file that is not a DRIFT file.
The file is not a DRIFT version xxxx file .	The DRIFT file version being read is not compatible with this version of DRIFT.
The initial cloud height is predicted to be higher than the atmospheric boundary layer.	The initial height of the cloud is predicted to be above the atmospheric boundary layer. DRIFT only models dispersion within the atmospheric boundary layer. Please check that the input source elevation and the predicted initial cloud height are both reasonable for your scenario.
The initial release is predicted to contain a pure liquid phase. Run terminated.	This message is issued when the release is predicted to be completely in the liquid phase and an instantaneous release is being modelled. This may occur if the release is a sub-cooled liquid. Due to relatively inefficient sub- cooled liquid break-up, DRIFT's instantaneous model is considered to be inappropriate for such releases and no run is performed.
The initial release is predicted to be all liquid. Mixing in the minimal amount of air necessary to run.	This message is issued when the release is predicted to be completely in the liquid phase and a continuous release is being modelled. This may occur if the release is a sub-cooled liquid. DRIFT will model the release as a finely atomised spray/mist. All the liquid that is not rained out immediately at the source (see Section 3.2.7) is assumed to remain airborne unless the liquid deposition is specified (see Section 3.8). The user should ensure that the release conditions are commensurate with the formation fine drops/mist – usually this would mean high pressure and small orifice dimension. A minimal amount of air is initially mixed into an all liquid release to allow DRIFT to run – this initial amount of air is so small it has no effect on predicted concentrations.
The input radius is unphysical. The cloud will be assumed to have a unit aspect ratio.	This indicates a problem with the input radius being too small for the instantaneous release. In this circumstance DRIFT will calculate the radius based on a unit aspect ratio (radius=height) cloud.
The source location is above the atmospheric boundary layer. Setting the height to be the mixing height.	The specified source height is above the atmospheric boundary layer (the inversion height). In this circumstance DRIFT assumes that the height is at the mixing height (equal to the inversion height). Please check the input data - in particular the source height and inversion height.
ToxicConcentrationField::convertFromToxicSubstanceCriteria. Cannot find substance.	No substance is found from which to extract toxic criteria. Please check that toxicity data has been entered for all toxic substances and that the substance property data source directories are correctly set (see Section

Warning Message	Additional Explanation/Guidance
	2.2)
Unable to run model.	Messages indicating reasons why DRIFT is unable to run the model.
Cloud radius is less than or equal to zero.	
Cloud mass is less than or equal to zero.	
Composition Data not set.	
Contaminant not set.	
Contaminant mass fraction is less than or equal to zero.	
Contaminant mass fraction is greater than unity.	
Duration is less than or equal to zero	
Exit Data not set	
Flammable Target Data not set	
Input Data not set.	
Liquid fraction greater than unity.	
Liquid fraction less than zero.	
Mixture Data not set	
Mixture information not set.	
One or more of the source radii is less than or equal to	
zero.	
Preferences not set	
Pressure less than or equal to zero.	
Rainout fraction exceeds unity.	
Rainout fraction less than zero.	
Release profile not set	
Release rate is less than or equal to zero	
Release rate negative.	
Release rate profile has a negative time entry.	
Release rate profile has been input in the wrong order.	
Source Data not set	
The orifice radius is less than or equal to zero.	
Temperature is less than or equal to absolute zero.	
Termination Criteria not set	
Toxic Target Data not set	
Weather Data not set	
Zero mass release: terminating calculation	A zero mass release is predicted. Please check the input data, in particular

Warning Message	Additional Explanation/Guidance
	the release mass, release rate, release duration and rainout fractions.

