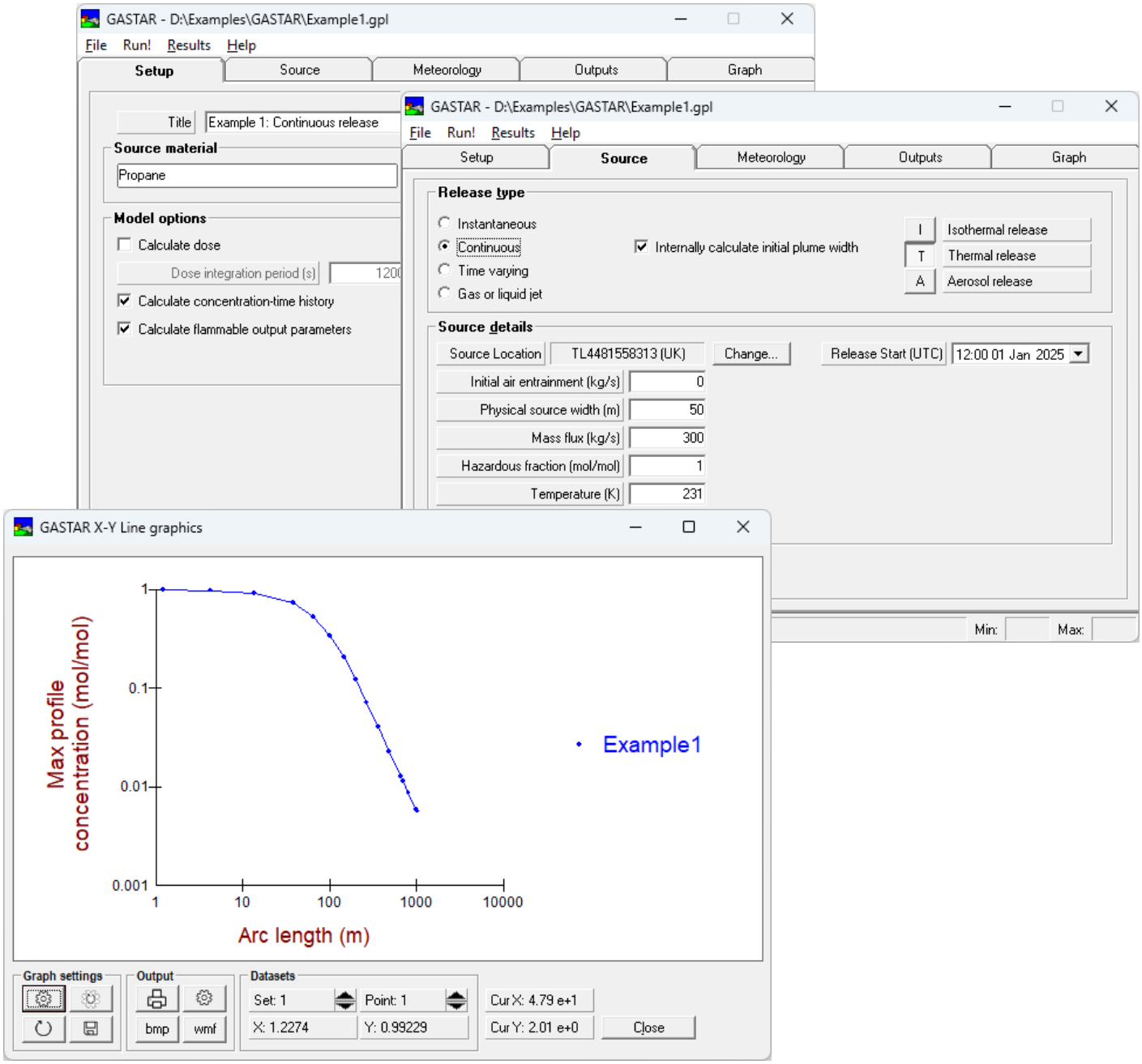
# GASTAR

## *Dense Gas Dispersion Modelling System Version 4.0*




# *User Guide* CERC

# GASTAR

Dense Gas Dispersion Modelling System

# User Guide

**Version 4.0**

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# Contents

# SECTION 1 Introduction

## 1.1 About GASTAR

GASTAR is an integral or box model, describing the evolution of a dense gas cloud in terms of properties integrated or averaged over the entire cloud or over sections through it. The model comprises a main dispersion calculation, determining the concentration and thermodynamic properties of the gas cloud, augmented by a variety of sub-models representing different features of the source giving rise to the cloud or the environment through which the gas cloud travels.

## 1.2 Model features

The capabilities of GASTAR include:

- continuous, instantaneous, time varying and three-dimensional jet release types
- a pool uptake model for creating a time varying source term based on pool evaporation
- a flash calculation for aerosol releases
- complex effects - sloping terrain and obstacles (separately or in combination)
- dose, concentration-time history, flammables and maximum range outputs for applicable source types
- an integrated graphical display for plotting model results
- gridded output for subsequent contour plotting

## 1.3 About this User Guide

This *GASTAR User Guide* is both a manual and a technical summary of the model.

### *Conventions*

To make this manual simpler to use, certain conventions have been followed with regard to layout and style.

- GASTAR interface controls are shown in **bold Arial** font, e.g. the **Setup** screen.
- Keyboard keys are shown in **bold**, e.g. press **Enter**.
- Directory and file names are shown in *italics*, e.g. *GASTAR.exe*, *<install_path>\Data*.
- Tips and other notes are shown thus:

  ---

  *Launching GASTAR and checking the licence details (though **Help**, **Licence details**) will give the location of the licence currently being used.*

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- Table and figure references are shown in **bold**, e.g. see **Table 3.2**, **Figure 2.1**.

# SECTION 2 Getting Started

## 2.1 System requirements

GASTAR is supported on a Windows 11 environment. Please visit our website[1] for the latest information regarding computer specifications, supported operating systems and third-party software.

## 2.2 Installation

The installation of GASTAR is straightforward. It uses an Installation Wizard, which guides the user through a short series of screens, collecting information on the user and installation parameters, before installing the software.

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*Please check with your own IT personnel for company procedures for installing software.*

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If you have an earlier version of GASTAR installed on your PC, you should uninstall this version before installing GASTAR 4.0. Proceed as explained in Section 2.2.1 and then follow instructions given in Section 2.2.2.

If you do not have any version of GASTAR installed on your PC, you should follow the instructions in Section 2.2.2.

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*The abbreviation <install_path> will be used in the rest of the User Guide to denote the directory in which GASTAR is installed, for example C:\Program Files (x86)\CERC\GASTAR.*

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### 2.2.1 Earlier versions of GASTAR

If you have an earlier version of GASTAR installed on your computer, this should be uninstalled before installing GASTAR 4.0.

To uninstall a previous version, log on as Local Administrator for the PC and click on the Windows button, type 'Settings' and hit **Enter**. Select **Apps** from the left menu and click **Installed apps** from the resulting list. Select GASTAR from the list of installed applications and then click **Uninstall** (see **Figure 2.1**).

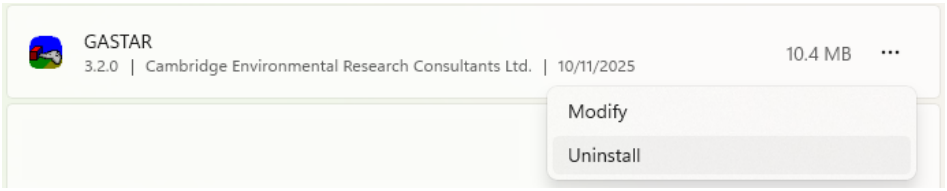



**Figure 2.1** − The **Uninstall** option.

[1] www.cerc.co.uk/systemrequirements

### 2.2.2 Installing GASTAR 4.0

The following steps lead you through the GASTAR installation process.

**Step 1** Log on as Local Administrator for the PC.

**Step 2** GASTAR will have been supplied by download link. Unzip the downloaded *.zip* file to a local directory.

*Do not choose a local directory with an excessively long pathname, as this may cause issues with file pathnames being longer than the allowed maximum of 256 characters.*

**Step 3** In Explorer, browse to this directory and double-click on the file '*setup.exe*'.

The screen shown in **Figure 2.2** will be launched.

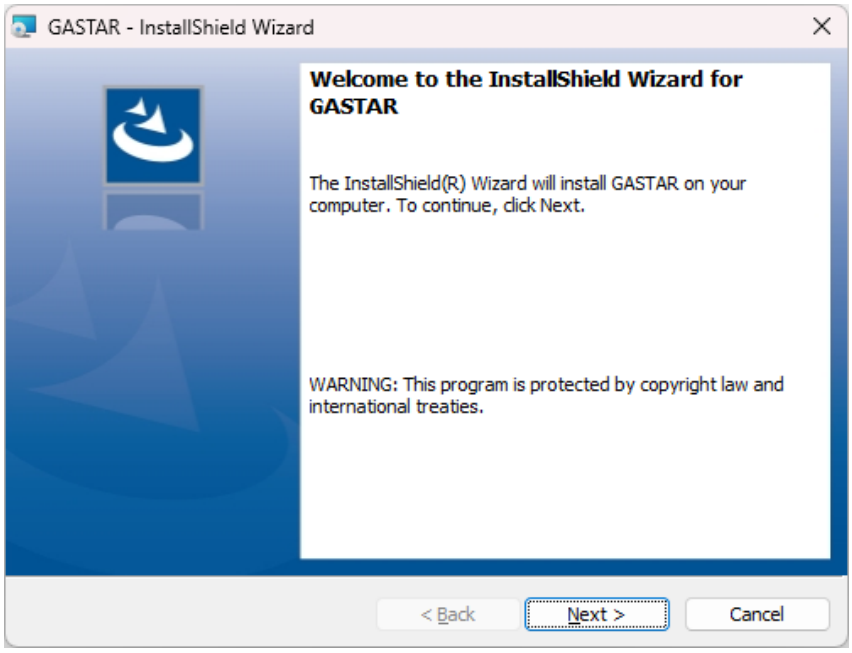



**Figure 2.2** – The **Welcome** screen.

**Step 4** Click **Next >** on the **Welcome** screen. Select **I accept the terms of the licence agreement**, and click **Next >** in the **Licence Agreement** screen, if you accept the licence terms. The **Customer Information** screen is then displayed, as shown in **Figure 2.3**.

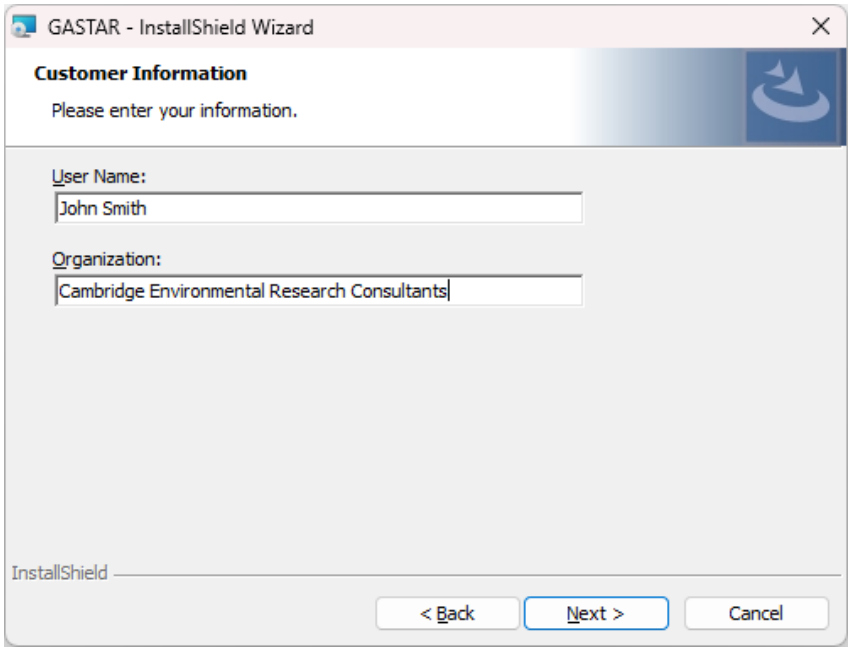



**Figure 2.3** − The **Customer Information** screen.

**Step 5** Enter your user name and organisation in the designated places. Click **Next >** to proceed to the **Destination Folder** screen, as shown in **Figure 2.4**.

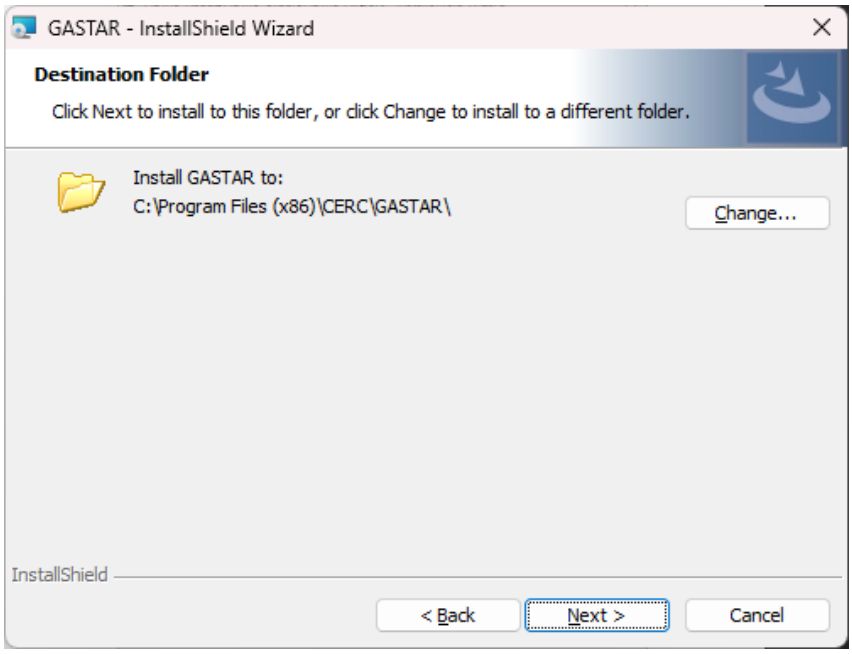



**Figure 2.4** − The **Destination Folder** screen.

**Step 6** You should select a drive with at least 1 GB of available disk space. The default installation directory is *C:\Program Files (x86)\CERC\GASTAR*. If required, use the **Change**... button to select your own installation directory. Click **OK** to return to the **Destination Folder** screen.

*Do not choose an installation directory with an excessively long pathname, as this may cause issues with file pathnames being longer than the allowed maximum of 256 characters.*

*It is advised to always choose a new installation directory rather than, for example, the directory of a previously uninstalled version of the same software.*

Click **Next >** to move to the **Ready to Install the Program** screen, as shown in **Figure 2.5**.

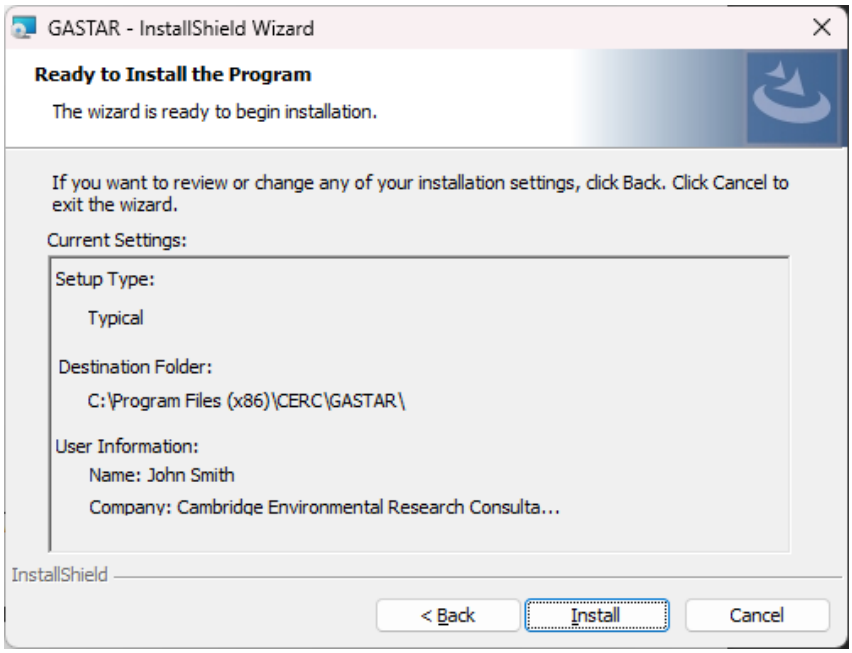



**Figure 2.5** – The **Ready to Install the Program** screen.

**Step 7** If you wish to amend any details, press the **< Back** and **Next >** buttons as appropriate. Once the **Install** button has been pressed, and GASTAR has been successfully installed, the final screen will appear, as shown in **Figure 2.6**.

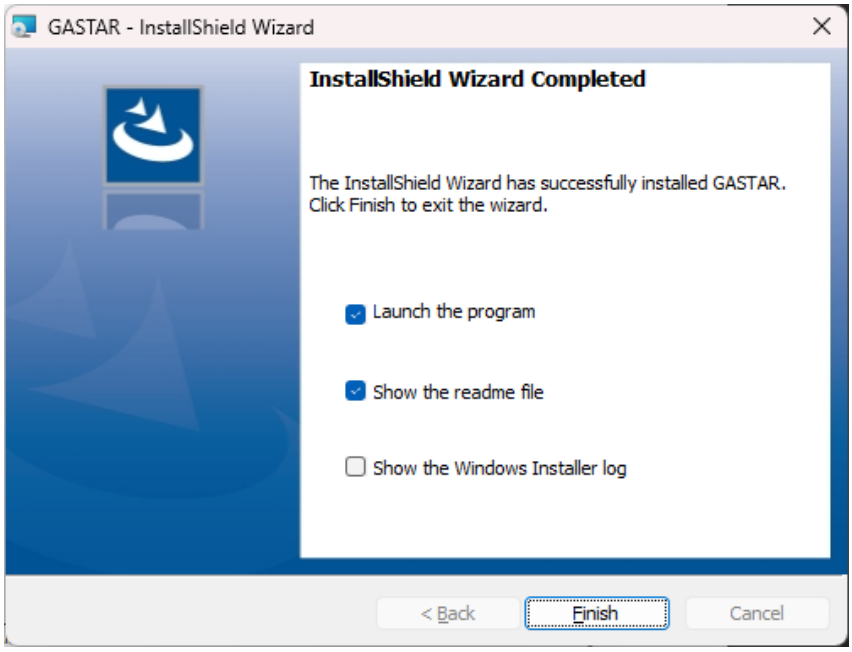



**Figure 2.6** – The **InstallShield Wizard Completed** screen.

**Step 8** Click **Finish** to complete the installation. The installation procedure automatically puts a shortcut to GASTAR on your Windows desktop. If the **Show the readme file** box is checked, a *What's New* document will be opened automatically once you click on **Finish**.

The installation is now complete.

You will have been provided with a unique licence file by email, which is required in order to run the model. It is important that you install this new licence file as instructed below.

**Step 9** To install the GASTAR licence, copy the supplied licence file to the <*install_path*> directory, renaming it to *GASTAR.lic* if necessary. Alternatively, drag and drop the supplied licence file onto the title bar of the GASTAR interface, this will automatically file and rename the licence file.

**Step 10** Depending on your licence type, the first time that you launch GASTAR after installation, it may be necessary to be connected to the Internet so that your licence can be registered. If there is no internet connection, the message shown in **Figure 2.7** will appear.

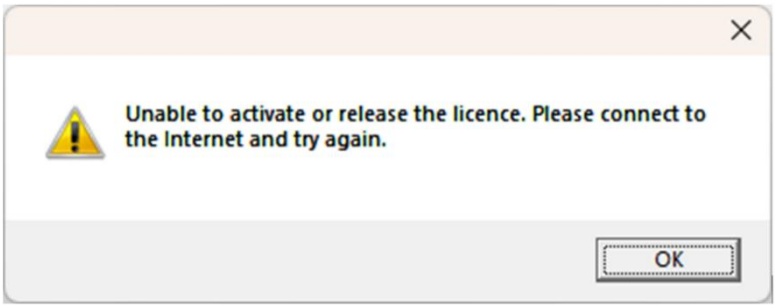



**Figure 2.7** – Licence registration failure.

**Step 11** Your licence will allow up to a certain number of concurrent users. Depending on the licence type, if the maximum number of users has already been reached, the message shown in **Figure 2.8** will appear. If you are issued this message, it is first necessary to release another user's licence (via the **Help**, **Release licence** menu item of the GASTAR interface on that user's PC) before launching GASTAR again on the current PC.


**Figure 2.8** – All licences in use.

*Launching GASTAR and checking the licence details (though **Help**, **Licence details**) will give the location of the licence currently being used.*

# 2.3 Getting around the interface

## 2.3.1 Mouse buttons

Unless otherwise stated, mouse instructions refer to the left button. If the mouse options have been used to reverse the button mapping (e.g. because you are left-handed), the right mouse button should be used instead.

## 2.3.2 Keyboard access

Most of the mouse instructions in this manual can be reproduced using keystrokes. A brief guide to these keystrokes is given in **Table 2.1**.

Often called shortcut keys, these are combinations of keys that perform some of the main commands. For example, menu commands that have one letter underlined are accessible by holding down the **ALT** key and then typing the underlined letter. For example, the menu command **Open**... located on the **File** menu, may be executed by typing **ALT + F** and then (keeping **ALT** held down) **O**.

| Key | Description |
|---|---|
| ***Moving the cursor between data entry boxes*** | |
| **TAB** | Move the cursor forwards through data entry boxes or buttons |
| **SHIFT + TAB** | Move the cursor backwards through data entry boxes and buttons |
| ***Entering data in a box*** | |
| **DELETE** | Delete the character immediately to the right of the cursor |
| **BACKSPACE** | Delete the character immediately to the left of the cursor |
| ← ↑ **arrows** | Move the cursor one space to the left in the current box |
| → ↓ **arrows** | Move the cursor one space to the right in the current box |
| **SHIFT + arrow** | Begin highlighting characters in the direction of the arrow (see above) |
| ***Highlighted text*** | |
| **DELETE** | Delete all highlighted characters |
| **(Type)** | Typing text replaces the highlighted text with new text |
| ***Radio buttons*** | |
| ← ↑ **arrows** | Move the cursor up through the radio buttons for the current item |
| → ↓ **arrows** | Move the cursor down through the radio buttons for the current item |
| ***Checkboxes*** | |
| **SPACEBAR** | Tick or untick the highlighted checkbox |
| ***Other buttons*** | |
| **RETURN** | Execute the action of a selected button |

**Table 2.1** − Keystrokes to enable you to move through the GASTAR interface.

## 2.4 Main menu options

The menu bar has four headings: **File**, **Run!**, **Results** and **Help**. All menu headings apart from **Run!** have drop-down lists of options (see for example the **File** menu options shown in **Figure 2.9**). **Table 2.2** gives the list of options and roles of each menu item.