A1.1 Axis Variables – Continuous Release

Axis Variable (Units)	Description
Ambient Density (kg/m ³)	Ambient air density at the height corresponding to cloud
	centroid height Z
Ambient Pressure (Pa)	Ambient pressure at the height corresponding to cloud
	centroid height Z
Ambient Temperature (K)	Ambient temperature at the height corresponding to
	cloud centroid height Z
Ambient Vertical	Ambient vertical diffusivity at the height corresponding
Diffusivity (m²/s)	to cloud centroid height Z
Ambient Wind Speed	Ambient wind speed at the height corresponding to
(m/s)	cloud centroid neight 2
Cioud Bulk Speed (m/s)	Speed of the cloud averaged over the plume closs-
Cloud Controling Valacity	X component of the cloud controline velocity
X (m/s)	
Cloud Centreline Velocity	Y-component of the cloud centreline velocity
Y (m/s)	
Cloud Centreline Velocity	Z-component of the cloud centreline velocity
Z (m/s)	
Cloud Centroid X (m)	X coordinate of the cloud centroid, defined as the mean
	height computed from the vertical concentration profile.
Cloud Centroid Y (m)	Y coordinate of the cloud centroid, defined as the mean
	height computed from the vertical concentration profile.
Cloud Centroid Z (m)	Z coordinate of the cloud centroid, defined as the mean
	height computed from the vertical concentration profile.
	This differs from Cloud Location Z when grounded but
	will be the same as Cloud Location Z in the limit of a
	fully elevated cloud.
Cloud Density (kg/m ²)	I he cloud density corresponding to the centreline
Cloud Dimonsionloss	
Moondor Paramotor	Parameter κ_{\uparrow} in the vertical meander model
kanna	
Cloud End Cap Profile	Length-scale a for the end-cap of the cloud (used in the
Parameter aEndCap (m)	finite duration model)
Cloud Excess Centreline	X-component of the vector difference between the
Velocity X (m/s)	plume velocity and the undisturbed ambient velocity
Cloud Excess Centreline	Y-component of the vector difference between the
Velocity Y (m/s)	plume velocity and the undisturbed ambient velocity
Cloud Excess Centreline	Z-component of the vector difference between the
Velocity Z (m/s)	plume velocity and the undisturbed ambient velocity
Cloud HF Monomer	The HF monomer vapour fraction, x_M
Vapour Fraction	
Cloud Half Width (m)	The cloud integral half-width, W
Cloud Height (m)	The cloud integral height, H
Cloud Lengthscale	Parameter used in the spreading model related to the
Omega (m)	half-width.
	Parameter used in the spreading model related to the
	ena-cap wiath.
Cloud Location X (M)	A location of the cloud

Axis Variable (Units)	Description
Cloud Location Z (m)	Z location of the cloud (zero for a ground-based cloud)
Cloud Maximum Concentration Distance (m)	Curvilinear distance along the locus of the maximum concentration
Cloud Maximum Concentration Locus X (m)	X coordinate of the locus of the maximum concentration (used for contouring).
Cloud Maximum Concentration Locus Y (m)	Y coordinate of the locus of the maximum concentration (used for contouring)
Cloud Maximum Concentration Locus Z (m)	Z coordinate of the locus of the maximum concentration (used for contouring)
Cloud Maximum Concentration Planar Distance (m)	Curvilinear distance along the locus of the maximum concentration projected onto the horizontal plane
Cloud Meander Parameter, chi_w (m ² s)	χ_w in the cloud vertical meander model
Cloud Mixing Height Contact Ratio (f_h)	A measure of the amount of contact between the cloud and the top of the mixing layer. $f_h = 0$ corresponds to
	no contact, $f_h = 1$ corresponds to full contact.
Cloud Molar Enthalpy Difference (J/mol)	The molar enthalpy difference of the cloud mixture at the cloud temperature and pressure. The difference is relative to a standard reference temperature and pressure.
Cloud Molar Volume (m ³)	The molar volume of the cloud mixture at the cloud temperature and pressure
Cloud Profile Factor Integral 1	The profile integral I_n with n = 1
Cloud Profile Factor Integral 2	The profile integral I_n with n = 2
Cloud Profile Factor Integral 3	The profile integral I_n with n = 3
Cloud Profile Lengthscale a (m)	Length scale parameter a used in concentration profile F_η
Cloud Profile Lengthscale b (m)	Length scale parameter b used in horizontal concentration profile, F_h
Cloud Profile Parameter f_g	Ground based to elevated cloud interpolation function, $f_g = 1$ corresponds to a fully grounded cloud, $f_g = 0$ corresponds to a fully elevated cloud
Cloud Profile Parameter s	The vertical profile parameter s
Cloud Profile Parameter w	The horizontal profile parameter w
Cloud Profile Parameter w_g	The ground based horizontal profile parameter w_g
Cloud Profile Sigma Y (m)	The standard deviation of the horizontal concentration profile (before the effects of time-averaging/lateral meander are applied).
Cloud Profile Sigma Y (incl. lateral meander) (m)	The standard deviation of the horizontal concentration profile (after the effects of time-averaging/lateral meander are applied).

Axis Variable (Units)	Description
Cloud Relative Density	The relative density difference between the cloud and
Difference (rho/rho_a-1)	$\rho - \rho_{a}$
	the surrounding air, $\Delta = \frac{\rho_a}{\rho_a}$ where ρ is the cloud
	density and $ ho_{a}$ is the air density
Cloud Relative	The relative temperature difference between the cloud
Temperature (T/Tref-1)	and the surrounding air
Cloud Richardson	The Richardson number for the cloud defined by
Number, Ri*	
	$B^{\prime} = g\Delta^{\prime}H$
	$Rl_* = -\frac{u^2}{u^2}$
	u_*
	where g is the acceleration due to gravity, Δ ' is the
	cloud relative density difference and u_{*} is the friction
	velocity which is a characteristic turbulent velocity scale
	in the atmosphere.
Cloud Stagnation	The cloud stagnation temperature corresponding to the
Temperature (K)	centreline concentration
Cloud Tangent Of Lean	The tangent of the angle that the cloud centroid axis
Over Angle	makes with the vertical, ζ
Cloud Temperature (K)	The cloud temperature corresponding to the centreline
	concentration
Cloud Tilt Parameter	The cloud tilt parameter
Cloud Total Liquid Molar	The cloud total liquid molar flux passing through the
Flux (mol/s)	cloud cross-section
Cloud Total Mass Flux	The cloud total mass flux passing through the cloud
(kg/s)	cross-section
Cloud Total Molar Flux	The cloud total molar flux passing through the cloud
(mol/s)	cross-section
Cloud Trajectory Angle To	The angle the cloud trajectory makes with the horizontal
Horizontal (rad)	
Cloud Travel Distance (m)	The curvilinear travel distance along the cloud centreline
	trajectory
Cloud Travel Time (s)	The travel time corresponding to the curvilinear travel
	distance along the cloud centreline trajectory
Cloud Vapour Fraction	The overall vapour mole fraction of the cloud mixture
Cloud Vertical Meander	The characteristic time t_{\uparrow} used in the vertical meander
Time (s)	model
Component Liquid Molar	The liquid molar flux for each substance component of
Flux (mol/s)	the cloud
Drop Radius (m)	The mean drop size radius for each distinct liquid phase
Liquid Fraction	The liquid moles for each distinct liquid phase as a
-	fraction of the total moles
Liquid Molar Flux (mol/s)	The molar flux of each distinct liquid phase liquid phase
Axis Variable (Units)	Description
------------------------------	---
Liquid Mole Fraction	Liquid mole fraction, x_i for each component substance
	in the cloud
	$r_{i} = \frac{\mu_{iL}}{\mu_{iL}}$ where μ_{i} is the liquid molar flux of
	μ_{iL}
	component <i>i</i> and $\mu_{\iota L}$ is the total liquid molar flux
Molar Flux (mol/s)	Molar flux (irrespective of phase) of each component
Mole Fraction	Mole fraction (irrespective phase) of each component
	substance in the cloud
Number Flux of Drops (/s)	Number of drops of each distinct liquid phase that pass
	through the cloud cross-section per second
Phase Balance	The phase balance of a component is defined by
	$y_i - x_i \gamma_i P_i / P$
	where y_i is the vapour mole fraction of component <i>i</i> , x_i
	is the liquid mole fraction, P_i is the pure substance
	vapour pressure and γ_i is the activity coefficient in the
	liquid mixture
Pure Vapour Pressure (Pa)	The pure substance vapour pressure P_i of each
	component
Vapour Molar Flux (mol/s)	Molar flux of substance in the vapour phase μ_{iv}
Vapour Mole Fraction	Vapour mole fraction, y_i for each component substance
	in the cloud
	$y_i = \frac{\mu_{iv}}{\mu_{iv}}$ where μ_{iv} is the vapour molar flux of
	component <i>i</i> and μ_{iv} is the total vapour molar flux

A1.2 Axis Variables – Instantaneous Release

Axis Variable (Units)	Description
Ambient Pressure (Pa)	Ambient pressure at the height corresponding to the
	plume centroid coordinate at time t
Ambient Temperature (K)	Ambient temperature at the height corresponding to the
	plume centroid coordinate at time t
Cloud Centroid X (m)	X coordinate of the cloud centroid, defined as the mean
	height computed from the vertical concentration profile.
Cloud Centroid Y (m)	Y coordinate of the cloud centroid, defined as the mean
	height computed from the vertical concentration profile.
Cloud Centroid Z (m)	Z coordinate of the cloud centroid, defined as the mean
	height computed from the vertical concentration profile.
	This differs from Cloud Location Z when grounded but
	will be the same as Cloud Location Z in the limit of a
	fully elevated cloud.
Cloud Density (kg/m ³)	The cloud density corresponding to the centreline
	concentration
Cloud Excess Velocity X	X-component of the vector difference between the
(m/s)	centroid velocity and the undisturbed ambient velocity
Cloud Excess Velocity Y	Y-component of the vector difference between the
(m/s)	centroid velocity and the undisturbed ambient velocity
Cloud Excess Velocity Z	Z-component of the vector difference between the
(m/s)	centroid velocity and the undisturbed ambient velocity
Cloud HF Monomer	The HF monomer vapour fraction, x_M
Vapour Fraction	
Cloud Height (m)	The cloud height, H
Cloud Lengthscale	Integral length scale Λ_2
Lambda Crosswind (m)	
	Integral length scale Λ_1
	Curvilinger distance clang the locus of the merimum
	curvilinear distance along the locus of the maximum
Distance (m)	concentration
Cloud Maximum	X coordinate of the locus of the maximum concentration
	(used for contouring)
(m)	(used for contourning)
Cloud Maximum	Y coordinate of the locus of the maximum concentration
Concentration Locus Y	(used for contouring)
(m)	
Cloud Maximum	Z coordinate of the locus of the maximum concentration
Concentration Locus Z	(used for contouring)
(m)	(acca ici conica in g)
Cloud Molar Enthalpy	The molar enthalpy difference of the cloud mixture at
Difference (J/mol)	the cloud temperature and pressure. The difference is
	relative to a standard reference temperature and
	pressure.
Cloud Molar Volume (m ³)	The molar volume of the cloud mixture at the cloud
	temperature and pressure
Cloud Profile Lengthscale	Cloud profile longitudinal length scale a
a_1 (m)	