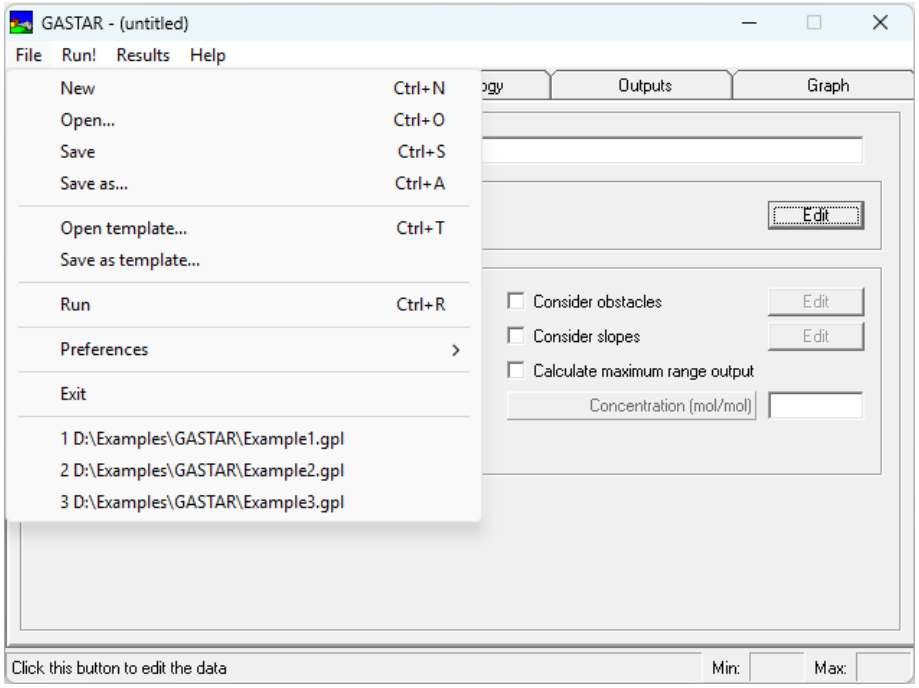



**Figure 2.9** − The **File** menu from the menu bar in GASTAR.

| Menu | | | Role | Ref. |
|---|---|---|---|---|
| File | New | | Reset parameters in model file to their defaults | 2.5.1 |
| | Open… | | Open a previously saved model file | 2.5.1 |
| | Save | | Save current parameters under current file name | 2.5.3 |
| | Save as… | | Save current parameters with a user-specified file name | 2.5.3 |
| | Open template… | | Open a previously saved template file | 2.5.6 |
| | Save as template… | | Save a set of data as a template file | 2.5.6 |
| | Run | | Run GASTAR code using current model file | 2.5.4 |
| | Preferences | Concentrations in ppm | Set concentration units to be either mol/mol or parts per million (ppm). | |
| | | Model execution | Choose options for run time window state and exit mode | 2.5.4 |
| | | Graph print setup | Set some of the commonly used printing options for graphics output | 5.2.4 |
| | | Viewing options | Choose application for viewing numerical results files in GASTAR (default application is Microsoft Excel) | 5.4.1 |
| | | Licence management | Specify whether the online licence should be released automatically when GASTAR is closed. (Only visible for some licence types). | * |
| | Exit | | Quit GASTAR | |
| | 1, 2, 3, … | | Names of the model files most recently opened in GASTAR (click on required file name to open selected model file) | |
| Run! | | | Run GASTAR code using current model file | 2.5.4 |
| Results | Contour plot | | Launch **2-D Output Plotter** for plotting contours in Surfer (if installed) | 5.3 |
| | Line plot | | Switch to **Graph** screen for 1-D plotting | 5.2 |
| | Log file | | Open log file of current model file in preferred viewing software | 5.1.3 |
| | Numerical output | | Open numerical output of current model file in preferred viewing software | 5.4 |
| | Results folder | | Open folder containing model file in an Explorer window | |
| Help | User guide | | Open User Guide in user's default PDF viewer | |
| | What's new | | Open *What's New* in user's default PDF viewer | |
| | Contact helpdesk | | Auto-address a new email to GASTAR helpdesk in user's default email client | |
| | CERC website | | Open CERC homepage in user's default internet browser | |
| | Licence details | | Show licensee and licence details including expiry date and licence number | |
| | Release licence | | Release licence from PC so it can be registered by another PC. (Only visible for some licence types). | * |
| | About GASTAR… | | Show model version number along with contact information for CERC and GASTAR helpdesk | |
| | Current directory | | Show/open/copy path of current working directory | |

**Table 2.2** − Options and roles of menu items. The last column (Ref.) indicates the section of this User Guide where the item is further described. *See 'Managing CERC Online Licences' document under *<install_path>/Support/Licence Management*.

## 2.5 Creating a model file and running the model

To generate results using GASTAR, there are several steps to complete:

- create a new model file;
- enter data to define the problem;
- save the model file;
- run the model; and
- display the output.

The first four of these steps are described in Sections 2.5.1 to 2.5.4 below. Entering model data is described in general terms here, and in detail in Sections 3 and 4. Displaying model output is covered in detail in Section 5. There is also an option to open/save template files, as described in Section 2.5.6.

### 2.5.1 Creating or opening an existing model file

When the GASTAR model interface is loaded or when you select **New** from the **File** menu, a new model file, or scenario, is created and default values are loaded into the screens for you to edit.

An existing model file for editing or running can be opened either in the GASTAR interface or from Explorer:

- To open a model file in the GASTAR interface, choose **Open**... from the **File** menu. (By default, GASTAR will only display files with the *.gpl* extension.)
- To open a model file from Explorer (identifiable by the GASTAR icon), either
  - right-click on the file and select **Open**, or
  - double click on the file, or
  - drag and drop the file onto the title bar of the GASTAR interface.

*The first two options above assume that GASTAR is set as the default application for opening* .gpl *files on the current PC. If this is not the case, but you want it to be, right-click on a* .gpl *file, choose* ***Open with > Choose another app > Choose an app on your PC*** *and browse to select GASTAR.EXE from the* <install_path> *directory, then click* ***Always****.*

*Files prepared in the previous version of GASTAR are converted into the current GASTAR format as they are loaded into the interface. Simply open the file you wish to convert, by selecting* ***Open...*** *from the* ***File*** *menu, and follow the instructions given on screen.*

*It is possible to have multiple instances of the GASTAR interface open simultaneously. This is particularly useful for comparing two model files side by side. A specific model file (*.gpl*) should not be open in more than one instance of the interface simultaneously.*

### 2.5.2 Entering information

#### *Changing values in the input screens*

To change a parameter value in an input screen, move the pointer until it is over the appropriate text box and click. Alternatively, use the **TAB** or **arrow keys** to move systematically through the sections contained in each screen. The selected area will be highlighted. Now type the new value, which will automatically replace what was highlighted. Alternatively, use **DELETE** and/or **BACKSPACE** to remove unwanted characters before typing in the new value.

*Note that a blank cell does not denote a value of zero.*

#### *The helpline*

This is a single line of text that appears at the bottom of the active screen. The information in the helpline changes when different controls on the screen are selected. It gives a brief description of the selected control's function. Where you are prompted for a numerical value, the helpline will give the minimum and maximum values allowed.

For example, when the **Wind speed (m/s)** box in the **Meteorology** screen is selected, the help bar will display the line:

*Wind speed in metres per second, Min: 0.1, Max: 20*

#### *Data validity and integrity checking*

As you enter data, the GASTAR model interface performs checks to ensure that all user-entered data are consistent with the model's logic and that minimum and maximum values are satisfied.

### 2.5.3 Saving input data to a model file

When you are ready to run the model, choose **Save** or **Save as**... from the **File** menu. If the current scenario has not been saved before, or if you chose **Save as**..., you will be prompted to choose a directory and file name. GASTAR model files are always saved with the extension *.gpl*.

### 2.5.4 Running GASTAR

After saving the current scenario as a *.gpl* file, select **Run!** from the menu bar to run the model (or select **Run** from the **File** menu). If you have never saved the current scenario or if you have changed anything in the interface since the scenario was last saved, then you will be prompted to save the modifications.

While the model is running, information is displayed in a progress window (see **Figure 2.10**). When the calculation has successfully completed, the progress window displays:

```
GASTAR Calculation on current data set complete
No Further Datafile arguments to run
```

If the **Exit Mode Option** is set to **Normal termination box** (see 'Runtime preferences' section below), the dialog box shown in **Figure 2.11** will also appear – click **Yes** to close the progress window or **No** to leave it open for reading (and later close using the close button or by selecting **File**, **Exit** from the menu bar).

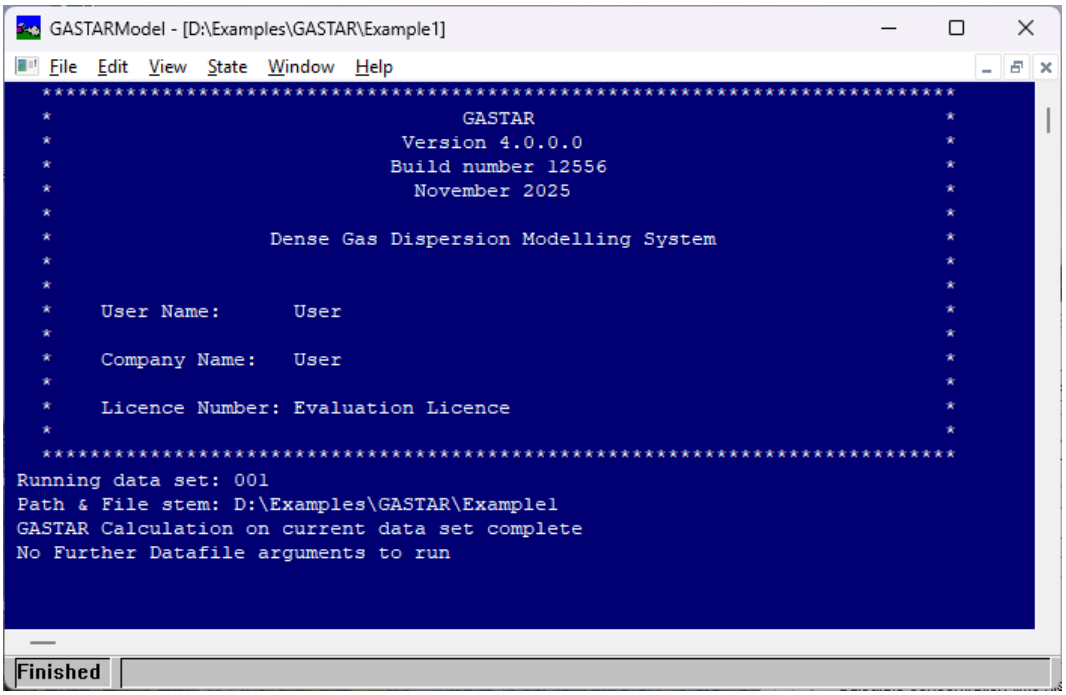



**Figure 2.10** − Progress window of a GASTAR run.

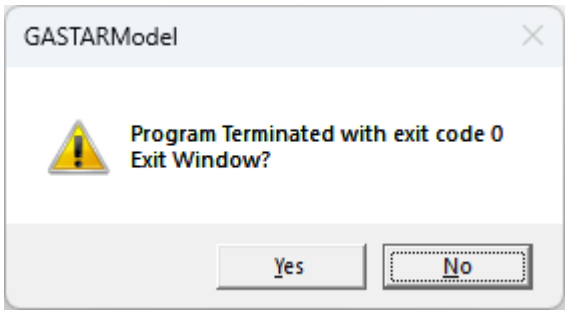



**Figure 2.11** – End-of-run dialog box.

### *Runtime preferences*

The user can edit the runtime options from the **File**, **Preferences**, **Model execution** menu. This will bring up the **Runtime Preferences** screen shown in **Figure 2.12**, divided into two sections:

- The **Window State Options** control the size and state of the run window: normal, minimized or maximised, with focus (active window) or without focus.
- The **Exit Mode Options** determine whether the run window closes after the run has completed. If **Normal termination box** is selected, a dialog box (**Figure 2.11**) appears at the end of the run asking whether you want the window to close. If **No termination box**, **window open** is selected, no dialog box is displayed and the progress window is kept open at the end of the run. If **No termination box**, **window closes** is selected, no dialog box is displayed and the progress window is closed at the end of the run.

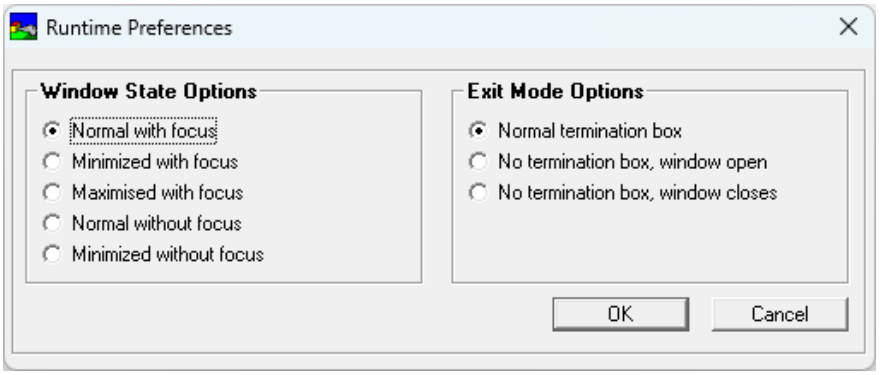



**Figure 2.12** – The **Runtime Preferences** screen.

#### *Batch file*

Alternatively, you can run the GASTAR model with a batch (*.bat*) file. Such a file allows you to run several files consecutively without opening and running each *.gpl* separately from the interface. The most common syntax for running GASTAR from a batch file is:

```
<model path name> <file path name> /e2
```

where `<model path name>` is the full path name of the GASTAR model executable file (*GASTARModel.exe* located in the model installation directory), enclosed in quotation marks (") if there are spaces in the path name

`<file path name>` is the full path name of the *.gpl* file you wish to run, enclosed in quotation marks (") if there are spaces in the path name,

`/e2` is an option to cancel the prompt window at the end of the model run, equivalent to the **No termination box, window closes** option in the **Runtime Preferences** screen. Change to `/e1` or `/e3` for behaviour equivalent to the **Normal termination box** or **No termination box, window open** option, respectively.

For example, if GASTAR is installed in directory *C:\Program Files (x86)\CERC\GASTAR* and the *.gpl* file to run is *D:\Work\Test.gpl*, the command will be:

```
"C:\Program Files (x86)\CERC\GASTAR\GASTARModel.exe" "D:\Work\Test.gpl" /e2
```

Repeat this line for each *.gpl* file you are running. Alternatively, you can list multiple *.gpl* files in a single command (separated by spaces) and/or specify the path to a separate list (*.lst*) file that contains a list of one or more *.gpl* files, each on a separate line.

The text in a *.bat* file is not case-sensitive. To start the model run(s), double-click on the *.bat* file in Explorer.

### 2.5.5 Displaying model output

Please refer to Section 5 for details about displaying output from GASTAR model runs.

### 2.5.6 Template files

When setting up a new problem, it is often most convenient to edit an existing set of data rather than start from scratch. One way to do this is to use an existing *.gpl* file, edit this and then use **File, Save as**... to create a new *.gpl* file. An alternative is to use the GASTAR templates feature, which is accessed via the **File** menu.

A GASTAR template is a complete input data file but with the extension *.gpt*. The interface provides the means both to open existing templates, and thereby provide the starting point for a new GASTAR input file, and to create new templates for later use.

To start a new input data set based on a template file, use the **File, Open template**... menu item: the GASTAR interface loads the data in the template file but sets the dataset name to (untitled) in the banner at the top of the interface window[1]. You can then edit these data and save as a new data file with **File, Save as**....

To create a new template file, simply edit an existing dataset in the interface – which may have been loaded as a *.gpl* or *.gpt* file or entered from scratch – and then use the **File, Save as template**... menu item to save the template with the desired path name and the *.gpt* extension.

[1] Note that you could also open a template (*.gpt*) file with **File, Open**... (provided you select **Template Files (*.gpt)** from the file type drop-down list), or using the recently-opened files list, but this would simply open the file "as is", and is not the recommended way of using template files. Similarly, **File, Save** and **File, Save as**... could be used to save template files, but again this is not recommended.

# SECTION 3 Model Input

Setting up a modelling problem requires the user to input information specifying the release conditions, meteorological conditions and details of the required output. This section provides an overall guide to the model interface. It describes the minimum input data required to run the model and briefly presents the additional modelling options available (full details on these options can be found in Section 4). Sections 3.1 to 3.4 give details of the data entered in each input screen of the GASTAR interface. Practice in use of the model can be obtained by following the three worked examples in Section 6.

There are four basic input screens associated with a GASTAR model run, as shown in **Figure 3.1**. The fifth (**Graph**) screen is used only for output. Data must be entered into each of these four screens for every model run. These screens are:

- **Setup**: source material and modelling options to be used;
- **Source**: release type and source details;
- **Meteorology**: meteorological conditions;
- **Outputs**: types of output and definitions.

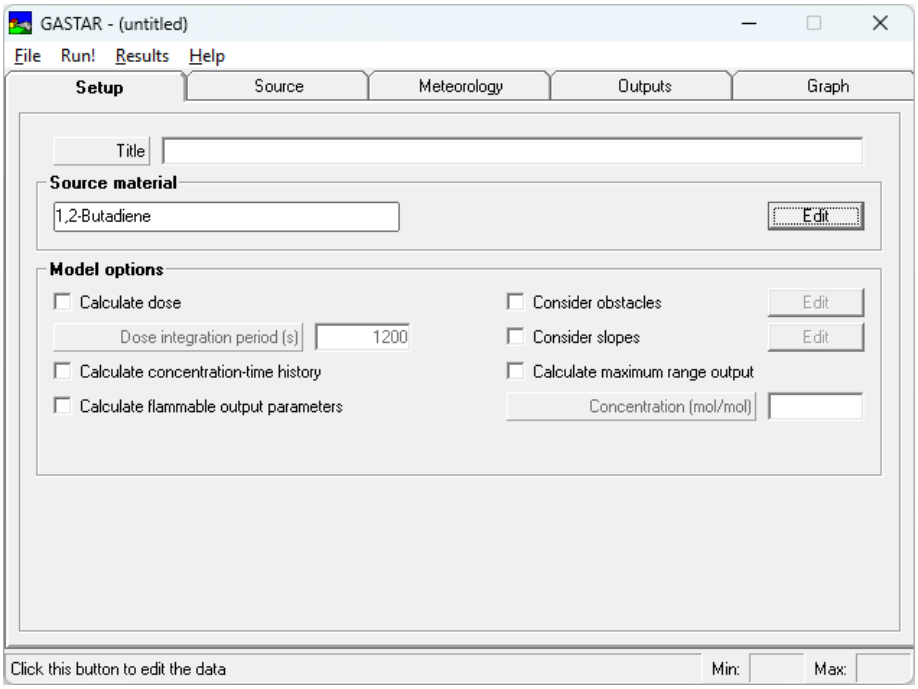



**Figure 3.1** − The **Setup** screen.

## 3.1 Setup screen

The **Setup** screen is shown in **Figure 3.1**. This is the screen that appears when GASTAR is first opened. The source material and modelling options are entered here.

### 3.1.1 Title

This is a string up to 80 characters in length. You might use this to name the run and give some descriptive details to help identify the run. It will be used as a title in the main output (*.gof*) file. This box may be left empty.

### 3.1.2 Source material

The selected source material for this run is displayed on the left of the **Source material** box. The source material can be changed, or its properties modified, by clicking the **Edit** button. This brings up the **Material properties** screen, as shown in **Figure 3.2**.

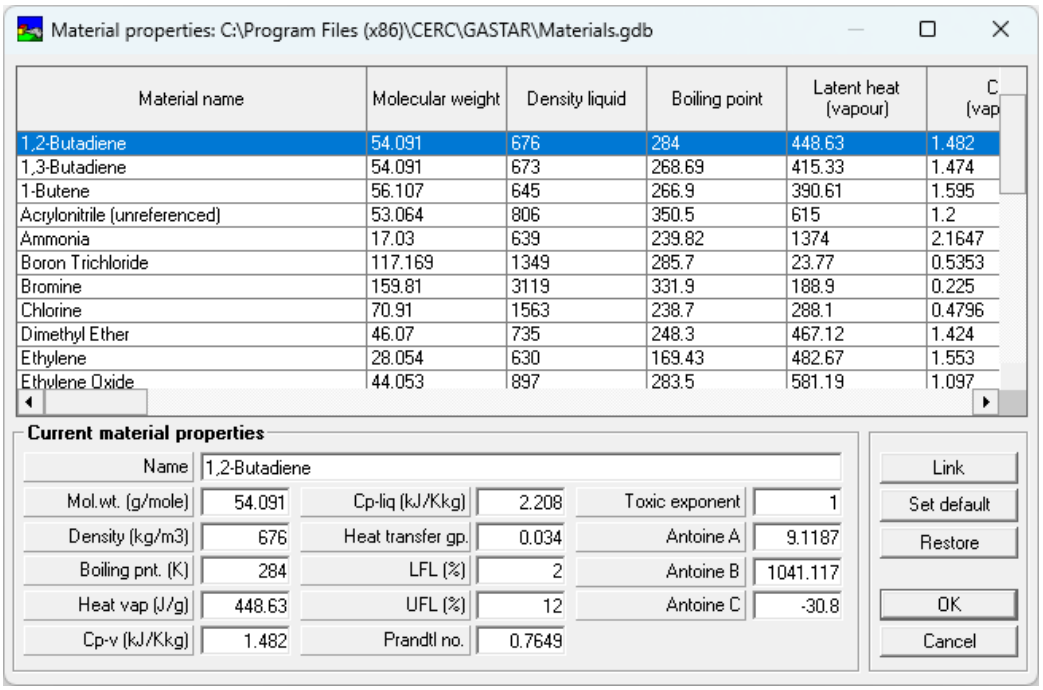



**Figure 3.2** − The **Material properties** screen.

The table in the upper half of the screen displays the data from the currently-linked materials database (*.gdb*) file. By default, *Materials.gdb* in the GASTAR install folder is linked. However, the **Link** button can be used to link to a new materials database file, which will then be remembered for future sessions. The complete properties for each material can be viewed by scrolling horizontally, or by maximising the screen via the window controls (depending on monitor size).

To select a new source material for the current run, double-click on the desired material from the table. This will update the **Current material properties** to the those of the selected material. If desired, individual material properties can be further modified by editing the relevant fields in the lower half of the screen. Note that this only modifies the material properties used for the current run, and not the values in the materials database itself – see the 'Editing the materials database' section further below if you would like to do this. Any values that differ from those stored in the materials database for a given material name will be highlighted as red text. Double-clicking on that material name in the upper table will reset all values back the ones stored in the materials database.

You can click **Restore** at any time to reset the current material properties back to the

values they took when the **Material properties** screen was opened. Click the **Set default** button if you would like the current material properties to be used as default in future sessions. Clicking **OK** closes the **Material properties** screen saving any changes made, while clicking **Cancel** closes the screen discarding any changes made.

**Table 3.1** lists the material properties that must be defined. While no field can be left blank, the values entered into fields that will not be used (see table caption) do not matter.

| Property | Units |
|---|---|
| Material Name | -- |
| Molecular Weight | g/mol |
| Density (liquid)* | $kg/m^3$ (at STP) |
| Boiling Point* | K (at SP) |
| Heat of Vaporisation | kJ/kg |
| Specific Heat Capacity (vapour) | kJ/K/kg |
| Specific Heat Capacity (liquid) | kJ/K/kg |
| Heat Transfer Group[1] | -- |
| Lower Flammability Limit† | % |
| Upper Flammability Limit‡ | % |
| Prandtl Number | -- |
| Toxic Exponent§ | -- |
| Antoine Coefficient (A)* | For p in Pa |
| Antoine Coefficient (B)* | For T in K |
| Antoine Coefficient (C)* | For T in K |

**Table 3.1** – Source material properties. *Only used for Aerosol releases. †Only used with flammables output option. ‡Not currently used. §Only used with dose output option.

### *Editing the materials database*

The materials database, *Materials.gdb*, is supplied as a read-only file in the GASTAR install folder. It has a simple tab-separated format. It is up to each licence holder to decide who should have the ability to edit *Materials.gdb* in order to add a new material that can then be used in any *.gpl* file, delete an existing material or edit the properties of an existing material. To make changes to *Materials.gdb*, firstly change the properties of the file from read-only so that it can be edited. You can do this by right clicking on *Materials.gdb* in Explorer, selecting **Properties** and unchecking the box labelled **Read-only** under **Attributes** on the **General** tab, before clicking **OK** to close the window. Then open the file in a text editor (see **Figure 3.3**) or Excel. The first line contains the names of the variables. Each following line contains the properties for each material. Materials can be added or deleted or properties edited. After the changes have been made and *Materials.gdb* saved, it is advisable to change the properties of *Materials.gdb* back to being read-only to prevent any future accidental changes. A copy of the original version of the materials database that is included with the install can also be found in the

[1] The Heat Transfer Group is a composite property that takes the value: $MW.c_{pg}.[\nu/(T.Pr)^2]^{1/3}$, where MW is the molecular weight and T is a representative temperature in K, taken to be 273.17K

<*install_path*> directory with the filename *Materials.original*, which can be used to perform a 'factory reset'.

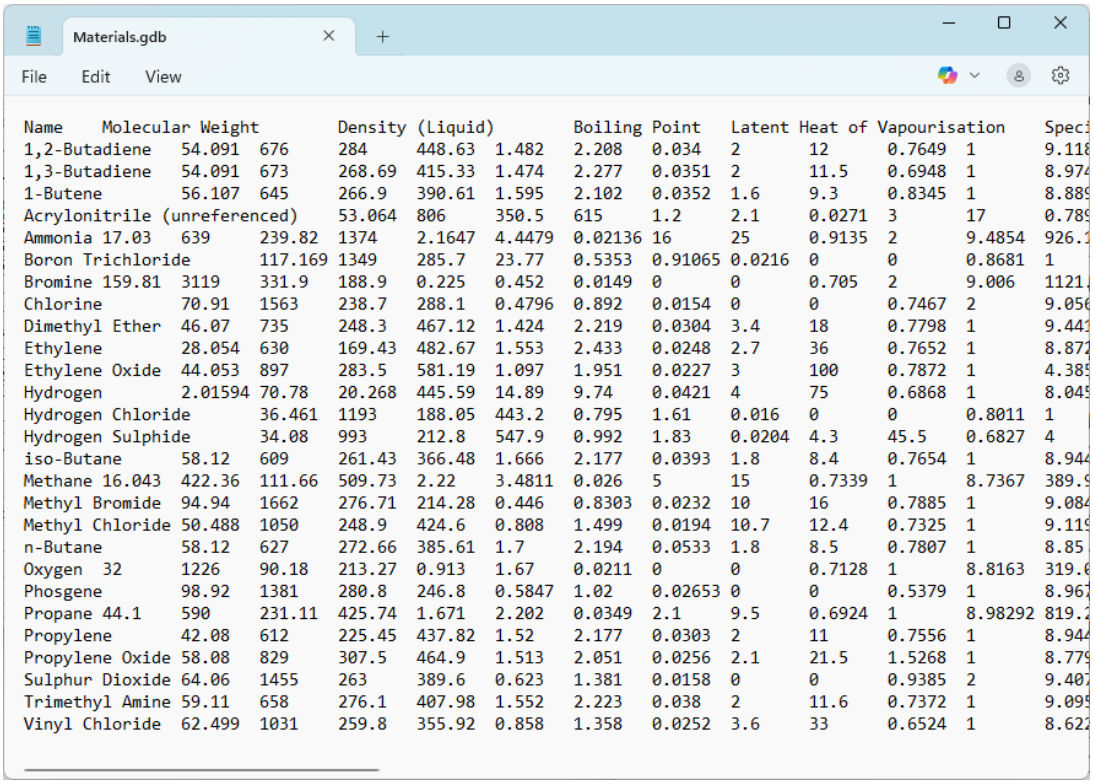



**Figure 3.3** – *Materials.gdb* opened in a text editor.

### 3.1.3 Model options

This box presents a choice of modelling options to be used in the GASTAR run. These options are fully described in Section 4.

---

*Any options that are not available to the currently selected release type will be greyed out.*

*If no model options are selected, GASTAR will still output the standard results table in the main output (.gof) file.*

---

## 3.2 Source Screen

The **Source** screen is shown in **Figure 3.4**. All source properties are entered here: release type, source location, release start and release conditions.

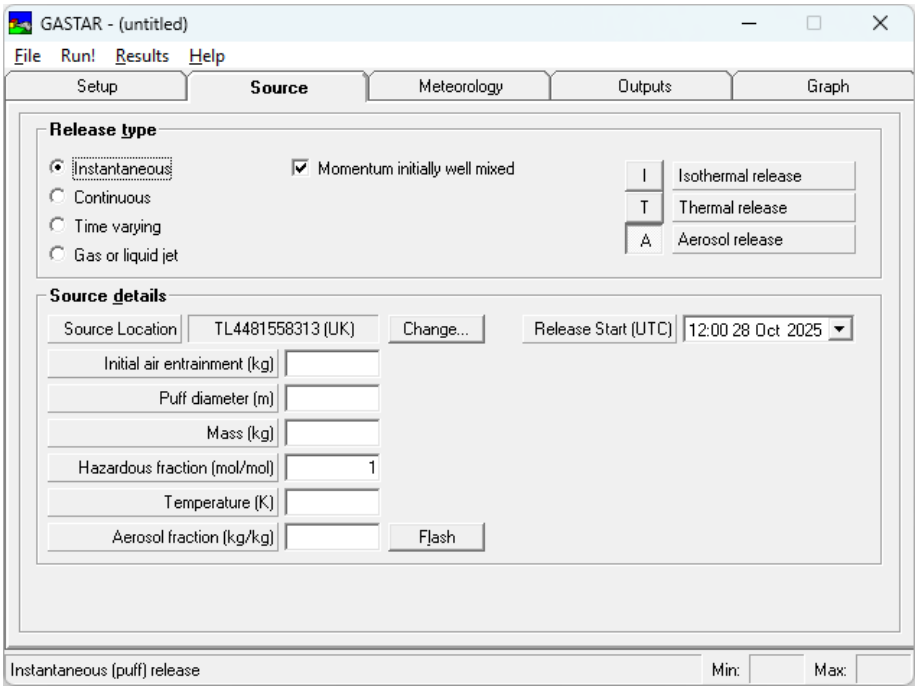



**Figure 3.4** − The **Source** screen.

### 3.2.1 Release type

There are two main choices for the **Release type**; the radio buttons to the left distinguish between **Instantaneous**, **Continuous**, **Time varying** and **Gas or liquid jet** releases, each described below, while the buttons to the right define whether the release is **Isothermal** (no temperature or phase changes), **Thermal** (temperature changes allowed but single phase) or **Aerosol** (two-phase with temperature/phase changes).

#### 3.2.1.1 Instantaneous release

For **Instantaneous** releases the initial volume, $V_0$, is calculated using the mass released and prevailing meteorological and source conditions. The initial puff diameter, $D_0$, is specified. The initial puff is assumed to be a right circular cylinder. The initial height of this cylinder is then given by $H_0 = V_0/(¼\ \pi\ D_0^2)$.

The initial temperature $T_0$ (for **Thermal** and **Aerosol** cases), initial aerosol fraction (for **Aerosol** cases), initial concentration $C_0$ and initial density $\rho_0$ are assumed to be uniform over the initial volume.

For instantaneous releases, use the **Momentum initially well mixed** checkbox to select whether the initial conditions of the puff momentum are well mixed or not well mixed. The default is for the momentum to be initially well mixed. This option is used to determine the initial conditions for puff momentum mixing. Typically, instantaneous releases are a result of some catastrophic event such as a tank rupture or explosion. In

these cases, it is easy to see that internally the puff will have a well-mixed momentum. For some situations this is not true, for example the Thorney Island instantaneous heavy gas dispersion trials. Here the cloud was created inside a large tent-like construction that dropped to the ground to release the puff. The material effectively appeared as a large stationary puff which slowly picked up speed as the wind advected it away. It would be more appropriate to model this case assuming the momentum was not well mixed initially. The effect of this is to make the cloud advection velocity start from zero and gradually grow. When the **Momentum initially well mixed** option is chosen, this reduction factor is not used and the cloud advection velocity is non-zero from the start of the modelling process.

#### 3.2.1.2 Continuous release

For **Continuous** releases, either the physical source width or the actual plume width can be specified. The mass flux, $M_0$, at the source is also specified. The initial plume cross section is assumed to be rectangular. The model will calculate the source density, $\rho_0$, in the same manner used by the Instantaneous release. The source height, $H_0$, is found such that the correct mass flux is obtained using $M_0 = H.W.U_a.\rho_0$, where $U_a$ is the (calculated) effective speed for the cloud based on the current wind speed profile (see Section 7.2.3).

The initial temperature $T_0$ (for **Thermal** and **Aerosol** cases), initial aerosol fraction (for **Aerosol** cases), initial concentration $C_0$ and initial density $\rho_0$ are assumed to be uniform over the initial section.

For continuous releases, you can tick the **Internally calculate initial plume width** checkbox if you wish GASTAR to determine the initial conditions for continuous release calculations, i.e. the source width and height are calculated *internally*. You must supply the physical source width. The effective (i.e. the actual plume) width, height and density are calculated from the source mass flux, temperature and prevailing meteorological conditions. This option produces a physically realistic plume aspect ratio.

If you do not choose to allow the model to calculate the initial plume dimensions, the value you enter for the plume width is assumed to be the initial plume width and will be retained by the model for the starting conditions, i.e. the user-specified width is *always* the effective source width. This option is useful if you know the actual plume width (e.g. modelling experimental results) or you wish to fix a certain width (e.g. you are using the results from another source model). It may also be required if the geometry of the release prevents lateral spreading of the plume beyond the physical source width.

#### 3.2.1.3 Time varying release

For **Time varying** releases, the initial conditions are specified as a sequence of piece-wise constant segments. The segments are specified by the time duration of each segment. The other details of the source specification are similar to the continuous case.

For each segment of the time varying release the physical source width, $D_0$, and mass flux, $M_0$, are specified. The initial condition is assumed to be a rectangular section with an effective source width $W_0$, effective source height $H_0$ and source density $\rho_0$.

The initial temperature $T_0$ (for **Thermal** and **Aerosol** cases), initial aerosol fraction (for **Aerosol** cases), initial concentration $C_0$ and initial density $\rho_0$ are assumed to be uniform

over the initial section.

The time varying segments can also be calculated by the **Pool Uptake** model. This considers the evaporation from a (developing) pool and calculates the dimensions of the developing cloud above the pool. For more details see Section 3.2.4.

#### 3.2.1.4 Gas or liquid jet release

For **Gas or liquid jet** releases, either the physical source diameter or the pseudo jet diameter can be specified. The mass flux, $M_0$, at the source is also specified. The jet cross section is assumed to be circular if airborne and semi-circular if the jet is grounded. The model will calculate the source density, $\rho_0$. There is no height dimension for jets, but the jet does have a height, *z*, to the centre of the circular cross-section.

The initial temperature $T_0$ (for **Thermal** and **Aerosol** cases), initial aerosol fraction (for **Aerosol** cases), initial concentration $C_0$ and initial density $\rho_0$ are assumed to be uniform over the initial section.

For jet releases, there are options for the source to be elevated, and to be orientated in any (3-D) direction (see **Figure 3.5** and **Figure 3.6**).

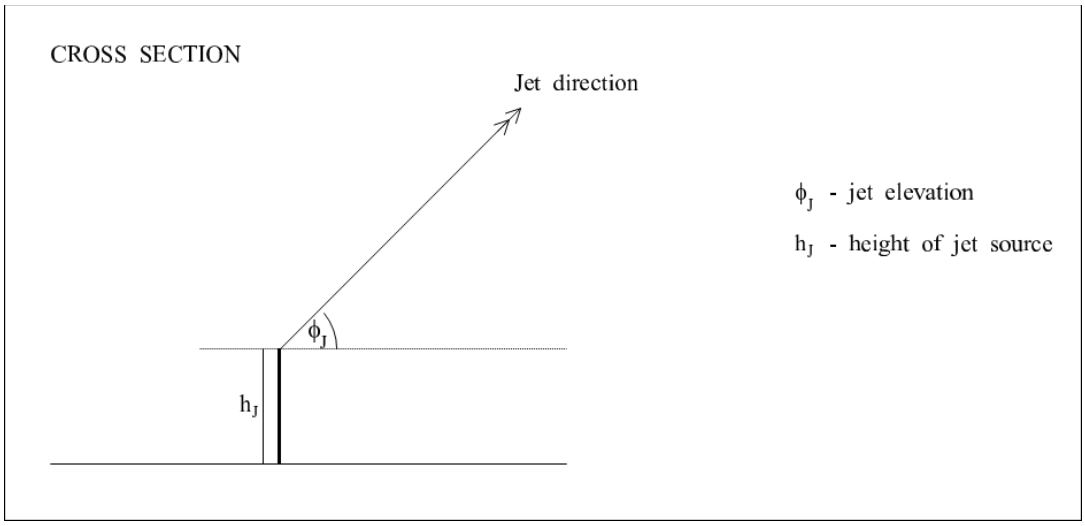



**Figure 3.5** − Definition of jet height and elevation (vertical cross section through jet).

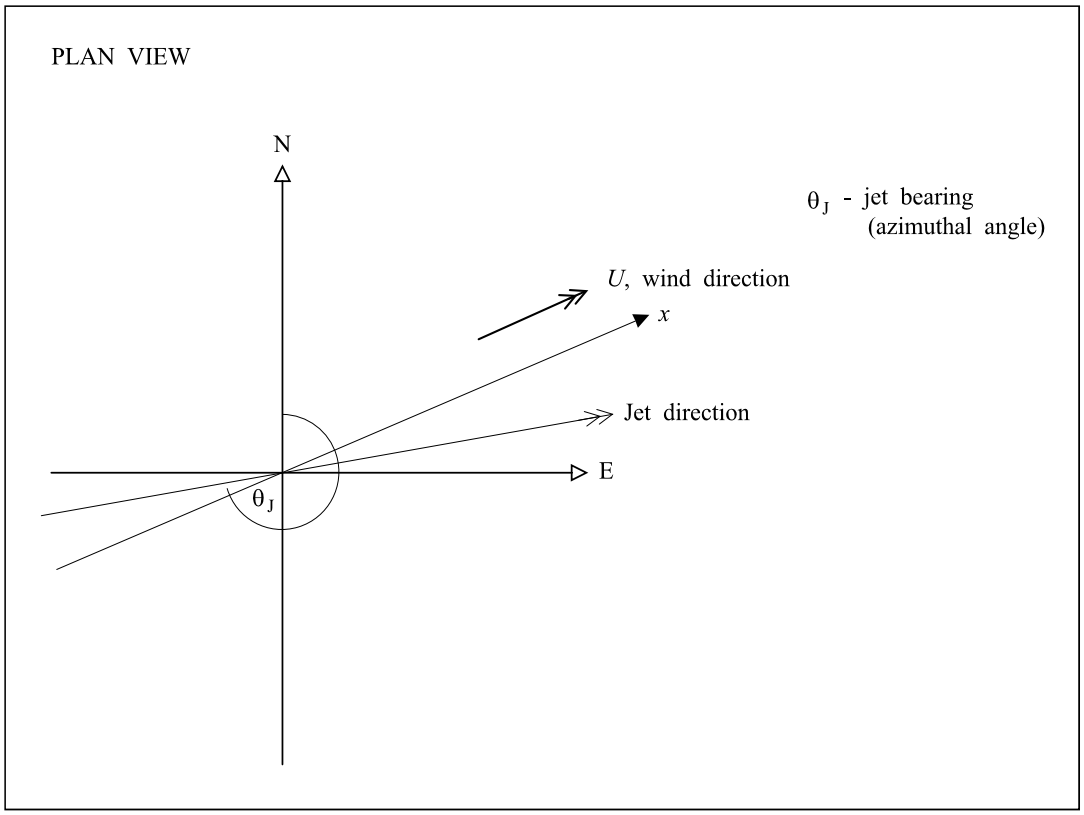



**Figure 3.6** − Definition of jet bearing (plan view of jet).

### 3.2.2 Source details

The exact requirements are dependent on the **Release type**.

#### *Source Location*

The **Source Location** can be entered in one of six formats that can be chosen by clicking the **Change**... button and selecting from the drop-down box labelled **Source Location Type** – see **Figure 3.7**. The available formats are:

- Latitude-longitude
- UK grid 6 digits
- UK grid 2x5 digits
- UK grid 2x6 digits
- Irish grid 2x3 digits
- Irish grid 2x5 digits

The **Source Location** must be entered by the user in the correct format for the **Source Location Type** selected. Advice on the format is given on the screen, as shown in **Figure 3.7**.

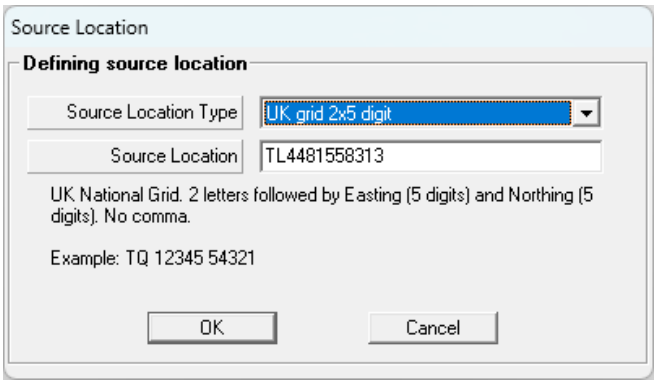



**Figure 3.7** – The **Source Location** screen.

The source location is not used by the GASTAR model code but is written to the main output file (*.gof*), and the *.ggd* file (if created).

### *Release Start (UTC)*

The **Release Start** time must be entered in UTC (hours and minutes) plus day of the month, month and year. The release start is not used by the GASTAR model code but is written to the main output file (*.gof*), and the *.ggd* file (if created).

### *Initial air entrainment*

Required for **Instantaneous**, **Continuous** and **Time varying** releases only. Enter the mass (for instantaneous releases) / mass flux (for the other release types) of air entrained at the start. Because of the nature of some releases, particularly explosive instantaneous, it is desirable to allow an initial mixing with air for the source term. Although it is unlikely in a real incident that the exact amount of air entrainment at the start would be known, a general rule of thumb for flashing releases is to assume instantaneous mixing with approximately ten times by the mass of air (Kaiser, 1979). The model assumes the entrained air to be at the air temperature and will use this together with the mass (flux) and temperature of released material to recalculate an overall cloud temperature and density.

This parameter gives the mass (flux) of the air initially entrained.

| | | |
|---|---|---|
| Minimum | 0.0 | kg (/s) |
| Maximum | 1,000,000.0 | kg (/s) |

### *Width/Diameter*

The definition of this parameter depends on the release type:

- **Instantaneous** releases: This is the initial diameter of the puff
- **Continuous** releases: This is the physical source width giving rise to the plume if the **Internally calculate initial plume width** option is chosen, otherwise it is the initial width of the plume.
- **Time varying** releases: This is the initial width of the current segment (as given in the **Current segment number** box).
- **Jet** releases: This is the initial diameter of the jet for ambient pressure releases, or the pseudo diameter if the release is under pressure, i.e. the diameter after expansion to ambient pressure.

| | | |
|---|---|---|
| Minimum | 0.01 | m |
| Maximum | 1,000.0 | m |

### *Mass (flux)*

This parameter gives the mass (for instantaneous releases) / mass flux (for the other release types) of material released. For **Instantaneous** releases, this is a single total amount measured in kilograms. For **Continuous**, **Time varying** and **Jet** releases, this is a mass flux for the source measured in kilograms per second. For **Instantaneous** and **Continuous** releases this does not include the air initially entrained (see above). For **Time varying** releases this entry will refer to the current segment, as given in the **Current segment number** box.

| | | |
|---|---|---|
| Minimum | 0.01 | kg (/s) |
| Maximum | 1,000,000.0 | kg (/s) |

### *Hazardous fraction*

This parameter gives the fraction of the release that is considered hazardous (not including any initial air entrainment). The input units are given in brackets and will be either mol/mol or ppm depending on whether or not **Concentrations in ppm** is ticked under the **File**, **Preferences** menu. For general use the hazardous fraction is the whole release: consequently, it has a default value of 1 mol/mol (1 million ppm). By changing this value, you may model the release of a dense gas (say $CO_2$) in which a small amount of a contaminant (say $H_2S$) was present. In this case, the dynamics of the cloud will depend on the main dense gas ($CO_2$), but the important concentration levels will be those of the contaminant in the release. The concentration of the *contaminant* will therefore be given directly in the model output. For **Time varying** releases this entry will refer to the current segment, as given in the **Current segment number** box.

| | | |
|---|---|---|
| Minimum | 0.000001 | mol/mol |
| | 1.0 | ppm |
| Maximum | 1.0 | mol/mol |
| | 1,000,000.0 | ppm |

### *Temperature*

For **Thermal** and **Aerosol** releases only. This parameter gives the temperature of the initial cloud of released gas and/or aerosol (after flashing but before any air entrainment). Some care is needed to ensure all source details are consistent. For example, if there is a spill of volatile material that is stored as a liquid under pressure at ambient temperature, you will need to perform a 'flashing' calculation (see Section 3.2.3) to determine the final temperature and aerosol fraction. In such cases, the storage temperature might not be the initial cloud temperature. It is the initial temperature of the released material that is required by the code. For **Time varying** releases this entry will refer to the current segment, as given in the **Current segment number** box.

| | | |
|---|---|---|
| Minimum | 10.0 | K |
| Maximum | 2,000.0 | K |

### *Aerosol fraction*

For **Aerosol** releases only. This parameter gives the fraction of the source material that

is in liquid state initially. This fraction can be found by using the **Flash** calculation (see Section 3.2.3). For **Time varying** releases this entry will refer to the current segment, as given in the **Current segment number** box.

| | | |
|---|---|---|
| Minimum | 0.0 | - |
| Maximum | 0.99 | - |

### *Number of segments*

For **Time varying** releases only. This parameter gives the number of distinct segments that the source term has been broken into in order to simulate the time varying release.

| | | |
|---|---|---|
| Minimum | 1 | - |
| Maximum | 100 | - |

### *Current segment number*

For **Time varying** releases only. This specifies the segment number associated with the currently displayed data. To change the current segment number, either use the up and down arrows (  ) or type the desired segment number directly into the text box.

| | | |
|---|---|---|
| Minimum | 1 | - |
| Maximum | Number of segments | - |

### *Segment duration*

For **Time varying** releases only. This parameter gives the time duration (in seconds) for the currently selected segment, as given in the **Current segment number** box.

| | | |
|---|---|---|
| Minimum | 1.0 | s |
| Maximum | 10,000.0 | s |

### *Height*

For **Jet** releases only. This parameter gives the height of the jet release point above ground level (see $h_J$ in **Figure 3.5**).

| | | |
|---|---|---|
| Minimum | 0.0 | m |
| Maximum | 100.0 | m |

### *Azimuthal angle*

For **Jet** releases only. This parameter gives the horizontal bearing of the jet at the source. This is measured in the same manner as a wind bearing; clockwise from North (in degrees) and represents the direction *from* which the jet is coming (see $\theta_J$ in **Figure 3.6**).

| | | |
|---|---|---|
| Minimum | 0.0 | ° |
| Maximum | 360.0 | ° |

### *Elevation angle*

For **Jet** releases only. This parameter gives the elevation angle of the jet at the source. This is measured from the horizontal and is positive if the jet is pointing upwards (see $\phi_J$ in **Figure 3.5**).

| | | |
|---|---|---|
| Minimum | -90.0 | ° |
| Maximum | 90.0 | ° |

### 3.2.3 Flash calculation

When choosing an **Aerosol** release type, the **Flash** calculation button will be enabled (to the right of the **Aerosol fraction** textbox). This utility is useful when you need to model the release of a material with a boiling point below ambient temperature stored in a pressurised container at ambient temperature. When suddenly released, these materials 'flash' producing a cold, dense cloud containing some material in liquid phase.

Clicking the **Flash** button brings up the **Flash calculation** screen – see **Figure 3.8**. The properties in the lower **Material details** box are based on the source material currently chosen in the **Setup** screen. In the **Storage conditions** box, fill in the **Storage temperature** (K) of the material, which is typically the ambient temperature, and the **Atmospheric pressure** (mb). If the **Air temperature** and/or **Atmospheric pressure** have already been defined in the **Meteorology** screen, these values are automatically copied to the **Flash calculation** screen. You may then choose to use these values or enter different ones before clicking the **Calculate** button to calculate the aerosol fraction and temperature of the released material. The model uses two slightly different algorithms to do this, and both sets of results are given. This is to give the most flexible approach for the modeller. The most commonly used method is labelled '**Normal method**'. The formula used for the normal method is

$$\text{Aerosol Fraction} = 1 - \left(C_{pl}\frac{T_{\text{storage}} - T_{BP}}{H_{LG}}\right) \tag{3.1}$$

and that for the **Exponential method** is

$$\text{Aerosol Fraction} = \exp\left(-C_{pl}\frac{T_{\text{storage}} - T_{BP}}{H_{LG}}\right) \tag{3.2}$$

where $T_{\text{storage}}$ is the storage temperature of the liquid, $T_{BP}$ is the boiling point of the released material, $H_{LG}$ is the specific heat of vaporisation of the released material and $C_{pl}$ is the specific heat capacity of the released liquid.

Note that if you change the **Storage conditions** from the values copied from the **Meteorology** screen, the changed values will not be copied back. This is to allow you to operate the **Flash** model as a tool or utility separately from the work you might be doing in the main GASTAR interface.

Clicking the **Use normal** button closes the **Flash calculation** screen and returns to the **Source** screen, copying the **Aerosol fraction** and **Source temperature** calculated via the **Normal method** into the relevant **Source details** fields, while clicking **Close** closes the screen without copying any data. To use the values from the **Exponential method** you must copy the data back manually.

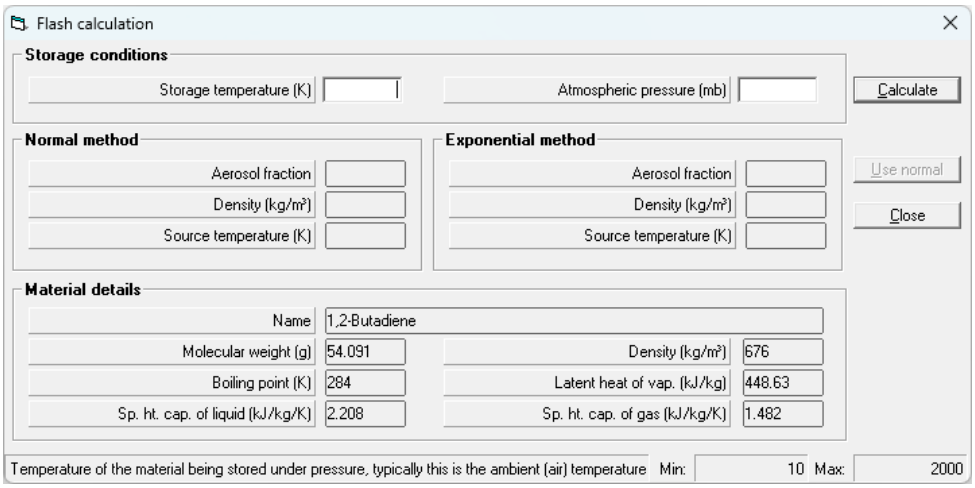



**Figure 3.8** – The **Flash calculation** screen.

### 3.2.4 Pool Uptake model

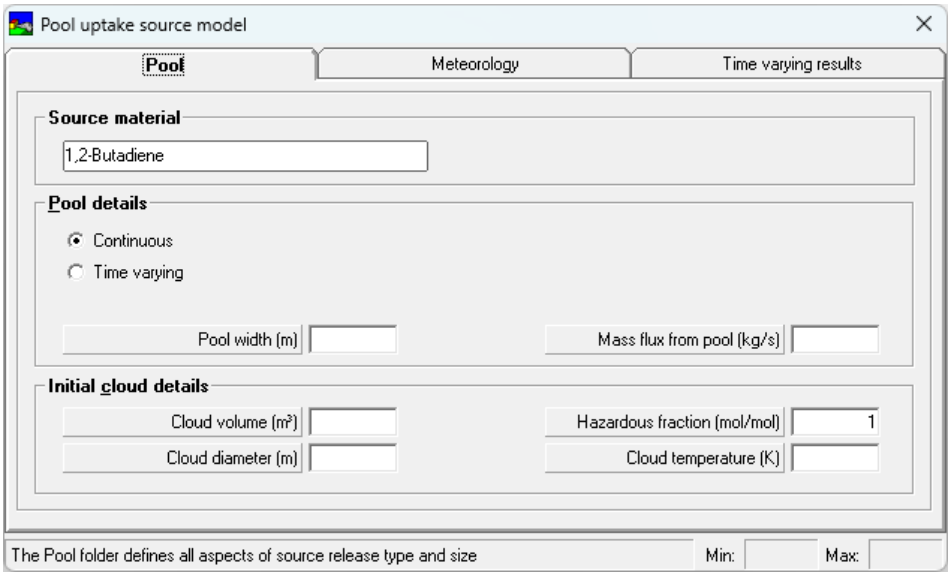



**Figure 3.9** – **Pool uptake source model**.

When modelling a **Time varying** release, the **Pool Uptake** button is enabled. Clicking this launches the **Pool uptake source model** (see **Figure 3.9**), which provides a simple way to create a time varying source term based on the evaporation of material from a pool. The model uses the supplied evaporation rates to calculate the subsequent cloud development above the pool which can then be used as a source term inside GASTAR. The Pool Uptake model does not calculate the vaporisation rates from the pool; in order to do this, a pool spill model is required.