Axis Variable (Units)	Description
Cloud Profile Lengthscale a_2 (m)	Cloud profile lateral length scale a_2
Cloud Profile Lengthscale a_3 (m)	Cloud profile vertical length scale a_3
Cloud Profile Parameter	Ground based to elevated cloud interpolation function,
f_g	$f_{a} = 1$ corresponds to a fully grounded cloud, $f_{a} = 0$
	corresponds to a fully elevated cloud
Cloud Profile Parameter s	The vertical profile parameter s
Cloud Profile Parameter w	The horizontal profile parameter w
Cloud Profile Parameter	The ground based borizontal profile parameter w
w_g	
Cloud Profile Sigma Y (m)	The standard deviation of the horizontal concentration profile
Cloud Relative Density	The relative density difference between the cloud and
Difference (rho/rho_a-1)	the surrounding air, $\Delta' = \frac{\rho - \rho_a}{\rho_a}$ where ρ is the cloud
	density and ρ_a is the air density
Cloud Relative	The relative temperature difference between the cloud
Temperature (T/Tref-1)	and the surrounding air
Cloud Richardson	The Richardson number for the cloud defined by
Number, Ri*	
	\mathbf{p} : $g\Delta' H$
	$Kl_* = \frac{u_*^2}{u_*^2}$
	where g is the acceleration due to gravity. Λ' is the
	cloud relative density difference and u is the friction
	volgeity which is a characteristic turbulent volgeity apple
	in the atmosphere
Cloud Stagnation	The cloud stgnation temperature corresponding to the
Temperature (K)	centreline concentration
Cloud Tangent Of Lean	The tangent of the angle that the cloud centroid axis
Over Angle	makes with the vertical, ζ
Cloud Temperature (K)	The cloud temperature corresponding to the centreline
	concentration
Cloud Tilt Parameter	The cloud tilt parameter
Cloud Total Mass (kg)	Total mass of the cloud
Cloud Total Number of	Total number of liquid moles in the cloud
Liquid Moles	Total number of males in the sloud
	Total number of moles in the cloud
Cloud Travel Distance (m)	Curvilinear distance of travel of cloud centroid
Cloud Travel Time (s)	The travel time corresponding to the plume centroid
Cloud Vapour Fraction	The vapour fraction of the cloud
Cloud Velocity X (m/s)	X-component of the cloud centreline velocity
Cloud Velocity Y (m/s)	Y-component of the cloud centreline velocity
Cloud Velocity Z (m/s)	Z-component of the cloud centreline velocity
Cloud Location X (m)	X location of the cloud
Cloud Location Y (m)	Y location of the cloud
Cloud Location Z (m)	Z location of the cloud (zero for a ground-based cloud)

Axis Variable (Units)	Description
Component Liquid Moles	The liquid molar flux for each substance component of
	the cloud
Drop Radius (m)	The mean drop size radius for each distinct liquid phase
Liquid Fraction	The liquid moles for each distinct liquid phase as a
	fraction of the total moles
Liquid Mole Fraction	The molar flux of each distinct liquid phase liquid phase
Liquid Moles	Liquid mole fraction, x_i for each component substance
	in the cloud
	$x_i = \frac{N_{iL}}{N_{tL}}$ where N_{iL} is the liquid moles flux of
	component <i>i</i> and N_{tL} is the total liquid moles
Mass Fraction	Mass fraction (irrespective of phase) of each component substance in the cloud
Mole Fraction	Mole fraction (irrespective phase) of each component
	substance in the cloud
Number of Drops	Number of drops of each distinct liquid phase
Number of Moles	Number of moles of each substance component