The Pool Uptake model is a separate utility that comprises three screens: two for input (**Pool** and **Meteorology**) and one for the results (**Time varying results**). Each screen is covered separately below. In order to ensure consistency, data items which are common between the main GASTAR interface and the Pool Uptake model are copied from the former to the latter when the Pool Uptake model is launched. It is therefore recommended that data are first entered into the four input screens of the main GASTAR interface (**Setup**, **Source**, **Meteorology**, **Outputs**) before accessing the Pool Uptake model and completing its

own screens.

*If you use the results of the Pool Uptake model, all the data common to the main GASTAR interface will be copied back, overwriting any data that is already there. If you do not wish to lose the data in the main GASTAR interface, you should save it before entering the Pool Uptake model.*

#### 3.2.4.1 Pool screen

The **Pool** screen of the Pool Uptake model (**Figure 3.9**) defines the details of the pool and cloud above it. A description of each of the fields on this screen is given below.

***Source material***

The **Source material** box shows the source material selected in the main GASTAR interface. This cannot be edited from the Pool Uptake model.

***Pool details: Pool type***

As material evaporates or boils off from the pool of spilled liquid, a cloud will form above the pool. The Pool Uptake model will provide information on the development of this cloud as it changes with time. However, it is also possible for the pool itself to be changing in time. Therefore, there is the option to have a **Continuous** or **Time varying** pool:

- A **Continuous** pool has a fixed rate at which material is leaving the pool and contributing to the cloud above it.
- A **Time varying** pool is one that changes over time. It is defined in a similar way to a **Time varying** release in GASTAR, in that the pool development is broken up into a number of "segments" with each lasting for a given time duration. The rate at which material is leaving the pool must be supplied for each segment of the pool development.

There are no links between any of the fields in the **Pool details** box and the fields in main GASTAR interface, since the details in the **Pool details** box relate to the pool while the source details in the main GASTAR interface relate to the cloud above the pool.

***Pool details: Pool width***

This parameter gives the physical width of the pool in metres. This is fixed over all segments for **Time varying** pools.

| | | |
|---|---|---|
| Minimum | 0.01 | m |
| Maximum | 1,000.0 | m |

***Pool details: Mass flux from pool***

This parameter gives the mass flux of material leaving the pool in kg/s. For **Time varying** pools this entry will refer to the current segment, as given in the **Current segment number** box.

| | | |
|---|---|---|
| Minimum | 0.01 | kg/s |
| Maximum | 1,000,000.0 | kg/s |

### *Pool details: Number of pool segments*

For **Time varying** pools only. This parameter gives the number of distinct segments that the pool development has been broken into in order to simulate the time varying pool.

| | | |
|---|---|---|
| Minimum | 1 | - |
| Maximum | 20 | - |

### *Pool details: Current segment number*

For **Time varying** pools only. This specifies the segment number associated with the currently displayed data. To change the current segment number, either use the up and down arrows (  ) or type the desired segment number directly into the text box.

| | | |
|---|---|---|
| Minimum | 1 | - |
| Maximum | Number of pool segments | - |

### *Pool details: Pool segment duration*

For **Time varying** pools only. This parameter gives the time duration (in seconds) for the currently selected pool segment, as given in the **Current segment number** box.

| | | |
|---|---|---|
| Minimum | 1.0 | s |
| Maximum | 2,000.0 | s |

### *Initial cloud details: Cloud volume*

This parameter gives the initial cloud volume in cubic metres. It is likely that you will have no information regarding the starting condition of the cloud, or you want the model to assume there is not any cloud initially. In these cases, you should give the initial cloud volume as zero.

| | | |
|---|---|---|
| Minimum | 0.0 | $m^3$ |
| Maximum | 100,000.0 | $m^3$ |

### *Initial cloud details: Cloud diameter*

This parameter gives the initial cloud diameter in metres. Although this parameter has fixed minimum and maximum values, it should not be less than the **Pool width** value defined above. This is because the Pool Uptake model assumes that the mass flux of material leaving the pool is uniform over the whole area of the pool. Consequently, if a cloud forms it must form at least over the whole width of the spill and never less. If you have no information regarding the starting condition of the cloud, or you want the model to assume there is no cloud initially, you should use the **Pool width** value defined above.

This parameter is linked with the **Width** field in the **Source** screen of the main GASTAR interface. The initial value will therefore be that given in the main GASTAR interface (for segment 1), and any changes made to this value in the Pool Uptake model will also be copied back to the main GASTAR interface should you end up using the Pool Uptake model results.

| | | |
|---|---|---|
| Minimum | 0.01 | m |
| Maximum | 1,000.0 | m |

### *Initial cloud details: Hazardous fraction*

This parameter gives the fraction of the cloud that is considered hazardous. The input units are given in brackets and will be either mol/mol or ppm depending on whether or not **Concentrations in ppm** is ticked under the **File, Preferences** menu.

This parameter is linked with the **Hazardous fraction** field in the **Source** screen of the main GASTAR interface. The initial value will therefore be that given in the main GASTAR interface (for segment 1), and any changes made to this value in the Pool Uptake model will also be copied back to the main GASTAR interface should you end up using the Pool Uptake model results. For more details, see the equivalent parameter in Section 3.2.2.

| | | |
|---|---|---|
| Minimum | 0.000001 | mol/mol |
| | 1.0 | ppm |
| Maximum | 1.0 | mol/mol |
| | 1,000,000.0 | ppm |

### *Initial cloud Details: Cloud temperature*

This parameter gives the initial cloud temperature over the pool in kelvin. It is linked with the **Temperature** field in the **Source** screen of the main GASTAR interface. The initial value will therefore be that given in the main GASTAR interface (for segment 1), and any changes made to this value in the Pool Uptake model will also be copied back to the main GASTAR interface should you end up using the Pool Uptake model results.

The source temperature will frequently be derived from a pool spill model (such as LSMS). This will also give the starting temperature for the cloud. As a guideline, if the material is classed as a cryogen then it will boil off and produce a cloud at the boiling point of the material. However, if it is considered to be volatile, then the cloud will be at the pool temperature.

| | | |
|---|---|---|
| Minimum | 10.0 | K |
| Maximum | 2,000.0 | K |

### 3.2.4.2 Meteorology screen

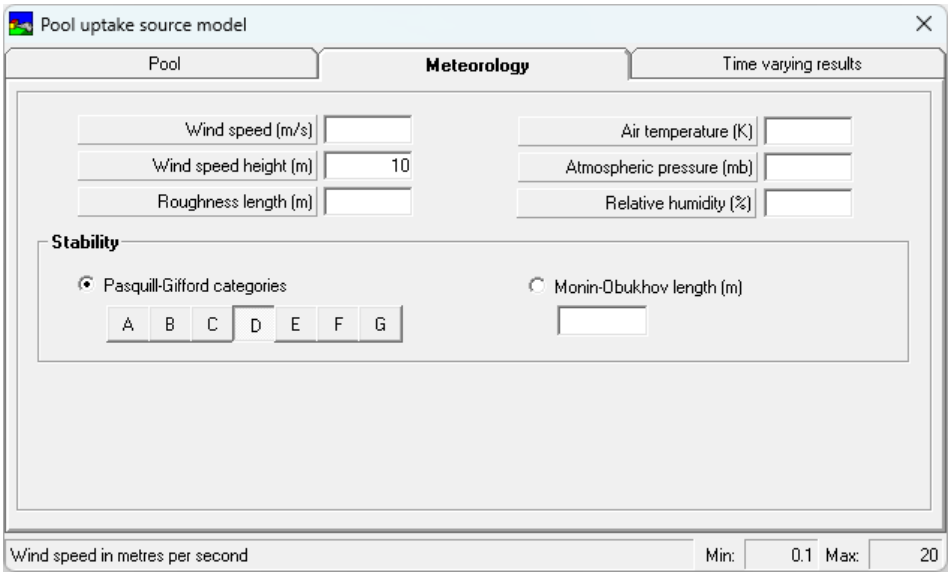



**Figure 3.10** – **Pool uptake source model** – **Meteorology** screen.

The **Meteorology** screen of the Pool Uptake model (**Figure 3.10**) shows a subset of the input in the **Meteorology** screen of the main GASTAR interface and the items have the same meaning – please refer to the Section 3.3 for a fuller explanation of these input parameters. The fields are linked, thus the initial values in this screen will be the same as those given in the **Meteorology** screen of the main GASTAR interface, and any changes made to these values in the Pool Uptake model will also be copied back to the main GASTAR interface should you end up using the Pool Uptake model results.

### 3.2.4.3 Time varying results screen

The **Time varying results** screen of the Pool Uptake model (**Figure 3.11**) allows the user to run the Pool Uptake model, view the resulting time varying source term that GASTAR would use to model the cloud above the evaporating pool spill, and use these results in a GASTAR run.

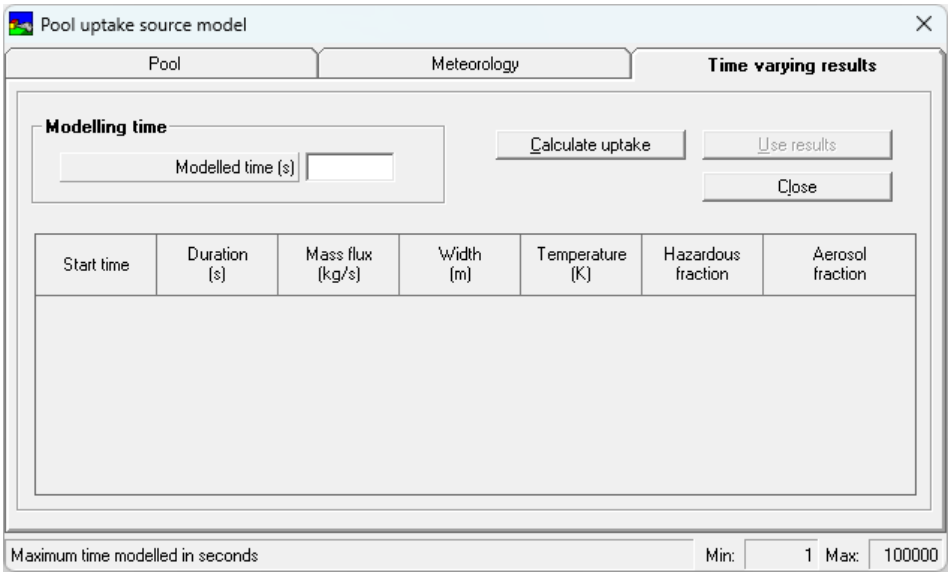



**Figure 3.11** – **Pool uptake source model** – **Time varying results** screen.

### *Modelled time*

This parameter gives the time (in seconds) from release start to which the code will model the cloud dispersion. It is linked with the **Modelled time** field in the **Outputs** screen of the main GASTAR interface. The initial value will therefore be that given in the main GASTAR interface, and any changes made to this value in the Pool Uptake model will also be copied back to the main GASTAR interface should you end up using the Pool Uptake model results.

| | | |
|---|---|---|
| Minimum | 1.0 | s |
| Maximum | 100,000.0 | s |

### *Calculate uptake*

When all the required data has been entered into the Pool Uptake model, click on the **Calculate uptake** button to run the Pool Uptake model. The results will appear in the table.

### *Use results / Close*

Once the results have been displayed in the table, you may choose to use them by clicking on **Use results**, in which case the Pool Uptake model will close and the results (and relevant inputs) will be copied back to the main GASTAR interface, or ignore them by clicking on **Close**, in which case the Pool Uptake model will close without copying the results back to the main GASTAR interface.

## 3.3 Meteorology screen

The **Meteorology** screen is shown in Figure 3.12. Below is a description of the each of the input parameters needed to define the meteorological conditions.

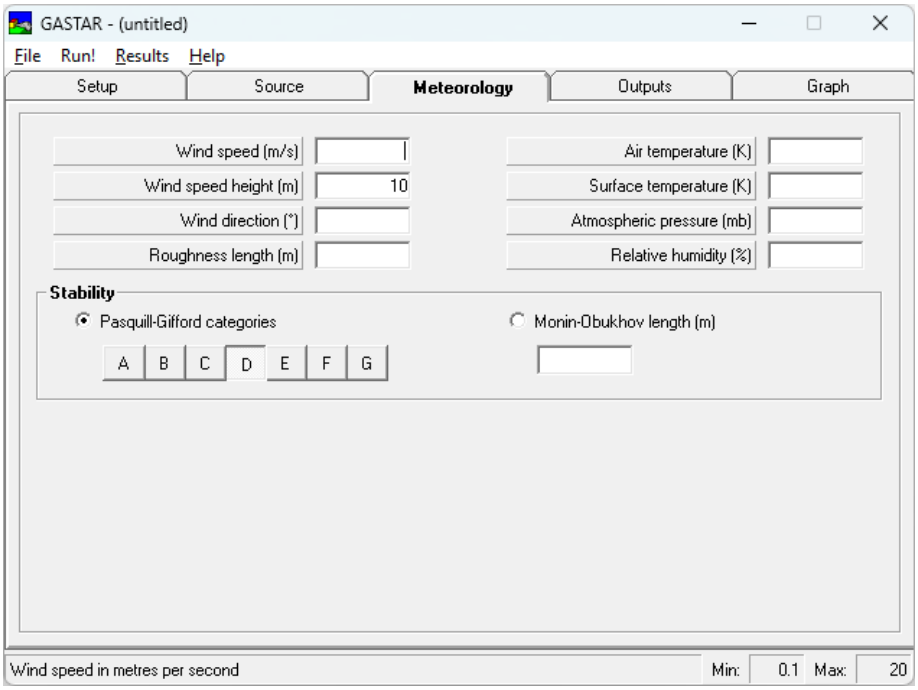



Figure 3.12 − The **Meteorology** screen.

### *Wind speed*

This parameter gives the wind speed, in metres per second, at a known height above the ground. If you have defined slopes with their own meteorological data, this field is disabled and the caption '**(Slopes On)**' appears in the textbox. In such circumstances, the cloud development is based on the conditions prevailing on the current slope – for more details see Section 4.5.3.

| | | |
|---|---|---|
| Minimum | 0.1 | m/s |
| Maximum | 20.0 | m/s |

### *Wind speed height*

This parameter defines the height above the ground, in metres, at which the wind speed measurement (above) was taken. If you have defined slopes with their own meteorological data, this field is disabled and the caption '**(Slopes On)**' appears in the textbox. In such circumstances, the cloud development is based on the conditions prevailing on the current slope – for more details see Section 4.5.3. It has been common practice to measure the wind height at 10m, and consequently a default value of 10 appears in this textbox.

| | | |
|---|---|---|
| Minimum | 0.1 | m |
| Maximum | 15.0 | m |

### *Wind direction*

This parameter defines the wind bearing, measured clockwise from North in degrees. Note that this uses the meteorological definition of wind bearing, namely the direction *from* which the

wind is coming.

| | | |
|---|---|---|
| Minimum | 0.0 | ° |
| Maximum | 360.0 | ° |

### *Roughness length*

This parameter gives the roughness length, in metres. The roughness length is a length scale that categorises the surface roughness by representing the eddy size at the surface. Some approximate values for a variety of land types are given in **Table 3.2**. If you have defined slopes with their own meteorological data, this field is disabled and the caption '**(Slopes On)**' appears in the textbox. In such circumstances, the cloud development is based on the conditions prevailing on the current slope – for more details see Section 4.5.3.

| | | |
|---|---|---|
| Minimum | 0.0001 | m |
| Maximum | 2.0 | m |

| Land type | Roughness length (m) |
|---|---|
| Cities, Woodland | 1.0 |
| Parkland, Open Suburbia | 0.5 |
| Agricultural Areas (max) | 0.3 |
| Agricultural Areas (min) | 0.2 |
| Root Crops | 0.1 |
| Open Grassland | 0.02 |
| Short Grass | 0.005 |
| Sandy Desert | 0.001 |

**Table 3.2** – Typical roughness length values for a range of surfaces.

### *Air temperature*

This parameter gives the ambient air temperature, in kelvin. Note that 0°C is approximately 273K. The air temperature also defines zero enthalpy.

| | | |
|---|---|---|
| Minimum | 220.0 | K |
| Maximum | 330.0 | K |

### *Surface temperature*

This parameter gives the surface temperature in kelvin. If the source release type is set to **Isothermal** on the **Source** screen, this parameter is not required and so this field is disabled with the caption '**(Isothermal)**' appearing in the textbox. In such cases the surface temperature is assumed to be the same as the air temperature.

| | | |
|---|---|---|
| Minimum | 220.0 | K |
| Maximum | 330.0 | K |

### *Atmospheric pressure*

This parameter gives the ambient air pressure, in millibars. Note that 1 standard atmosphere (atm) is equal to 1,013.25 mb.

| | | |
|---|---|---|
| Minimum | 800.0 | mb |
| Maximum | 1,200.0 | mb |

### *Relative humidity*

This parameter gives the relative humidity of the air as a percentage.

| | | |
|---|---|---|
| Minimum | 0.0 | % |
| Maximum | 100.0 | % |

### *Pasquill-Gifford / Monin-Obukhov definition*

Radio buttons allow a mutually exclusive choice between entering the atmospheric stability conditions in terms of the Pasquill-Gifford stability category or the Monin-Obukhov length (see Section 7.3 for more on the relationship between the Monin-Obukhov length and Pasquill-Gifford stability categories):

- **Use Pasquill-Gifford categories**: This is defined by a mutually exclusive choice of 7 buttons each representing a letter between A and G. This is a method of indicating the relative importance of heat convection and mechanical turbulence by dividing the meteorological conditions into fairly simple bands. For instance, A represents extremely unstable conditions and therefore strong convection with large vertical dispersion, D represents neutral conditions in which turbulence is purely mechanical, and G represents very stable conditions in which the mechanical turbulence is strongly damped by stratification.
- **Use Monin-Obukhov length**: This parameter also defines the atmospheric stability via the relative importance of heat convection and mechanical turbulence, but on a continuous scale, measured in metres. Theoretically, it can take all values between ±∞, but in reality, its modulus is unlikely to fall below about 2.

  | | | |
  |---|---|---|
  | Minimum modulus | 2.0 | m |
  | Maximum modulus | 1,000,000.0 | m |

## 3.4 Outputs screen

The **Outputs** screen is shown in **Figure 3.13**. Details relating to the locations and/or times of the model output are specified in this screen, as well as the averaging time.

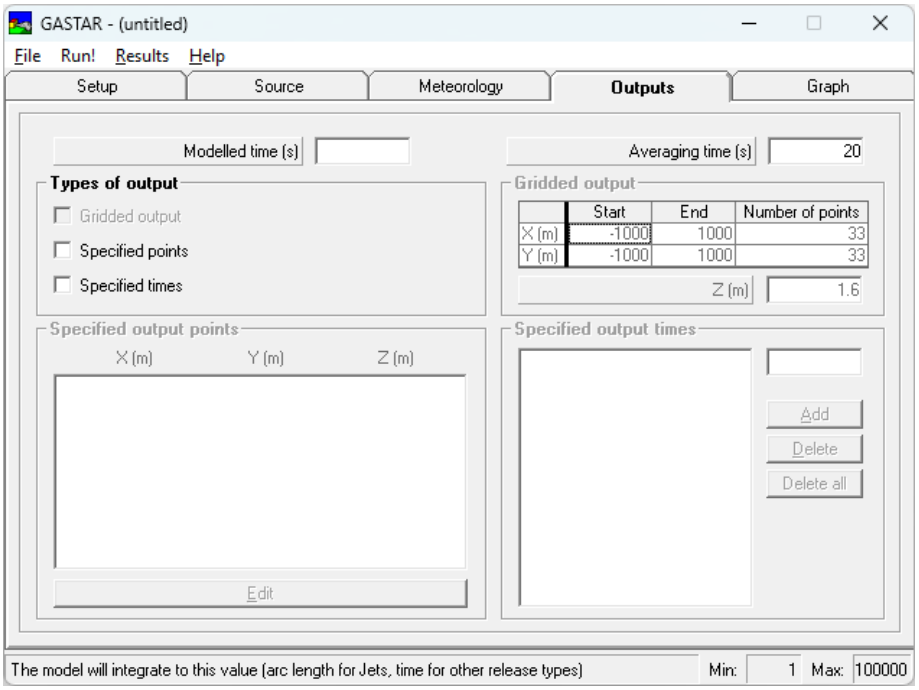



**Figure 3.13** − The **Outputs** screen.

### 3.4.1 Modelled time / Modelled arc length

For **Instantaneous**, **Continuous** and **Time varying** releases, the **Modelled time** gives the time (in seconds) from release start to which the code will model the cloud dispersion.

| | | |
|---|---|---|
| Minimum | 1.0 | s |
| Maximum | 100,000.0 | s |

For **Jet** releases, this field is instead labelled **Modelled arc length** and gives the *approximate* arc length (in metres) from the source to which the code will model the cloud dispersion.

| | | |
|---|---|---|
| Minimum | 1.0 | m |
| Maximum | 100,000.0 | m |

It is important to select an appropriate modelled time/arc length that is large enough to cover the dispersion region/period of interest but is not so large as to lead to unnecessarily sparse output data. It may be advisable to perform a preliminary model run using an initial 'best-guess' value, check the model output and increase/decrease the value accordingly for the main model run.

### 3.4.2 Averaging time

Required for **Continuous**, **Time varying** and **Jet** releases only. For **Instantaneous** releases,

this is disabled and the caption '**(Puff)**' appears in the text box. The model sets the averaging time internally to 20 seconds.

This parameter accounts for plume meander due to short-term changes in mean wind direction, affecting the lateral spread in the dispersion calculations. Longer averaging times result in wider plumes with smaller peak concentrations. While there is no consensus on the most appropriate averaging time, a value of 600 seconds is often supported for non-instantaneous releases, e.g. HSE (2015).

| | | |
|---|---|---|
| Minimum* | 1.0 | s |
| Maximum | 3,600.0 | s |

*It is typically not advised to use a value less than 20 s. This reflects the observation that when $T_{avg} \approx 20$s, plume width correlations revert to puff width correlations: the plume can never be narrower than the puff.

### 3.4.3 Types of output

Use the checkboxes to select which type(s) of output are required for this run; the options are **Gridded output**, **Specified points** and **Specified times**, each of which are described further below. Note that if none of these checkboxes are ticked, the run will still produce the standard results table in the main output (*.gof*) file (see Section 5.1.1).

Any types of output that are not available to the currently selected release type will be greyed out. **Table 3.3** summarises which types of output are available for each release type, as well as which results include output for that particular output type – more details are also given in the sections below, as well as in the model options (Section 4) and output files (Section 5.1) sections.

| | | **Release type** | | | |
|---|---|---|---|---|---|
| | | **Instantaneous** | **Continuous** | **Time varying** | **Gas or liquid jet** |
| **Type of output** | **Gridded output** | ✓[1] | ✓ | × | × |
| | **Specified points** | ✓<br>• Standard results<br>• Dose<br>• Concentration-time history | ✓<br>• Standard results<br>• Dose<br>• Concentration-time history | ✓<br>• Dose<br>• Concentration-time history | × |
| | **Specified times** | ✓<br>• Standard results<br>• Flammables<br>• Gridded output[1] | ✓<br>• Standard results | ✓<br>• Standard results (additional snapshots) | ✓<br>• Standard results |

**Table 3.3** – Output type compatibility with release type. Bullet points list which results include output for that particular output type. [1]Gridded output given at each specified output time for instantaneous releases.

### 3.4.4 Specified output points

Available for **Instantaneous**, **Continuous** and **Time varying** releases only. To define up to

1024 additional specified output points, first tick the **Specified points** checkbox in the **Types of output** box. Then click the **Edit** button in the **Specified output points** box to bring up the **Define Specified Output Points** screen (**Figure 3.14**).

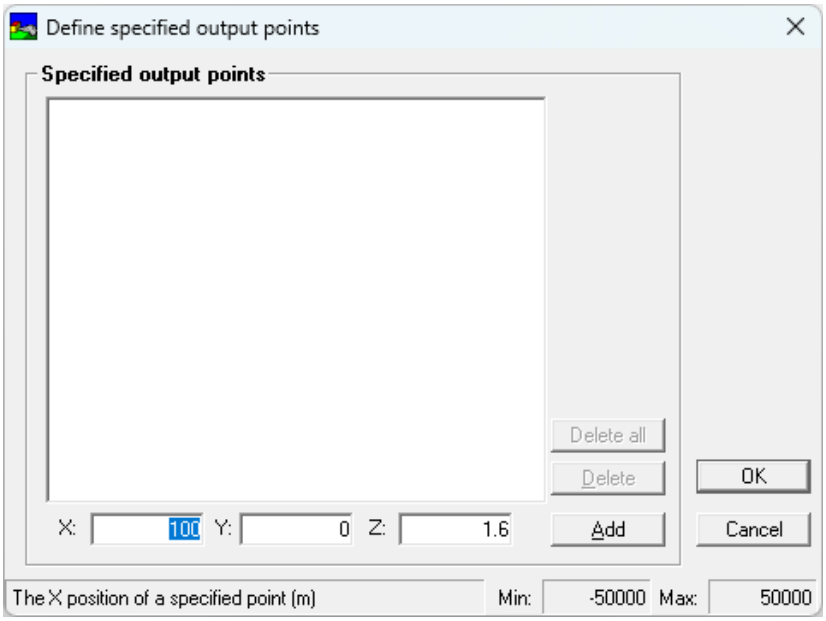



**Figure 3.14** − The **Define Specified Output Points** screen.

Enter values for the *x*, *y* and *z* coordinates of a point in the respective boxes and then click on **Add** or press **Space bar** to add the point to the list. These should be in ***source-centred wind-aligned*** coordinates, i.e. with the source at the origin and positive *x*-axis pointing downwind. To remove a point from the list, highlight it and either click on the **Delete** button, use the **Delete** key, or double click with the mouse (this last method also copies the coordinates of the point being deleted into the *x*, *y*, *z* boxes). The list of points is sorted numerically by *x* then *y* then *z* as they are added. No points may be repeated. Click **OK** (or hit **Enter**) to return to the main GASTAR interface with the specified output points copied into the relevant table of the **Outputs** screen, or click **Cancel** (or hit **Esc**) to return without copying the specified output points.

| | | |
|---|---|---|
| Minimum (*x*, *y*) | -50,000.0 | m |
| (*z*) | 0.0 | m |
| Maximum (*x*, *y*) | 50,000.0 | m |
| (*z*) | 10,000.0 | m |

Note that the numerical method that integrates the model equations in time will attempt to adjust the timestep so that the *x*-coordinate of the cloud hits that of each specified output point (provided the **Modelled time** is large enough for the cloud to have travelled that far). Defining specified output points will therefore likely affect results in general. The travel time associated with each specified output point will also be added to the standard results table in the main output (*.gof*) file for **Instantaneous** and **Continuous** releases.

The specified output points are also used for any dose output (see Section 4.1) and any concentration-time history output (see Section 4.2).

### 3.4.5 Specified output times

Available for all release types. To define up to 50 additional specified output times, first tick the **Specified times** checkbox in the **Types of output** box. This enables the **Specified output times** box – you may then enter the time(s) in the text box and either click on **Add** or press **Space bar** to add each time to the list. To remove a time from the list, highlight it and either click on the **Delete** button, use the **Delete** key, or double click with the mouse. The times are sorted numerically as they are added to the list. No times may be repeated.

| | | |
|---|---|---|
| Minimum | 0.1 | s |
| Maximum | 100,000.0 | s |

Note that the numerical method that integrates the model equations in time adjusts the timestep so that the integration hits each specified output time (that is before the **Modelled time**, or provided the **Modelled arc length** is large enough for the cloud to have travelled for that long for **Jet** releases). Defining specified output times will therefore likely affect results in general. The specified output times will also be added to the standard results table in the main output (*.gof*) file for **Instantaneous**, **Continuous** and **Jet** releases.

For **Time varying** releases, for which the standard results table is a snapshot at the **Modelled time**, additional snapshots are also generated at each specified output time that is before the modelled time, with the results given underneath the main table.

For **Instantaneous** releases, the specified output times are also used for any flammables output (see Section 4.3) and any gridded output (see Section 3.4.6).

### 3.4.6 Gridded output

Available for **Instantaneous** and **Continuous** releases only. To obtain gridded output at a given height above ground, first tick the **Gridded output** checkbox in the **Types of output** box. Then enter the minimum (**Start**) and maximum (**End**) X and Y coordinates for the gridded output, the **Number of points** in the X and Y directions (i.e. the fineness of the results grid) and the height **Z** above ground level at which the output will be calculated. This defines a grid of points in ***source-centred wind-aligned*** coordinates, i.e. with the source at the origin and positive *x*-axis pointing downwind.

| | | | |
|---|---|---|---|
| Minimum | (*x*, *y*) | -50,000.0 | m |
| | (*z*) | 0.0 | m |
| | (*Number of points*) | 1 | - |
| Maximum | (*x*, *y*) | 50,000.0 | m |
| | (*z*) | 10,000.0 | m |
| | (*Number of points*) | 501 | - |

By default, gridded output will be written to a *.gtd* (for **Instantaneous** releases) or *.gst* (for **Continuous** releases) file, both of which have formats recognised by the **2-D Output Plotter** utility for plotting contours in Surfer (see Section 5.3). For consistency with older versions of GASTAR, there is also an option to write the gridded output to a *.ggd* file – this file format includes a metadata header (a full description is given in Section 5.1.4) but is not recognised by the **2-D Output Plotter** and so is not typically recommended. To generate a *.ggd* file instead, run the *.gpl* from a batch file (see Section 2.5.4) and add the

`/G2` option to the command.

For **Continuous** releases, the gridded output file will contain a single set of concentrations reflecting the steady-state solution.

For **Instantaneous** releases, gridded concentrations will be given for each **Specified output time** (see Section 3.4.5); if there are no specified output times, no gridded output will be given.

# SECTION 4 Additional Model Options

This section describes the additional model options available in GASTAR. These options are available via the **Model options** section of the **Setup** screen, as shown in **Figure 4.1**. Some of these options require only basic model input, while others require further information to be entered in separate screens. Options that are not available to the currently selected release type will be greyed out. **Table 4.1** summarises which model options are available to which release types.

| | | Release type | | | |
|---|---|---|---|---|---|
| | | **Instantaneous** | **Continuous** | **Time varying** | **Gas or liquid jet** |
| **Model option** | **Dose** | ✓ | ✓ | ✓ | × |
| | **Concentration-time history** | ✓ | ✓ | ✓ | × |
| | **Flammables** | ✓ | ✓ | × | × |
| | **Obstacles** | ✓ | ✓ | ✓ | × |
| | **Slopes** | ✓ | ✓ | ✓ | × |
| | **Maximum range** | ✓ | × | × | × |

**Table 4.1** – Model option compatibility with release type.

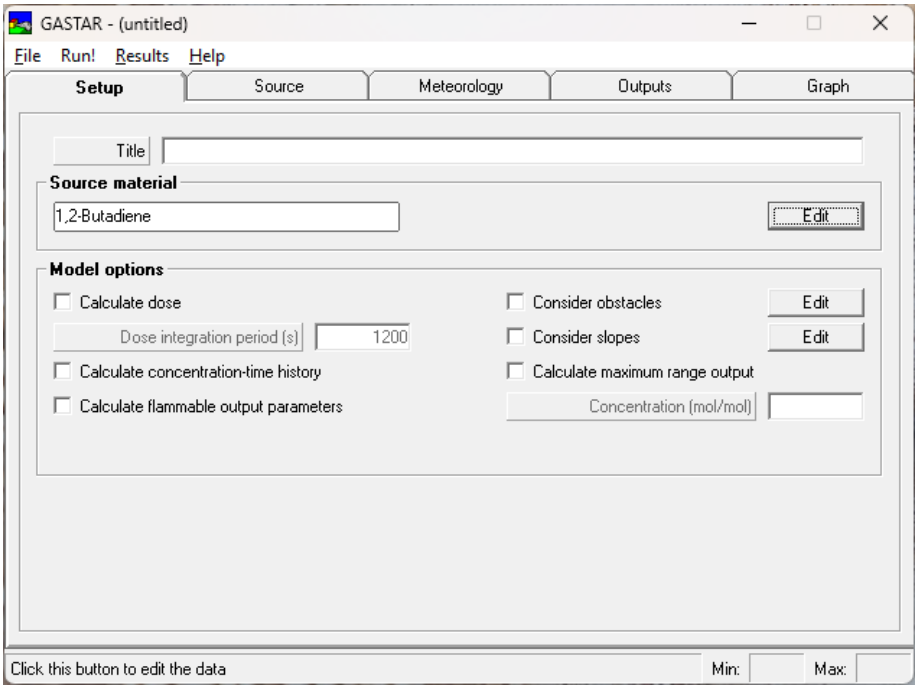



**Figure 4.1** − The **Setup** screen.

## 4.1 Dose

Available for: **Instantaneous, Continuous, Time varying** releases

Tick the Calculate **dose** checkbox on the **Setup** screen to produce dose (and toxic load) output at each **Specified output point** defined in the **Outputs** screen. The output is written to the 'DOSE RESULTS' section of the *.gof* file.

The time interval over which the dose is calculated depends on the release type:

- **Instantaneous** releases: The dose is calculated over the **Modelled time**, as defined in the **Outputs** screen. For output points where the concentration is still significant at the modelled time (specifically, the concentration is greater than 1% of the maximum cloud concentration at the modelled time), the comment 'Still covered' is given in the results table. For output points where the cloud has not yet reached that point at the modelled time, the comment 'Not reached' is given.
- **Continuous** releases: The cloud has a steady-state solution and so the concentration at a given output point is constant in time. The dose is thus simply proportional to the dose integration period. The user must therefore specify a value for the **Dose integration period** in the relevant textbox (minimum value 1 s, maximum value $10^5$ s). For output points that have an associated travel time beyond the **Dose integration period**, the comment 'Not reached' is given.
- **Time varying** releases: The cloud has a defined release start and end time, and so the dose is calculated over all time. However, the dose will not be calculated at any output points that have an associated travel time beyond the **Modelled time** – for these points, the comment 'Not reached' is given in the results table.

For any output points upwind of the source, the comment 'Behind source' is given in the results table.

The dose, $D$, at a given output point, $\mathbf{x}$, is defined by

$$D(\mathbf{x}) = \int_T c(t;\mathbf{x})dt \tag{4.1}$$

where $c(t;\mathbf{x})$ is the concentration (after the relevant concentration profiles have been applied to the integral concentration value) at $\mathbf{x}$ as a function of time $t$, and $T$ is the period of integration as defined above for each release type.

The toxic load $\Gamma(\mathbf{x})$ is calculated as

$$\Gamma(\mathbf{x}) = \int_T \{c(t;\mathbf{x})\}^n dt \tag{4.2}$$

where $n \geq 1$ is the toxic exponent for the source material, as given in the materials database or supplied by the user.

## 4.2 Concentration-time history

Available for: **Instantaneous**, **Continuous**, **Time varying** releases

Tick the **Calculate concentration-time history** checkbox on the **Setup** screen to produce concentration-time history output at each **Specified output point** defined in the **Outputs** screen. The output is written to the 'CONCENTRATION - TIME HISTORY' section of the *.gof* file.

The contents of the results table depend on the release type:

- **Instantaneous** releases: The table gives the concentration at different elapsed times since release (table rows), up to the **Modelled time**, at each specified output point (table columns). There is also a column giving the *x*,*y*,*z* coordinates of the cloud centre at each time since release. With these results, you may see the concentration at a given output point rise and fall as the cloud puff approaches and then passes beyond that point.
- **Continuous** releases: The cloud has a steady-state solution and so the concentration at a given output point is constant in time. Thus, the table simply gives, for each specified output point (table rows), a single steady-state concentration, as well as the travel time from the source to that point.
- **Time varying** releases: The cloud has a piecewise steady-state solution, i.e. the concentration at a given output point is constant while a given segment is passing that point, but is likely to change from one segment to the next. The table thus gives, for each specified output point-segment combination (table rows), the steady-state concentration associated with that segment at that output point, as well as the arrival time (since the start of the release) of the leading edge of that segment at that point. The segment duration is also given, from which the time at which the trailing edge of a given segment passes that point can also be calculated. Note that this time may be slightly different to the arrival time of the next segment; this is because the individual segments are integrated independently and will likely experience slightly different dispersion conditions due to their different initial properties (for example a lower initial height will result in a slightly lower initial advection speed).

In all cases, the concentrations are the concentrations after the relevant concentration profiles have been applied to the integral concentration value.

## 4.3 Flammables

Available for: **Instantaneous, Continuous** releases

Tick the **Calculate flammable output parameters** checkbox on the **Setup** screen to produce flammables output in the 'FLAMMABLES RESULTS' section of the *.gof* file. The output consists of information on the flammable part of the cloud (for releases of flammable materials). Specifically, the following properties of the cloud for both the Lower Flammability Limit (LFL) and half-LFL concentration contours are given:

- downwind and crosswind radius and downwind range (cloud downwind distance plus downwind radius) of the contour for **Instantaneous** releases; maximum (crosswind) width and (downwind) range of the contour for **Continuous** releases;
- maximum height of the contour;
- volume enclosed within the contour;
- mass of flammable material enclosed within the contour.

For **Continuous** releases, for which the cloud has a steady-state solution, a single set of values is given. For **Instantaneous** releases, a set of values is given for each **Specified output time** defined in the **Outputs** screen; if no times are specified, no flammables output will be given for this release type.

No flammables output will be given for non-flammable source materials, i.e. those with an LFL of zero.

The **Hazardous fraction** of the release, as given in the **Source** screen, must also be unity in order to obtain flammables output.

## 4.4 Obstacles

Available for: **Instantaneous, Continuous, Time varying** releases

This option allows the effects of obstacles in the path of the dispersing cloud to be considered. For full details refer to Section 7.14. To enable this option, tick the **Consider obstacles** checkbox on the **Setup** screen and then click the **Edit** button next to this to bring up the **Obstacles** screen, as shown in **Figure 4.2**.

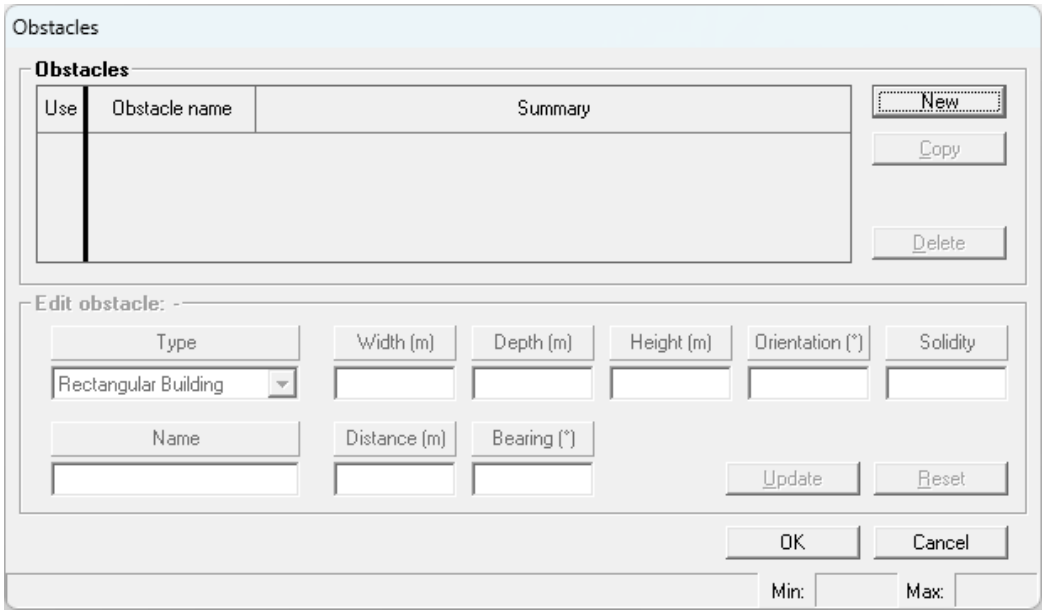



**Figure 4.2** − The **Obstacles** screen.

### 4.4.1 Adding obstacles

Click **New** to add a new obstacle to the table. The properties of that obstacle (which will initially have default values) can then be edited in the **Edit obstacle** box below the table. A description of each property is given further below. Once all the obstacle properties have been defined appropriately, click **Update** to save the edits (or click **Reset** to reset the properties back to the currently saved values). This will update the relevant row of the table, which has three columns:

- **Use**: This first column will respond to the mouse click, or hit the spacebar when it is selected to toggle the tick icon (or use the **Y** and **N** keys). This allows you to turn on/off the effects of obstacles on an individual basis.
- **Obstacle name**: The obstacle name.
- **Summary**: A single-line text summary of the obstacle properties.

The order in which obstacles appear in the table is the order in which they were entered; there is no importance, inferred or otherwise, to their order. Use the **Copy** button to create a copy of the currently selected obstacle in the table. The properties of the copied obstacle can then be updated independently. Use the **Delete** button to delete the currently selected obstacle from the table. The **Edit obstacle** box will show the properties of the currently selected obstacle in the table, which may then be edited and updated if desired. Clicking **OK** will return to the **Source** screen saving any edits made, while clicking **Cancel** will return to the **Source** screen discarding any changes made.

Note that any data stored in the **Obstacles** screen will still be saved with the *.gpl* file even if the **Consider obstacles** checkbox on the **Setup** screen is subsequently unticked. This is useful when you wish to run comparisons with and without the effects of obstacles, or because you have changed the wind direction and know that the obstacles are no longer important. Switching off their effect allows you to keep the data without having to delete it from the data file.

### 4.4.2 Obstacle type

Use the **Type** dropdown to select the obstacle type, using either the mouse or the arrow keys (or use the **R**, **C** or **F** keys). There are three types of obstacle that can be modelled in GASTAR: Rectangular buildings, circular buildings and fences. The properties will change according to the type of obstacle being added, so it is recommended that you select the obstacle type first, before entering other data.

#### *Rectangular building*

Rectangular buildings are defined by a height, the location of the centre point of the building (via a distance and bearing from the source), a width and depth and the orientation of the building – see **Figure 4.3**.

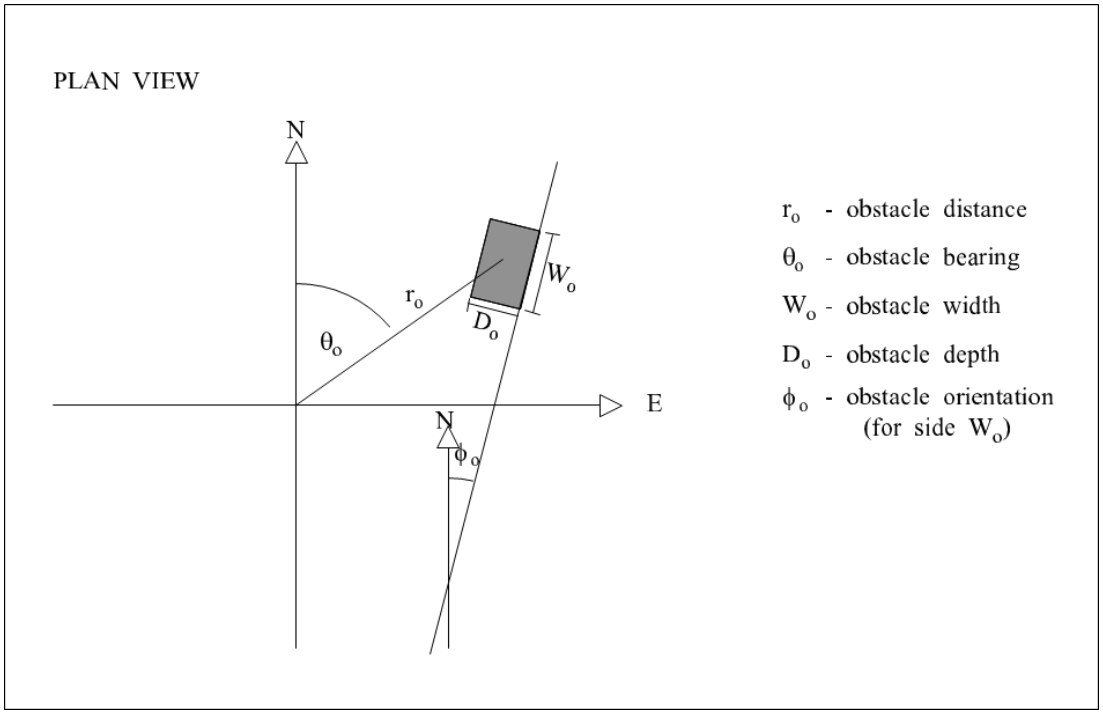



**Figure 4.3** – Definition of a rectangular building.

#### *Circular building*

Circular buildings are defined by a height, the location of the centre point of the building (via a distance and bearing from the source) and a width/diameter – see **Figure 4.4**.

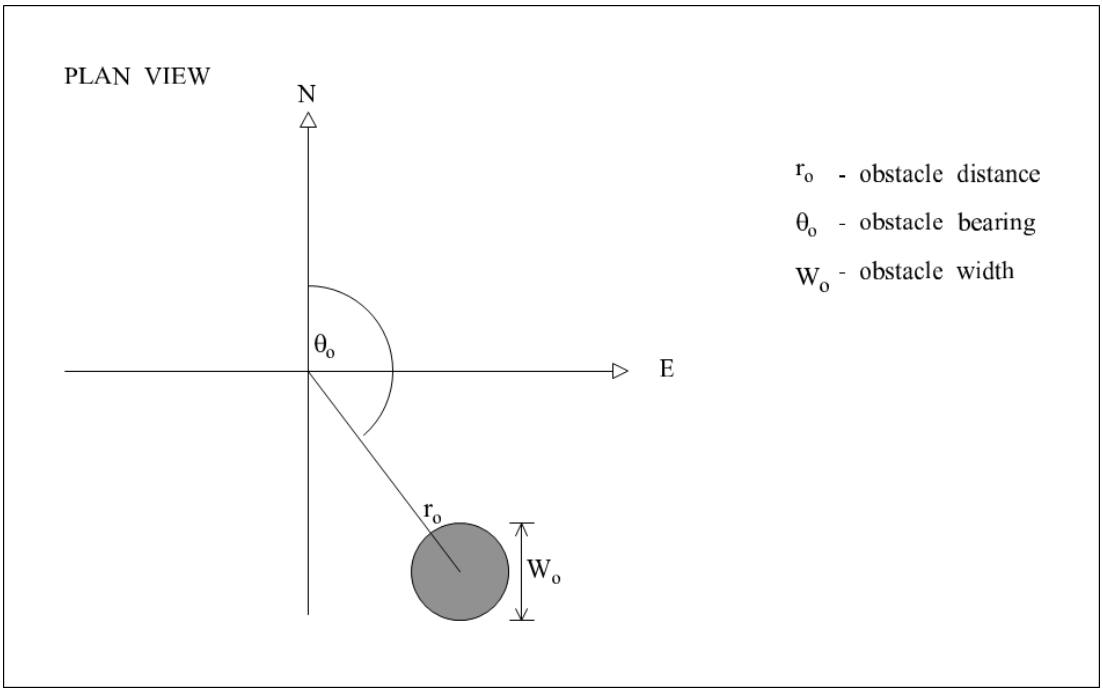



**Figure 4.4** – Definition of a circular building.

### *Fence*

Fences are defined by a height, the location of a point along the fence (via a distance and bearing from the source) and the orientation of the fence – see **Figure 4.5**

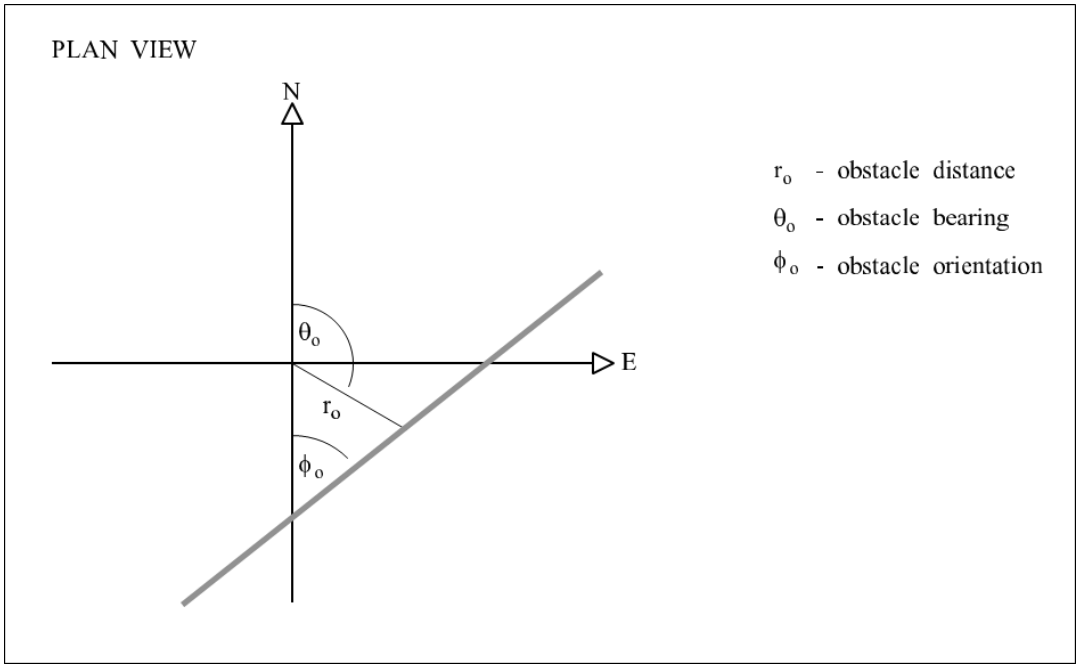



**Figure 4.5** – Definition of a fence.

### 4.4.3 Obstacle properties

#### *Name*

Give the obstacle a name to help you identify it in the table (and output files). The model will tell you if the cloud passed over and interacted with the obstacle or not, so a descriptive name is recommended.

#### *Width/Diameter*

This obstacle dimension is only required for buildings. With a circular building, it is the diameter in metres. For rectangular buildings it can be either of the horizontal dimensions of the obstacles – see the definition of the obstacle orientation below, which is linked to this parameter.

| | | |
|---|---|---|
| Minimum | 1.0 | m |
| Maximum | 1,000.0 | m |

#### *Depth*

This obstacle dimension is only required for rectangular buildings. It represents the *other* horizontal dimension of the building to that given above as the obstacle width, in metres. Please read the definition of the obstacle width and orientation for more explanation.

| | | |
|---|---|---|
| Minimum | 1.0 | m |
| Maximum | 1,000.0 | m |

#### *Height*

This is the obstacle height. All types of obstacle require their height in metres to be entered.

| | | |
|---|---|---|
| Minimum | 1.0 | m |
| Maximum | 500.0 | m |

#### *Orientation*

Fences and rectangular buildings must have their orientation with respect to North defined so that the model can calculate the interaction effects. Circular buildings, by definition, cannot have an orientation.

For rectangular buildings, the relevant angle is the bearing of the side defined as the building *width* above measured in degrees clockwise from North. The angle chosen is the smallest positive value and consequently will be less than 180 degrees.

For fences, the orientation is the bearing of the fence measured clockwise from North. As with rectangular buildings, the angle chosen is the smallest positive value. It is also important to remember that the model considers fences to be infinitely long, so any error on your definition of the fence orientation will become magnified as you move away from the point on the fence defining its position (see obstacle distance and bearing).

| | | |
|---|---|---|
| Minimum | 0.0 | ° |
| Maximum | 180.0 | ° |

### *Solidity*

The solidity allows the effect of the obstacle to be faded in or out. It represents the ratio of the 'blocked out' surface area of the obstacle to the complete surface area including any 'holes', projected into the wind. As a general rule, buildings are not porous and have a solidity of 1. The parameter is usually only applied to fences which are often not solid. For example, if the fence is a picket type where the slats are the same width as the gaps between them, an appropriate solidity factor would be 0.5.

| | | |
|---|---|---|
| Minimum | 0.0 | - |
| Maximum | 1.0 | - |

### *Distance*

This parameter, together with the obstacle bearing, will position the obstacle relative to the source.

For buildings this is the distance, in metres, from the source to the centre of the building.

For fences, this is the distance to any point along the fence. However, this parameter is linked with the obstacle bearing, so you will need to know the bearing of this line defining the distance. Depending where you are obtaining the obstacle data, you may consider a number of strategies to reduce the effect of any errors in your measurement data. One way would be to measure the distance to the fence along a well-defined direction, such as North, South, East or West, thereby removing the error in the obstacle bearing. Another might be to find the nearest point along the fence to the source, so that the fence orientation and bearing are 90 degrees apart. For cases where the orientation of the fence is quite oblique to the cloud trajectory, you may wish to define the point along the fence that lies in the path of the trajectory. In this case you may have to run the model without considering the fence, i.e. turn if *off* by double clicking in the first column of the summary table or unchecking the **Consider obstacles** checkbox on the **Setup** screen. Having discovered the trajectory of the cloud, you will know approximately where it will interact with the fence and can define a point near to that in the obstacle distance and bearing parameters.

| | | |
|---|---|---|
| Minimum | 1.0 | m |
| Maximum | 5,000.0 | m |

### *Bearing*

The obstacle bearing, together with the obstacle distance, will position the obstacle relative to the source.

For buildings this is the bearing, measured clockwise from North in degrees, of the imaginary line drawn from the source to the centre of the building.

For fences this is the bearing, measured clockwise from North in degrees, of the imaginary line drawn from the source to a point along the fence whose length is the obstacle distance defined above.

| | | |
|---|---|---|
| Minimum | 0.0 | ° |
| Maximum | 360.0 | ° |

## 4.5 Slopes

Available for: **Instantaneous, Continuous, Time varying** releases

This option allows the effects of slopes on the dispersing cloud to be considered. For full details refer to Section 7.15.

The slopes module allows for simple slopes to be modelled. Such slopes can be visualised as resembling a sheet of card, folded along *parallel* lines. The folds are the boundaries between the rectilinear plane slope segments. Each segment has a finite along-slope length but is assumed to extend laterally to ± infinity. Note that the direction of maximum slope need not be aligned with the wind direction, allowing for crosswind slopes.

To enable this option, tick the **Consider slopes** checkbox on the **Setup** screen and then click the **Edit** button next to this to bring up the **Slopes** screen, as shown in **Figure 4.6**.

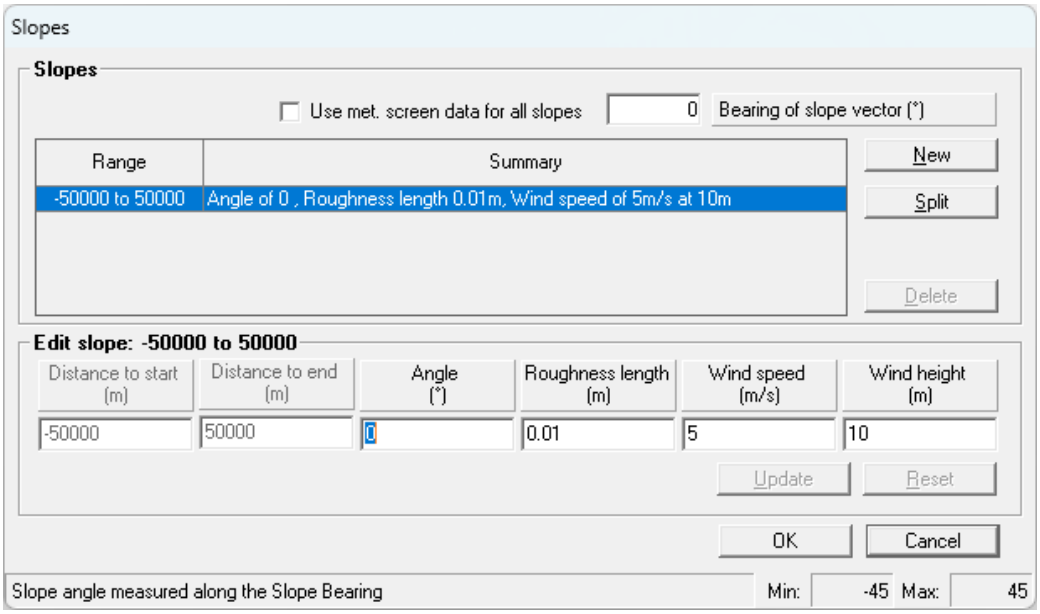



**Figure 4.6** − The **Slopes** screen.

### 4.5.1 Slope vector and meteorological data

The **Bearing of slope vector** field in the **Slopes** box defines the bearing, measured clockwise from North in degrees, of the line of maximum slope for the slope segments (minimum value 0°, maximum value 360°) – see $\theta_S$ in **Figure 4.7**. The bearing is measured in the same manner as the wind direction. For example, if you have the same value for the slope and wind bearing, they will be aligned such that moving along the slope vector in the negative direction is upwind, and in the positive direction is downwind. This form of definition allows you to separate a slope segment's angle from the wind direction, because a slope segment's angle is measured relative to the slope vector and is the incline seen by someone moving in the positive direction along the slope vector. You can reverse the wind direction simply by adding $180^o$ to the wind bearing and the ground will not be altered, i.e. the effective reversal of the slopes seen by the cloud will be accounted for by the slope vector.

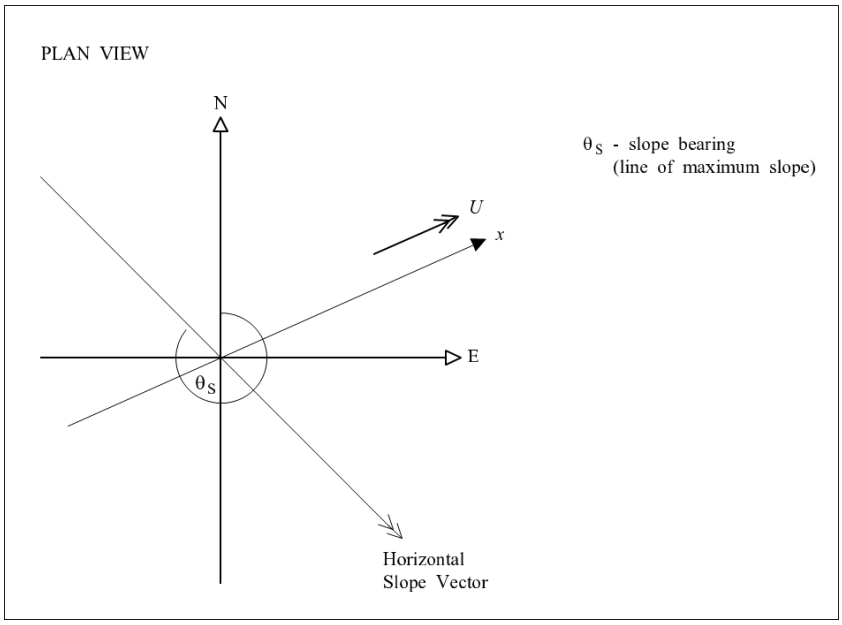



**Figure 4.7** − Definition of slope bearing.

The **Use met. screen data for all slopes** checkbox in the **Slopes** box is unticked by default. This means that, for each slope segment, the user must supply not only the slope parameters but also values for the ground roughness length, wind speed and height of the wind speed measurement associated with that segment. Accordingly, the equivalent fields in the **Meteorology** screen of the main GASTAR interface will display the text '(**Slopes On**)' and will not be editable. Alternatively, if you wish to use the **Meteorology** screen data for all slope segments, tick the **Use met. screen data for all slopes** checkbox; all fields in the **Meteorology** screen of the main GASTAR interface will now be editable. While ticking this checkbox will grey out any meteorological data associated with the slope segments (to indicate it will not be used by the model), note that the information is still retained/saved with the *.gpl* file so that it can be reinstated if you decide to untick the checkbox again.

### 4.5.2 Adding slope segments

The table in the **Slopes** box summarises the currently defined slopes. There are two columns in the table: The first column gives the range of each slope segment measured in metres, along the slope vector, relative to the source; the second column gives a data summary for each slope segment.

Initially, the table will by default contain one entry which defines a single flat 'slope' segment (i.e. an angle of 0 $^{o}$) extending the full permissible range either side of the source, i.e. from -50,000 to 50,000 m. The properties of this (or any) slope segment can be edited in the **Edit slope** box below the table; click **Update** to save the edits (or click **Reset** to reset the properties back to the currently saved values). A description of each property is given in Section 4.5.3 below.

Click **New** or **Split** to split the currently selected segment into two separate segments:

- Using the **New** button means that the new segment will be given default properties

- Using the **Split** button mean that the new segment will keep the same properties as the segment being split

By default, the split point will be taken as the mid-point of the segment being split, however this can be modified by editing the **Distance to start** of the 'new' segment, i.e. the segment further along the (positive) slope vector.

Use the **Delete** button to delete the currently selected slope segment from the table. Since there can be no gaps between slope segments, the range covered by the deleted segment will be automatically absorbed into the definition of the preceding segment. There is no warning before the slope segment is removed.

The slope segments in the table are always ordered with adjoining segments next to each other, moving in the positive direction along the slope vector. The **Edit slope** box will show the properties of the currently selected slope segment in the table, which may then be edited and updated if desired.

Clicking **OK** will return to the **Source** screen saving any changes made, while clicking **Cancel** will return to the **Source** screen discarding any changes made.

Note that any data stored in the **Slopes** screen will still be saved with the *.gpl* even if the **Consider slopes** checkbox on the **Setup** screen is subsequently unticked. This is useful when you wish to run comparisons with and without the effects of slopes. Switching off their effect allows you to keep the data without having to delete it from the data file.

### 4.5.3 Slope segment properties

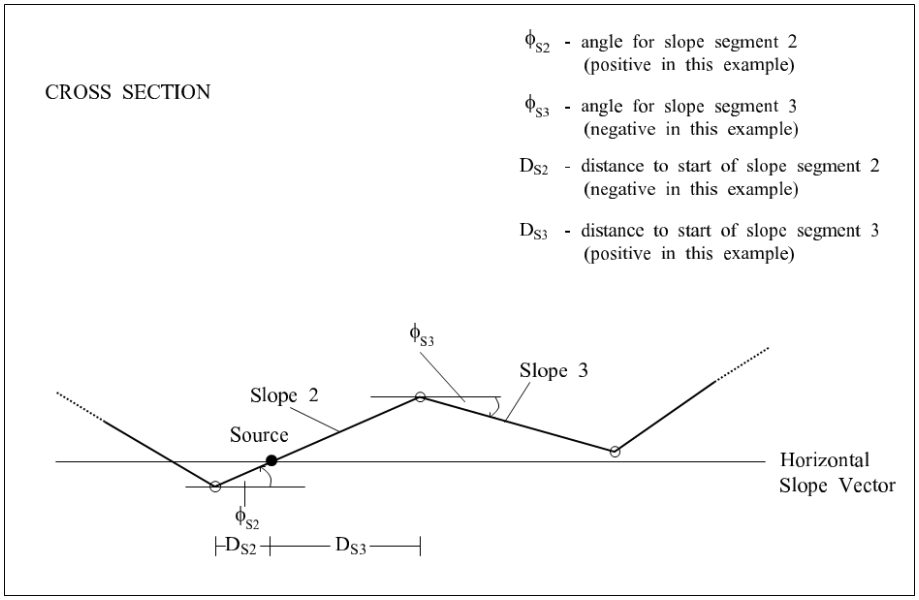



**Figure 4.8** − Vertical section through the sloping ground parallel to the slope vector.

#### *Distance to start*

This parameter gives the distance along the slope vector from the source to the start of this slope segment, in meters (see **Figure 4.8**). Note that this field is not editable for the first segment in the table, which will always be set to -50,000 m.

| | | |
|---|---|---|
| Minimum | -50,000.0 | m |
| Maximum | 50,000.0 | m |

### *Distance to end*

This parameter gives the distance along the slope vector from the source to the end of this slope segment, in meters (see **Figure 4.8**). This value is calculated automatically (i.e. it is not editable by the user) and is displayed for information purposes only. Since there can be no gaps between slope segments, the **Distance to end** of a given segment will, for all but the last slope segment, be equal to the **Distance to start** of the segment that follows it. For the last segment, the **Distance to end** will always be set to 50,000 m.

| | | |
|---|---|---|
| Minimum | -50,000.0 | m |
| Maximum | 50,000.0 | m |

### *Angle*

This parameter gives the angle of incline (positive values) or decline (negative values) of the current slope segment measured in degrees from the horizontal as you move along the positive slope vector (see **Figure 4.8**).

| | | |
|---|---|---|
| Minimum | -45.0 | ° |
| Maximum | 45.0 | ° |

### *Roughness length*

This parameter gives the roughness length, in metres, for the current slope segment. It has the same definition as the roughness length parameter on the **Meteorology** screen (see Section 3.3). This field is only editable if the **Use met. screen data for all slopes** checkbox is unticked, otherwise it will be greyed out.

| | | |
|---|---|---|
| Minimum | 0.0001 | m |
| Maximum | 2.0 | m |

### *Wind speed*

This parameter gives the wind speed, in metres per second, at a known height above ground over the current slope segment. This field is only editable if the **Use met. screen data for all slopes** checkbox is unticked, otherwise it will be greyed out.

| | | |
|---|---|---|
| Minimum | 0.1 | m/s |
| Maximum | 20.0 | m/s |

### *Wind height*

This parameter defines the height above the ground, in metres, at which the wind speed measurement for the current slope segment was taken. This field is only editable if the **Use met. screen data for all slopes** checkbox is unticked, otherwise it will be greyed out.

| | | |
|---|---|---|
| Minimum | 0.1 | m |
| Maximum | 15.0 | m |

## 4.6 Maximum range

Available for: **Instantaneous** releases

Tick the **Calculate maximum range output** checkbox on the **Setup** screen to output the maximum range (in metres) from the source to a user-defined (ground-level) concentration, along with the time and location at which the corresponding concentration occurred. The output is written to the 'MAXIMUM RANGE RESULTS' section of the *.gof* file. The calculation considers all time up to the **Modelled time**, as given in the **Outputs** screen; a warning will be written to the *.gof* file if the true maximum range is expected to be greater than the value given due to the relevant contour still existing at the modelled time. A warning will also be written if the maximum range occurred around the same time as an interaction with an obstacle.

The user-defined concentration whose maximum range is to be found should be entered in the **Concentration** field, which becomes editable once the **Calculate maximum range output** checkbox is ticked (see **Figure 4.9**). The input units are given in brackets and will be either mol/mol or ppm depending on whether or not **Concentrations in ppm** is ticked under the **File, Preferences** menu.

| | | |
|---|---|---|
| Minimum | 0.000,000,01 | mol/mol |
| | 0.01 | ppm |
| Maximum | 0.999,999 | mol/mol |
| | 999,999.0 | ppm |

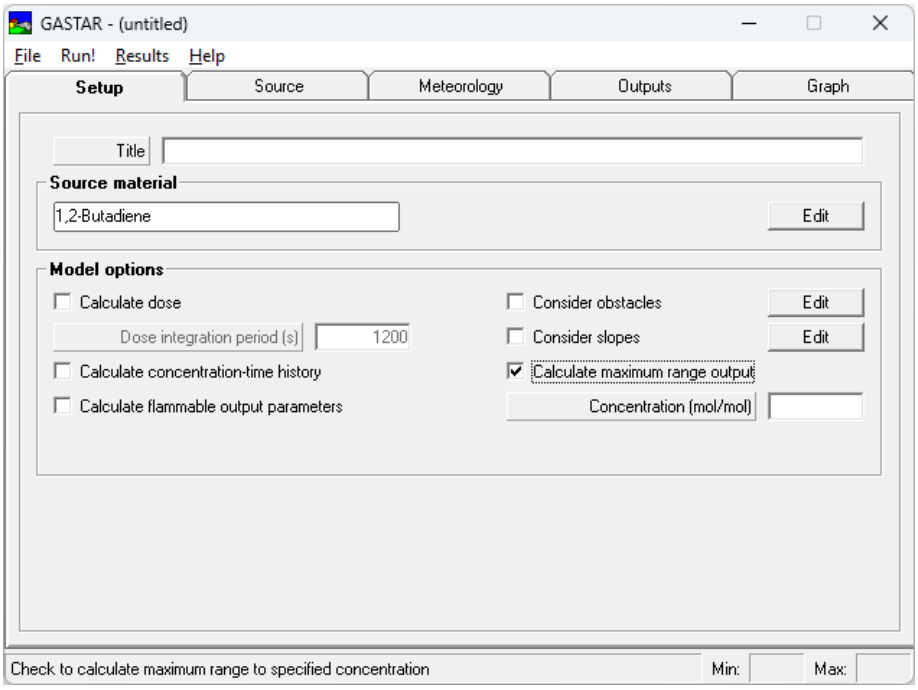



**Figure 4.9** − The **Setup** screen with **Calculate maximum range output** ticked.

# SECTION 5 Model Output

The output file(s) produced by GASTAR depend on the run configuration. This section describes each possible output file and presents the tools available in GASTAR to visualise the results of a run.

Section 5.1 describes the different types of files produced by GASTAR. Section 5.2 describes the **Graph** screen of the GASTAR interface, which can be used for 1-D plotting. Section 5.3 describes how 2-D contour plots can be created in Surfer (a third-party software application) if it is installed.

## 5.1 Output files

### 5.1.1 .gof file

The *.gof* file is GASTAR's main formatted output file and is created for every run. It is designed to be human-readable in a text editor such as Notepad. It can also be easily imported into a spreadsheet editor, such as Excel, as a *tab delimited* file.

The top part of the *.gof* file contains model version information, the date and time at which the model run was started, and licence file information. Below this is a summary of the model set up parameters entered in the GASTAR interface and saved in the *.gpl* file (and some derived parameters), including the source material name, release type, meteorological parameters ('METEOROLOGICAL INPUT' section) and source details ('SOURCE DEFINITION' section) – see **Figure 5.1**.

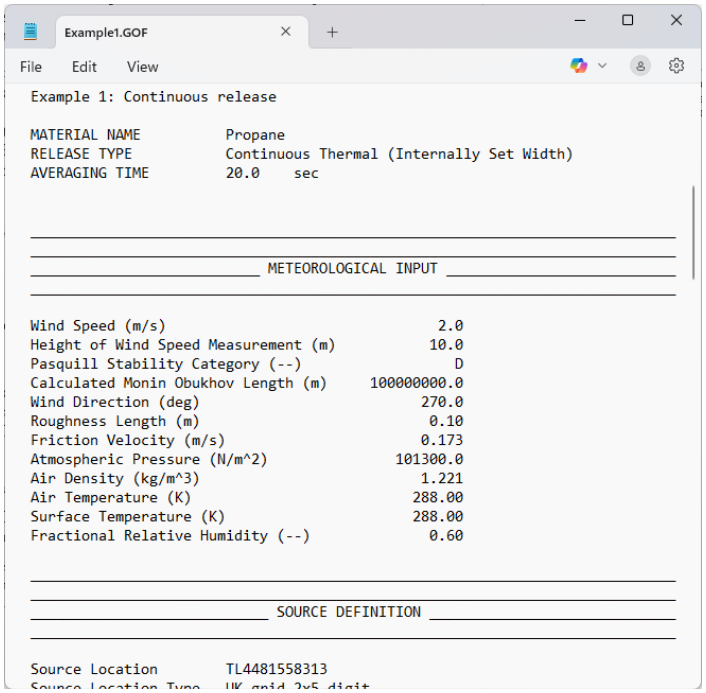



**Figure 5.1** – Part of an example *.gof* file.

This is followed by one or more additional sections, depending on the run configuration. Each possible section is described below.

### *RESULTS section*

The 'RESULTS' section is included for every run and contains values of the main integration variables, together with some other derived variables. The meaning of each output parameter is given in **Table 5.1**; those that are derived are indicated with an asterisk*.

The interpretation of the data table(s) in this section depends on the release type:

- **Instantaneous** releases: The table gives the cloud properties at different elapsed times since release, from zero up to the **Modelled time**.
- **Continuous** releases: The table gives the steady-state cloud properties at different travel times from the source, from zero up to the **Modelled time**.
- **Time varying** releases: The first table gives a snapshot of the cloud properties at the **Modelled time**, at different travel times from the source, up to the modelled time. If the source is still emitting at the modelled time, the travel times will start from zero, otherwise they will start from the travel time associated with the trailing edge of the cloud at the modelled time. Additionally, for each **Specified output time** defined in the **Outputs** screen (that is before the modelled time), an additional table will be written out that gives a snapshot of the cloud properties at that output time.
- **Gas or liquid jet** releases: The table gives the steady-state cloud properties at different travel times from the source, from zero up to the first integration time for which the associated arc length is greater than the **Modelled arc length**.

For **Instantaneous**, **Continuous** and **Jet** releases, the times in the table are all times that were actually hit during the integration calculations, i.e. no interpolation is necessary. This includes any **Specified output times** and the times associated with any **Specified output points**[1] (as long as these occur before last time in the table). For **Time varying** releases, for which each table gives a snapshot of the cloud at a given time since release start, the times in the table are equally spaced, interspersed with any travel times associated with the boundaries between two segments (for which the properties given represent the average of the two segments); interpolation of the integration results is therefore necessary in this case.

Note that GASTAR uses an adaptive integration timestep that is optimised for short run times, so that the timestep tends to be significantly larger at the end of the simulation (when cloud properties change relatively slowly) than at the beginning (when cloud properties change relatively quickly). This means that the resolution of cloud properties is typically relatively coarse at the end of the simulation compared with the start. The specified output times and points can be used to augment the integration times, thus increasing the resolution later in the simulation if desired.

[1] Since the model integrates in time, the adaptive timestep can be set to exactly hit each specified output time. The model also tries to hit the times where the downwind distance of the cloud centre(line), Xc or X, is equal to the *x*-coordinate of each specified output point, however this is only approximate and so the corresponding entries in the RESULTS table may have a slightly different X coordinate.

For **Jet** releases, the model transitions from using the jet integration routines to the 'standard' dense gas integration routines (as used for the other non-directional release types) when the jet velocity reduces to some predetermined level *and* jet 'touchdown' has occurred (see Section 7.13.3 for more details). Information about this transition (if it occurred) is also written to the RESULTS section of the *.gof* file, underneath the main table.

| Parameter | Units | Description |
|---|---|---|
| Time since release or travel time | s | Instantaneous releases: Time since release<br>Continuous and jet releases: Travel time from source (steady-state solution)<br>Time varying releases: Travel time from source at given snapshot time |
| Arc length | m | Distance along cloud centre/centreline trajectory |
| Xc or X | m | Instantaneous releases: Downwind distance to cloud centre at given time since release<br>Other release types: Downwind distance to cloud centreline at given travel time |
| Yc or Y | m | Instantaneous releases: Crosswind distance to cloud centre at given time since release<br>Other release types: Crosswind distance to cloud centreline at given travel time |
| Z | m | Jet releases: Height of jet centreline at given travel time<br>Other release types: Always zero |
| C | mol/mol or ppm | Integral/top-hat cloud concentration (hazardous fraction only) |
| Cmax* | mol/mol or ppm | Instantaneous releases: Maximum concentration within cloud after along-wind, crosswind and vertical concentration profiles applied (hazardous fraction only)<br>Other release types: Maximum concentration within cloud after crosswind and vertical concentration profiles applied (hazardous fraction only) |
| Mass Fr | -- | Reciprocal of dilution factor of cloud by mass, i.e. ratio of mass (flux) at release to current cloud mass (flux). Mass (flux) at release does not include any initial air entrainment but current mass (flux) does. |
| W | m | Instantaneous releases: Cloud diameter<br>Other release types: (Lateral) cloud width |
| H | m | (Vertical) cloud depth |
| V or V flux | $m^3$ or $m^3/s$ | Instantaneous releases: Cloud volume<br>Other release types: Cloud volume flux |
| U | m/s | Cloud advection speed |
| M or M flux | kg or kg/s | Instantaneous releases: Total mass of cloud<br>Other release types: Mass flux of cloud |
| E or E flux | kJ or kJ/s | Instantaneous releases: Total enthalpy of cloud<br>Other release types: Enthalpy flux of cloud |
| T | K | Cloud temperature |
| Rho | $kg/m^3$ | Cloud density |
| AF | -- | Cloud aerosol fraction – mass (flux) of liquid as a fraction of total cloud mass (flux) |
| Ri | -- | Richardson number based on friction velocity, cloud density and depth |
| Xle | m | Output for instantaneous releases only. Downwind distance from source to leading edge of cloud (= Xc + W/2) |
| Xte | m | Output for instantaneous releases only. Downwind distance from source to trailing edge of cloud (= Xc – W/2) |
| Wtot* | m | Lateral width of cloud taking into account turbulent spreading ($\sigma_y$). Mainly important for passive clouds. |
| Wdisp* | m | Output for instantaneous releases only. Longitudinal width of cloud taking into account turbulent spreading ($\sigma_x$) and shear dispersion ($\sigma_s$). Mainly important for passive clouds. |
| Area | $m^2$ | Output for instantaneous releases only. Plan-view area of cloud ($=\pi W^2/4$) |

**Table 5.1** – Output parameters in the RESULTS table of the *.gof* file. *Derived variables

#### *DOSE RESULTS section*

This section is included if the **Calculate dose** model option is selected in the **Setup** screen (available for **Instantaneous**, **Continuous** and **Time varying** releases). The table gives the dose (and toxic load) at each **Specified output point** defined in the **Outputs** screen – see **Table 5.2** below for column descriptions. The time interval over which the dose is calculated depends on the release type – refer to Section 4.1 for more details.

| Column name | Units | Description |
|---|---|---|
| Point | -- | Output point counter |
| X | m | Output point x-coordinate |
| Y | m | Output point y-coordinate |
| Z | m | Output point z-coordinate |
| Dose | mol/mol minute or ppm minute | Concentration dose at output point |
| Toxic load | $(mol/mol)^n$ minute or $(ppm)^n$ minute | Toxic load at output point |
| Comment | -- | Information on status of point relative to cloud that might affect the value calculated – see Section 4.1 for details |

**Table 5.2** – Columns in the DOSE RESULTS table of the *.gof* file. n in the toxic load units is the toxic exponent of the source material.

#### *CONCENTRATION-TIME HISTORY section*

This section is included if the **Calculate concentration-time history** model option is selected in the **Setup** screen (available for **Instantaneous**, **Continuous** and **Time varying** releases). The contents of the results table depend on the release type – see Section 4.2 for more details.

#### *FLAMMABLES RESULTS section*

This section is included if the **Calculate flammable output parameters** model option is selected in the **Setup** screen (available for **Instantaneous** and **Continuous** releases only). The contents of the results table depend on the release type – see Section 4.3 for more details.

#### *MAXIMUM RANGE RESULTS section*

This section is included if the **Calculate maximum range output** model option is selected in the **Setup** screen (available for **Instantaneous** releases only). It gives the maximum range (in metres) from the source to a user-defined (ground-level) concentration, along with the time and location at which the corresponding concentration occurred. See Section 4.6 for more details.

### 5.1.2 .gph file

The *.gph* file is also created for every GASTAR run. This tab-delimited file includes the same data as that found in the standard RESULTS table of the *.gof* file (and the FLAMMABLES RESULTS table if present), but in a format that is readable by the **Graph** utility.

### 5.1.3 .log file

The *.log* file is also created for every GASTAR run includes any info, warning and/or error messages issued during the model run.

*You can open the .log file of the current model file in the preferred viewing software using the **Results, Log file** menu item.*

### 5.1.4 .gst, .gtd and .ggd files

The *.gst*, *.gtd* and *.ggd* files are all associated with gridded output, which is available for **Instantaneous** and **Continuous** releases only and is generated if the **Gridded output** checkbox is ticked in the **Outputs** screen.

By default, gridded output will be written to a *.gtd* file for **Instantaneous** releases or a *.gst* file for **Continuous** releases, both of which have formats recognised by the **2-D Output Plotter** utility for plotting contours in Surfer (see Section 5.3). However, the legacy *.ggd* file can be generated instead by adding the `/G2` flag if running GASTAR from the command line or a batch file. This file format is not recognised by the **2-D Output Plotter** and so is not typically recommended. It differs from the *.gst*/*.gtd* file format only by the inclusion of a metadata header (described further below) above the main data table.

The main data table is in comma-separated format and includes 8 columns: Year, Day, Hour, Time, X, Y, Z and Conc (concentration) – see **Table 5.3** below for column descriptions. The output points use ***source-centred wind-aligned*** coordinates, i.e. with the source at the origin and positive *x*-axis pointing downwind. The concentration units will be either mol/mol or ppm depending on whether or not **Concentrations in ppm** is ticked under the **File, Preferences** menu. For **Continuous** releases, a single set of concentrations is given, reflecting the steady-state solution. For **Instantaneous** releases, concentrations are given for each **Specified output time** defined in the **Outputs** screen; if there are no specified output times, no output will be given.

| Column name | Units | Description |
|---|---|---|
| Year | -- | Year of release start |
| Day | -- | Julian day of release start, e.g. Jan 1st = 1, Dec 31st = 365 or 366 |
| Hour | -- | Hour of release start |
| Time(s) | s | Instantaneous releases: Time since release<br>Continuous releases: Always -999 |
| X(m) | m | x-coordinate of output point |
| Y(m) | m | y-coordinate of output point |
| Z(m) | m | z-coordinate of output point |
| Conc… | mol/mol or ppm | Concentration at this output point (at the given time since release for instantaneous releases) |

**Table 5.3** – Columns in the main data table of the gridded output file.

The metadata header in the *.ggd* file contains the following information:

| Line | Parameter | Description |
|---|---|---|
| Line 1 | Title | "GASTAR gridded data output file" |
| Line 2 | FILE_VERSION | *.ggd* file version: Currently 1.0 |
| Line 3 | FILE_STEM | Input file stem (i.e. filename excluding *.gpl*) |
| Line 4 | PATH | Full pathname of directory in which *.gpl* file is located |
| Line 5 | WIND_DIRECTION | Wind direction (°); included so that the output (x,y) coordinates (which are always aligned so that the positive x-axis is downwind) can be translated to a fixed coordinate system if required |
| Line 6 | COORD_SYSTEM | Coordinate system in which the source location is given |
| Line 7 | SOURCE_LOCATION | Source location, in the above coordinate system |
| Line 8 | RELEASE_DATE_AND_TIME | Release date and time, in the format YYYY/MM/DD HH:MM |
| Line 9 | TIME_ZONE | Time zone; currently always UTC |
| Line 10 | POLLUTANT_NAME | Source material name |
| Line 11 | CONCENTRATION_UNITS | Concentration units; either mol/mol or ppm |
| Line 12 | AVERAGING_TIME_SECONDS | Averaging time (s) |
| Line 13 | END_OF_HEADER_SECTION | Separator line |
| Line 14 | NX | Number of x-values in the output grid |
| Line 15 | NY | Number of y-values in the output grid |
| Line 16 | NZ | Number of z-values in the output grid; currently always 1 |
| Line 17 | NT | Number of output times. Always 1 for continuous releases |
| Line 18+ | Time X | List of output times since release (s). Always one value of -999 for continuous releases. |

**Table 5.4** – Contents of metadata header in *.ggd* file.

## 5.2 Graph screen

Once a GASTAR run is complete, the **Graph** screen (shown in **Figure 5.2**) can be used for 1-D plotting of the resulting output data.

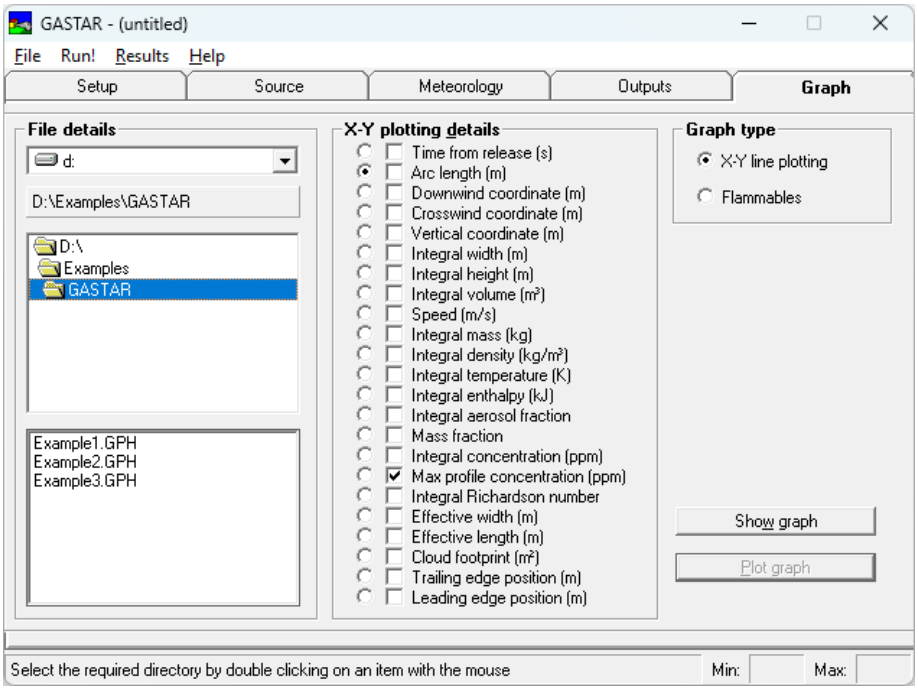



**Figure 5.2** − The **Graph** screen.

### 5.2.1 Selecting data to plot

This involves selecting one or more graphical data (*.gph*) files using the controls in the **File Details** box.

Use the Drive dropdown list at the top to select the drive from which you wish to plot data. This conforms to the Windows standard and will show any drive that is currently mapped by your system. To map a new drive, use the **Map network drive** option under the ellipses (...) after selecting **This PC** in Explorer. Alternatively, you can paste or drag-drop a UNC path from Explorer onto the path label to access "\\servername\" type paths.

You can then use the Directory list in the middle to navigate to the correct directory on the drive. Once there, all the available output data files in that directory will appear in the File list at the bottom.

Click on the data file you wish to plot in the File list. If you wish to plot from multiple files do so in the normal Windows way by holding down the **SHIFT** key and clicking on the final data file you want to plot. To select multiple isolated files from the list, hold down the **CTRL** key and click on those files you want to plot. When you have selected one or more *.gph* files the **Plot Graph** button will become enabled, signifying that data are available to plot.

If you have just run the model in the directory currently displayed but the new data file has not appeared, try clicking with the right mouse button in the file list box. This will request it to update and display the current contents of the directory.

Next, select the **Graph type** using the appropriate radio button in the top right box. There are two types of graph available, namely **X-Y line plotting** and **Flammables** graphical output, and which one you choose determines the form of the rest of the display on the **Graph** screen.

#### *X-Y line plotting*

This is likely the graph type you will want to use in the majority of cases, as it allows you to plot any of the core output data. With this graph type selected, the central box of the **Graph** screen displays the variables that may be plotted against each other.

The dependent variable (*x*-axis) is selected using the (circular) radio buttons. Only one dependent variable may be selected. By default, the Arc length is selected.

The independent variable(s) (*y*-axis) are chosen using the checkboxes. You may choose to plot more than one variable at the same time. Note, however, that variables with very different magnitudes may lead to a graph that is difficult to interpret. The variables available for plotting will vary depending on the release type.

#### *Flammables*

This graph type is available for **Instantaneous** and **Continuous** releases of flammable materials, providing the flammables model option was selected (see Section 4.3). With this graph type selected, the central box of the **Graph** screen displays a series of checkboxes, one for each variable that may be plotted. Tick the variable(s) you wish to plot. Above the checkboxes is a list containing the concentrations that may be plotted, i.e. the Lower Flammability Limit (LFL) and half-LFL associated with the flammable source material: highlight one or both of these to select them for plotting. If multiple files are selected but are associated with source materials with differing LFLs, only data from the files with the selected LFL will be plotted.

### 5.2.2 Plotting data

Whichever graph type you have selected, once you have chosen the variable(s) and dataset(s) you wish to plot, click on the **Plot Graph** button to update the graphical display. If you have not chosen any variables to plot, a warning message is issued. For X-Y plotting, this means checking at least one of the output variable checkboxes, while for Flammables plotting this means in addition selecting at least one concentration.

Note that any changes made in the **Graph** screen do not occur immediately: it is necessary to click on the **Plot Graph** button, which then updates the plot. If you just want to bring the graphical display to the foreground without re-plotting any data, use the **Show Graph** button. This will restore the graphical display window without the update.

### 5.2.3 Graph display features

A typical example of a graph produced after clicking the **Plot Graph** button is shown in **Figure 5.3**. In this section we describe other aspects of the display.

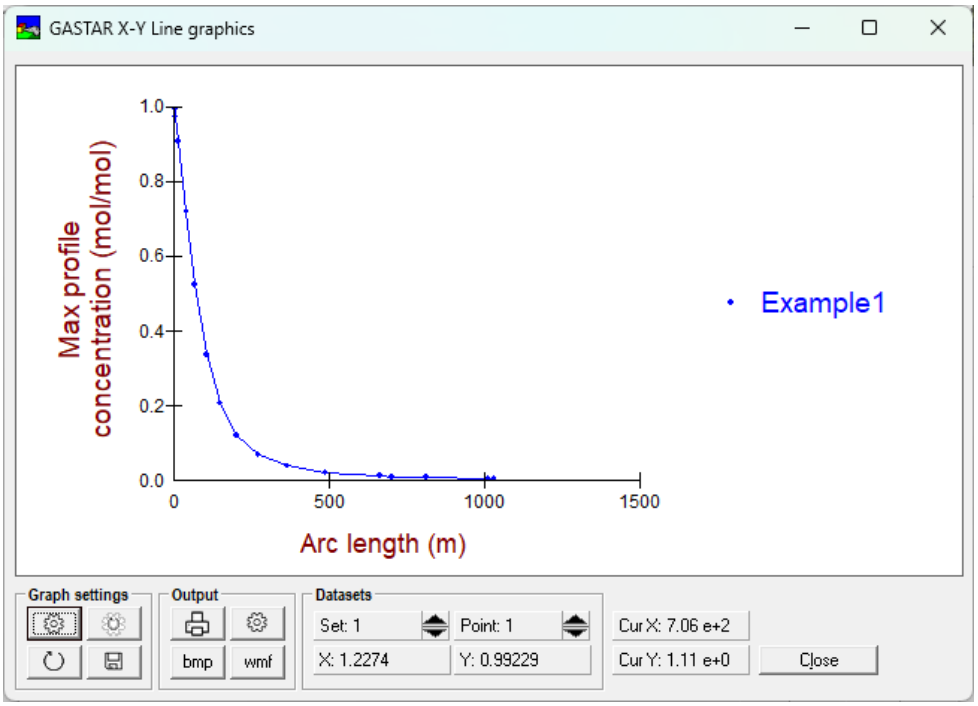



**Figure 5.3** – Example X-Y line graph.

### *Viewing data values*

The actual data values behind the graph can be obtained in a number of ways:

- The **Datasets** box below the graph gives the actual values plotted on the independent ($x$) and dependent ($y$) axes. The set and point being displayed can be changed using the up and down arrows (  ).
- The graph can also respond to mouse clicks – if you position your cursor over a point and click the left mouse button, the corresponding data value will be displayed in the **Datasets** box. Alternatively, as you move the cursor over the graph, the **Cur X** and **Cur Y** panels below the graph will display the current cursor location; thus, to obtain an indication of the value of any plotted point, hold the cursor over the point and read the values given in these panels.
- Finally, the complete datasets are available from the **Data** tab in the **Graph Design** dialog box, which is accessed via the  button in the **Graph settings** box below the graph.

### *Zooming in on a graph*

You may use the mouse to select and zoom into a region of the graph. To do this, move the cursor to one corner of the desired region, use the right mouse button to click and drag a region in the graph. Releasing the right mouse button at some other point over the graph will allow the region selected to fill the display. If the region you select is too small, the graph will ignore the selection, assuming you have accidentally clicked the right mouse button over the graph. To reset the axes, click the **Reset Axes** button which appears to the right of the **Cur X**/**Cur Y** panels once you have made a zoom on the current graph.

### *Configuring the graph*

The ability to change much of a graph's appearance is configurable through the **Graph Design** dialog box, which is accessed via the button in the **Graph settings** box below the graph. There is no attempt here to fully describe the configuration options available, but some of the most useful options are highlighted below:

- The **Style** tab can be used to select whether to display symbols and/or lines on the plot, and whether to use linear or log axes for *x* and *y* separately.
- The **Titles** tab can be used to give the graph a title and/or change the axis titles from the defaults.
- The **Fonts** tab can be used to alter the font size and style of various elements of the plot, including the graph title, axis titles, axes labels and legend.
- The **Markers** tab can be used to alter the colour, symbol and line type used for a particular set of values. Select a series (set) to modify by clicking on a point that belongs to that set in the top left box, then change the **Color**, **Symbol** etc. as desired.

The configuration properties in the **Graph Design** dialog box will be reset to default values whenever the graphics screen is closed and reopened. However, there is an option in the **Graph settings** box of the graphics screen to save the current settings as the new defaults (the button). The button can be used to refresh the settings by re-reading from this file, and the button can be used to restore the factory default settings.

By default, the series colours and symbols repeat every 20 sets. If desired, the user can change this by modifying the `NumColours` and/or `NumSymbols` fields directly in the *Gastar.ini* file (in the <*install_path*> directory) in a text editor. For example, if both fields were changed to 3, the first and fourth series, second and fifth series etc. of a plot would use the same colour and symbol. The colour codes in the `[PlottingColours]` section of the *.ini* file for the default 'rainbow' palette (`Palette=6`) are given in **Figure 5.4** below.

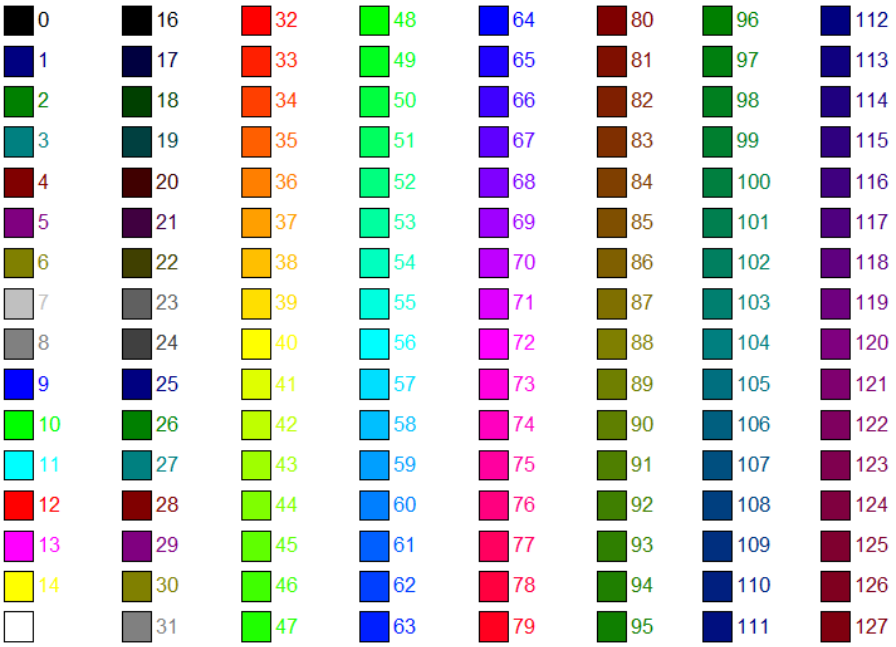



**Figure 5.4** – Rainbow palette colour codes.

### 5.2.4 Copying/printing the graph

Once satisfied with the appearance of a graph, it can be copied to the clipboard for pasting into a separate application, or printed.

The buttons in the **Output** box below the graph can be used to copy the graph to the clipboard as a bitmap (**bmp**) file or as a Windows metafile (**wmf**); the latter is a vector format and may therefore be better for including in documents if using a compatible application (e.g. Microsoft Word).

The  button prints the graph using the printer settings specified in the **Graphics print settings** screen (see **Figure 5.5**), accessed via the  button in the **Output** box or via the **File, Preferences, Graph print setup** menu item from the main GASTAR interface. This screen allows you to set some of the commonly used printing options, including the printer, the size and position of the graph on the page and the overall page title (this is not the same as the graph title, which must be set for each individual graph).

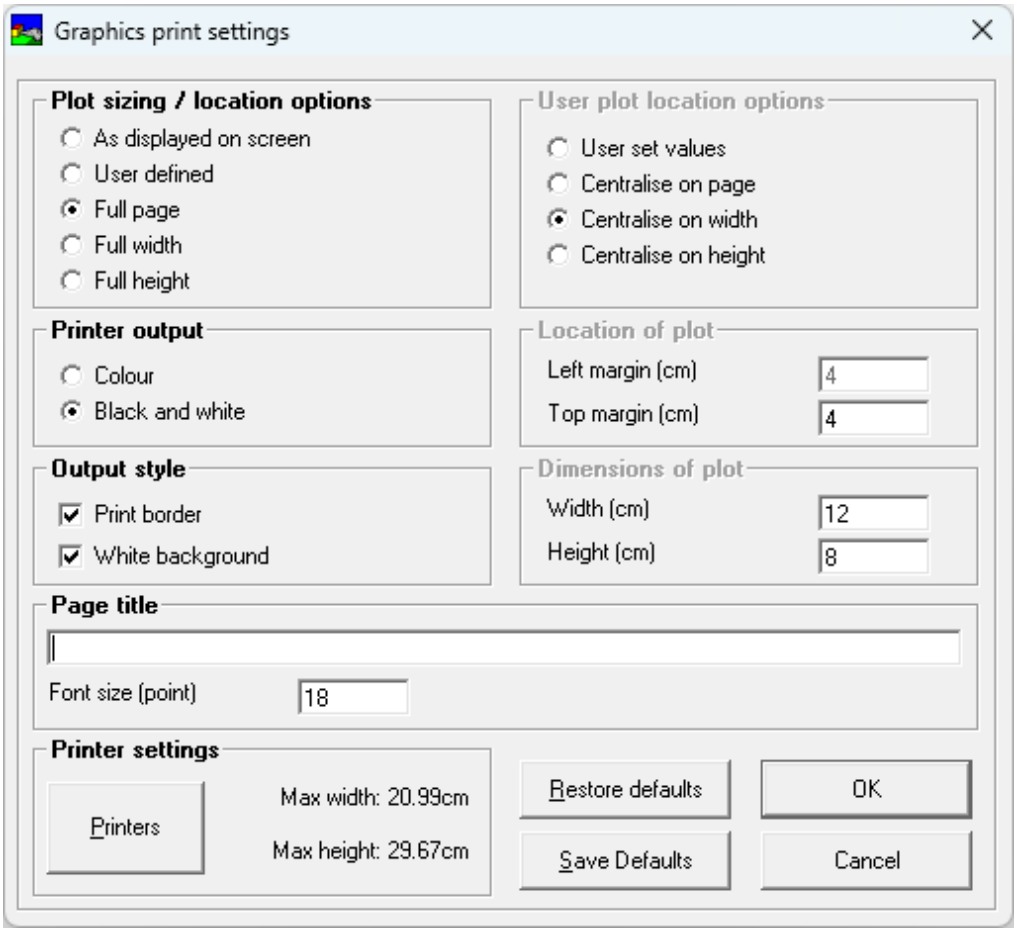



**Figure 5.5** – **Graphics print settings** screen.

## 5.3 Contour plots

This section outlines how to produce contour plots in Surfer (if installed) from standard gridded GASTAR output data using the **2-D Output Plotter** utility, launched from the GASTAR interface via the **Results**, **Contour plot** menu item. This brings up the screen shown in **Figure 5.6**.

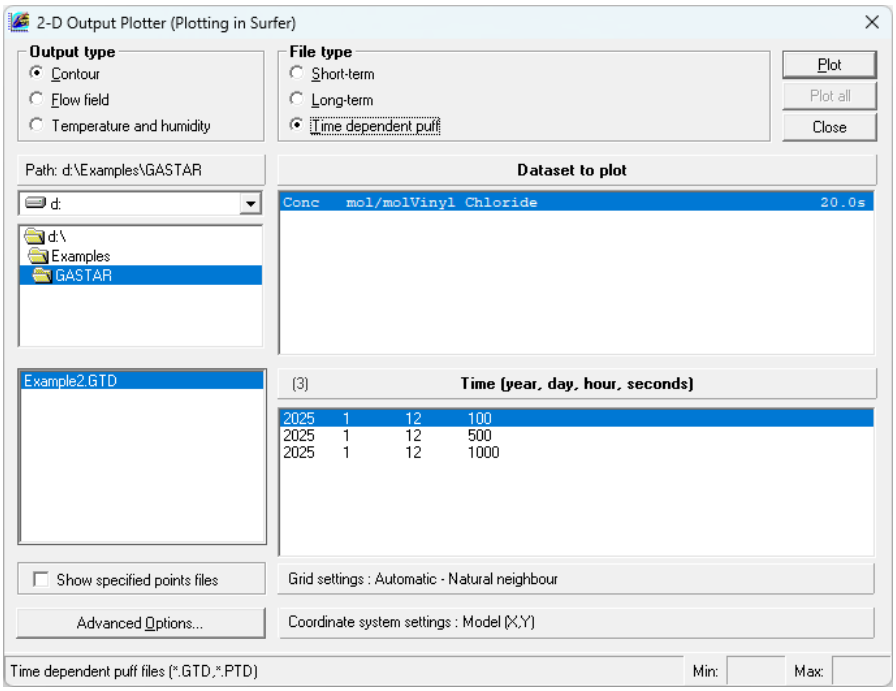



**Figure 5.6** – The **2-D Output Plotter** screen.

The **2-D Output plotter** allows for plotting many different types of gridded output. However, the only **Output type** relevant to GASTAR is **Contour** output, and so this radio button should be selected in the top right box of the screen.

Here are the steps to follow in order to create a contour plot of data:

**Step 1** Ensure **Contour** is selected under **Output type** (top left of the screen).

**Step 2** Choose the **File type** (top right of the screen). This defines the types of files listed in the lower left-hand box. If **Short-term** is chosen, all the files with the extension *.gst* (in the chosen directory) are listed. This option is appropriate for plotting standard gridded output from **Continuous** releases. If **Time dependent puff** is chosen, all files with the extension *.gtd* are listed. This option is appropriate for plotting standard gridded output from **Instantaneous** releases. The **Long-term** option is not relevant to GASTAR and so should never be selected. Note that the **2-D Output plotter** cannot be used to plot gridded output data in *.ggd* files.

**Step 3** Using the boxes on the left, select the appropriate folder and click on the name of the file containing the data to plot. Right-clicking on **Path:** allows the path of a file or directory to be pasted in. Files or directories can also be dragged from Explorer onto **Path:** to use that file or directory.

**Step 4** Click on the dataset to plot (**Dataset to Plot** box) and, for **Instantaneous** releases, also click on the time for which the data are to be plotted (**Time (year, day, hour, seconds)** box).

The **Dataset to Plot** box shows a list of all the variables that can be used for the plot; for GASTAR there should only be one. This record shows the type of output (e.g. 'Conc' for concentration), the units of output (e.g. 'mol/mol' or 'ppm'), the pollutant name (e.g. 'Chlorine') and the averaging time (e.g. '600 s').

For **Instantaneous** releases only, a list of multiple **Time (year, day, hour, seconds)** entries may also be displayed. The year, day, hour fields are the year, Julian day and hour of the release start. The last field gives the time since release in seconds, i.e. the relevant **Specified output time** from the **Outputs** screen.

**Step 5** Optionally, click on the **Advanced Options**... button to set some properties of the plot, including the **number of grid lines** (resolution of the contour plot), user-specified **Contour levels**, an option to convert your output from X-Y coordinates to longitude-latitude coordinates, and the **Contour gridding method**. Information about the available gridding methods can be found in the Surfer user guide. The **Natural neighbour** method is recommended in most cases. Click **OK** to return to the main screen.

*If the **Specify number of grid lines** option is not selected, the **2-D Output Plotter** will choose the resolution based on the resolution of the results to be plotted.*

**Step 6** Click on **Plot** to plot the selected data in Surfer.

The GASTAR gridded output file is converted to a grid file (.grd) for Surfer to plot. Save this to an appropriate location.

In the upper right-hand corner, the **Close** button closes the **2-D Output Plotter**. The **Plot all** button is not relevant to GASTAR and is greyed out.

If you do not have Surfer installed but you do have another CERC model installed that comes with the Mapper (e.g. ADMS 6, ADMS-Urban, ADMS-Roads), you can produce contour plots in the Mapper instead. Launch the **2-D Output Plotter** from the model with the Mapper via the **Results, Contour plot, Mapper** menu item and create a contour plot of data following the same steps as above. Once the contour (and contour lines) layer has been generated in the Mapper plot window, you should make sure to deselect all other layers from the **Layers** tab as these will be relevant to the other model that is linked to the Mapper and not GASTAR.

Note that care is needed if wanting to overlay the contour plot on a map, as the coordinate system used by the contour plot is wind-aligned and not 'compass-aligned'.

## 5.4 Viewing numerical output

The numerical output files created by GASTAR are mainly tab-delimited or comma-separated text files. Output files can be accessed from the GASTAR interface, via the **Results**, **Numerical output** menu item, and viewed in Notepad, WordPad, Microsoft Excel or some other application of the user's choice. The application used to view output files is set in the **File Viewing Preferences** screen as described in Section 5.4.1.

An alternative way of opening the output files in Microsoft Excel is outlined in Section 5.4.3.

### 5.4.1 Choosing application to view output

To change the preferred viewing application for output files, select **File**, **Preferences**, **Viewing options** from the menu bar of the GASTAR interface. This will bring up the **File Viewing Preferences** screen shown in **Figure 5.7**.

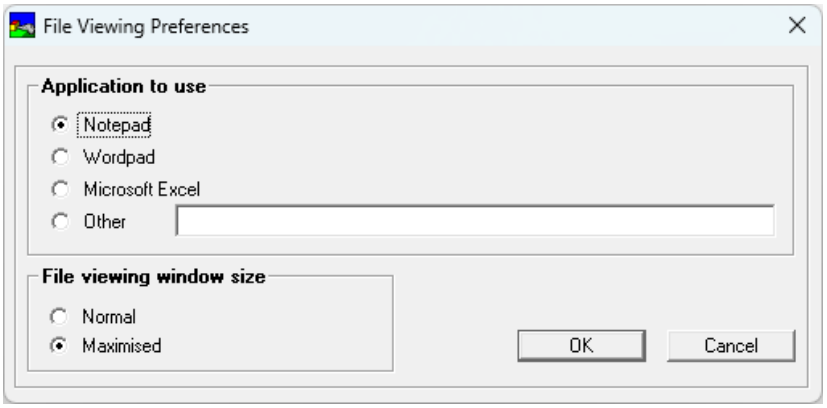



**Figure 5.7** – The **File Viewing Preferences** window.

**Application to use** allows the user to select which application to use to view output files. If an application other than Notepad, WordPad or Microsoft Excel is to be used, then select **Other** and enter the full path of the application executable.

**File viewing window size** defines the size of the viewing window when it is opened. Choices are either **Normal** (size of the last used window) or **Maximised** (full screen).

### 5.4.2 Viewing output from the GASTAR interface

The output files associated with the *.gpl* file that is currently open in the interface can be viewed using the **Results**, **Numerical output** menu item. A screen will appear showing all of the main output (*.gof*) files in the folder containing the current *.gpl* file. By changing **Output files (*.gof)** to **All files (*.*)** in the lower right corner, you can also view the other files in this folder. After selecting a file and clicking **Open**, the file will be opened with the application selected in the **File Viewing Preferences**, as described in Section 5.4.1

If the file is being opened in Microsoft Excel, it will automatically be opened as a comma-separated file. If the file you are opening is tab-delimited rather than comma-separated (e.g. the *.gof* file), select the first column in Excel, choose **Text to Columns** from the **Data** ribbon, and use the resulting Wizard to convert to tab delimited (see Section 5.4.3 below).

### 5.4.3 Use of Microsoft Excel to view numerical output

The numerical output files can be opened using Microsoft Excel without using the GASTAR interface, proceeding as follows. These instructions relate to Microsoft Excel 2019.

**Step 1** Start Microsoft Excel.

**Step 2** Select **File > Open** from the ribbon, and browse through the directories to locate the relevant file, making sure that **All files (*.*)** is selected in the lower right drop-down menu. You can also type, e.g. '*.gof' in the **File name** box and press **Enter** to see just those files that end with the extension *.gof* in the current directory.

**Step 3** Click on the file and then click **Open**. This starts the Microsoft Excel **Text Import Wizard** shown in **Figure 5.8**.

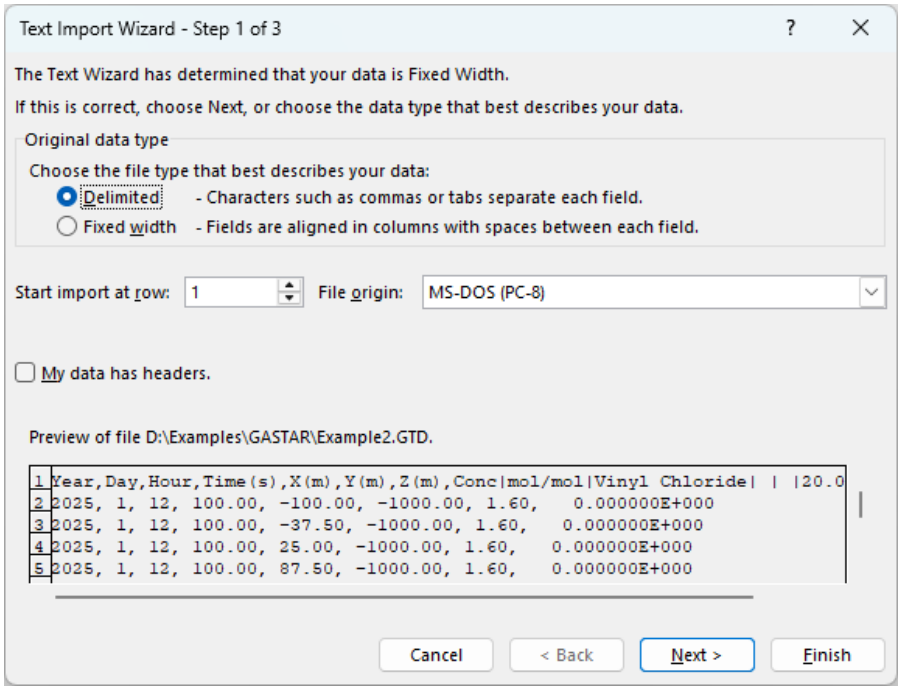



**Figure 5.8** − Step 1 of the Microsoft Excel **Text Import Wizard**.

**Step 4** The human-readable numerical output files created by GASTAR are either tab-delimited (*.gof*) or comma-separated (*.gst*, *.gtd*, *.ggd*) text files so they can be imported easily into many standard packages.

Select the **Delimited** option and click on **Next >** to move to the next step, shown in **Figure 5.9**.

*Double-click on the option to select it and to move directly to the next step.*

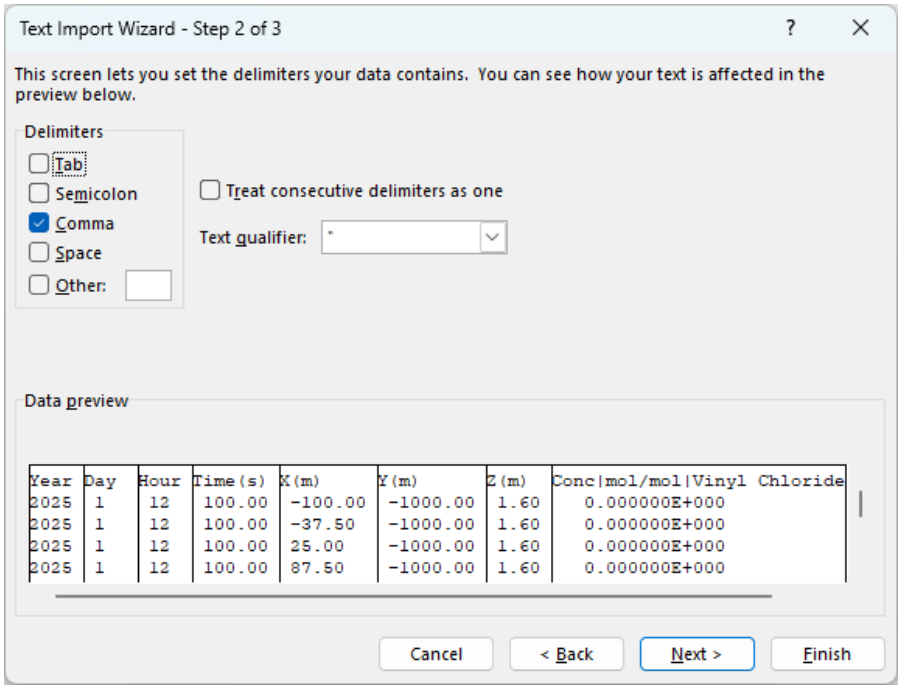



**Figure 5.9** − Step 2 of the Microsoft Excel **Text Import Wizard**.

**Step 5** In the **Delimiters** box, select only the relevant checkbox (**Tab** or **Comma**) and click on **Next >** to move to the last step, shown in **Figure 5.10**.

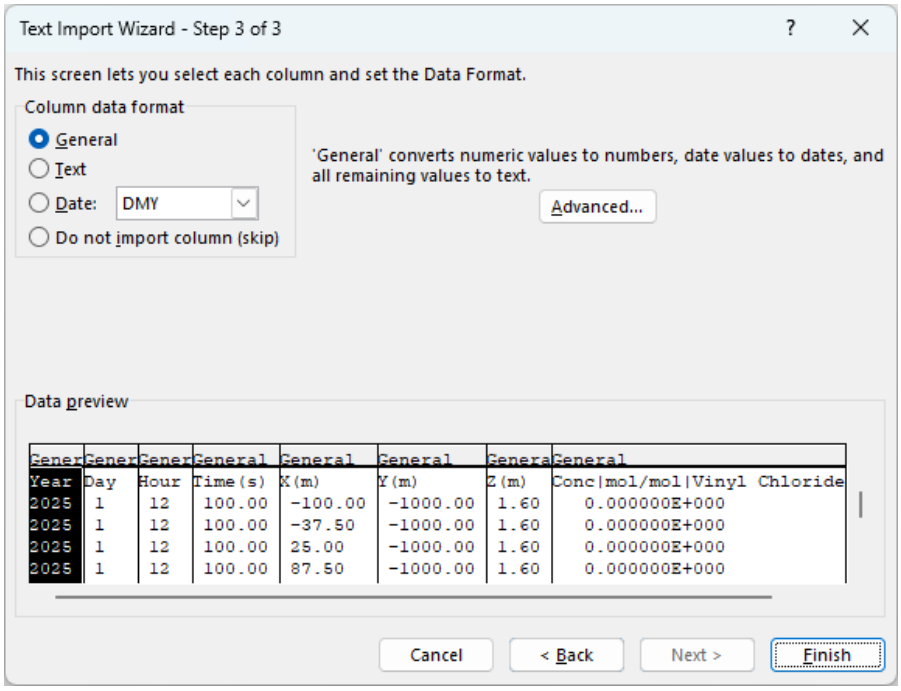


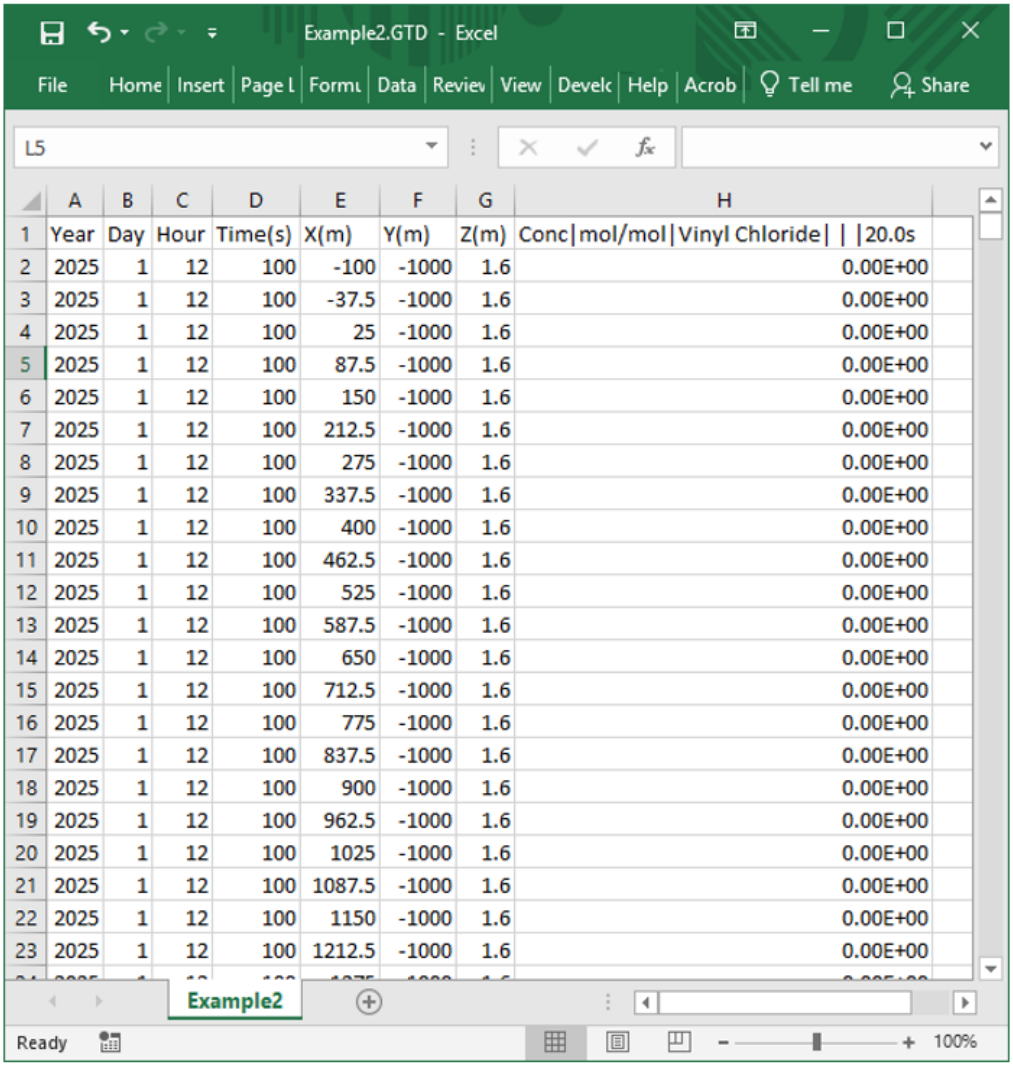

**Figure 5.10** − Step 3 of the Microsoft Excel **Text Import Wizard**.

**Step 6** In the **Data Preview** box, ensure that the file has been properly separated and click on **Finish** to import the data.

An example of imported data from a *.gtd* file in Microsoft Excel is shown in **Figure 5.11**.

If the column headings are not visible because the columns are too narrow, select all the

columns containing data and use the **Format** button in the **Cells** section of the **Home** tab and select **AutoFit Column Width** to increase the column widths to fit the longest entry in each column.




| | A | B | C | D | E | F | G | H |
|---|---|---|---|---|---|---|---|---|
| 1 | Year | Day | Hour | Time(s) | X(m) | Y(m) | Z(m) | Conc\|mol/mol\|Vinyl Chloride\| \| \|20.0s |
| 2 | 2025 | 1 | 12 | 100 | -100 | -1000 | 1.6 | 0.00E+00 |
| 3 | 2025 | 1 | 12 | 100 | -37.5 | -1000 | 1.6 | 0.00E+00 |
| 4 | 2025 | 1 | 12 | 100 | 25 | -1000 | 1.6 | 0.00E+00 |
| 5 | 2025 | 1 | 12 | 100 | 87.5 | -1000 | 1.6 | 0.00E+00 |
| 6 | 2025 | 1 | 12 | 100 | 150 | -1000 | 1.6 | 0.00E+00 |
| 7 | 2025 | 1 | 12 | 100 | 212.5 | -1000 | 1.6 | 0.00E+00 |
| 8 | 2025 | 1 | 12 | 100 | 275 | -1000 | 1.6 | 0.00E+00 |
| 9 | 2025 | 1 | 12 | 100 | 337.5 | -1000 | 1.6 | 0.00E+00 |
| 10 | 2025 | 1 | 12 | 100 | 400 | -1000 | 1.6 | 0.00E+00 |
| 11 | 2025 | 1 | 12 | 100 | 462.5 | -1000 | 1.6 | 0.00E+00 |
| 12 | 2025 | 1 | 12 | 100 | 525 | -1000 | 1.6 | 0.00E+00 |
| 13 | 2025 | 1 | 12 | 100 | 587.5 | -1000 | 1.6 | 0.00E+00 |
| 14 | 2025 | 1 | 12 | 100 | 650 | -1000 | 1.6 | 0.00E+00 |
| 15 | 2025 | 1 | 12 | 100 | 712.5 | -1000 | 1.6 | 0.00E+00 |
| 16 | 2025 | 1 | 12 | 100 | 775 | -1000 | 1.6 | 0.00E+00 |
| 17 | 2025 | 1 | 12 | 100 | 837.5 | -1000 | 1.6 | 0.00E+00 |
| 18 | 2025 | 1 | 12 | 100 | 900 | -1000 | 1.6 | 0.00E+00 |
| 19 | 2025 | 1 | 12 | 100 | 962.5 | -1000 | 1.6 | 0.00E+00 |
| 20 | 2025 | 1 | 12 | 100 | 1025 | -1000 | 1.6 | 0.00E+00 |
| 21 | 2025 | 1 | 12 | 100 | 1087.5 | -1000 | 1.6 | 0.00E+00 |
| 22 | 2025 | 1 | 12 | 100 | 1150 | -1000 | 1.6 | 0.00E+00 |
| 23 | 2025 | 1 | 12 | 100 | 1212.5 | -1000 | 1.6 | 0.00E+00 |

**Figure 5.11** – GASTAR output data from a *.gtd* file imported into Microsoft Excel.

# SECTION 6 Worked Examples

In order to help the user learn how to use GASTAR, a few worked examples have been set up to cover many of the main functions of the model.

You can launch GASTAR in several different ways:

- double-click on the desktop icon
- search for GASTAR via the Windows search bar
- go to the GASTAR install directory and double-click on the file GASTAR.EXE

---

*It is strongly recommended to create a directory for setting up and running these examples in order to keep them separate from the examples provided in the <install_path>/Examples directory supplied with the model.*

---

## 6.1 Example 1: Modelling a continuous release

In this worked example you will:

- Model a continuous dense gas release (plume)
- Calculate the plume concentration at a sensitive receptor
- Calculate flammability information
- View numerical and graphical results

### 6.1.1 Setting up the run

This example models the fictitious case of a plume of propane gas emanating from a spill of liquefied petroleum gas (LPG) in a bunded (contained) area of width 50 m and a known (maximum) boil-off rate of 300 kg/s. Maximum concentration and flammability information at a sensitive receptor located 700 m from the spill is of particular interest.

**Step 1** Start GASTAR or click **File, New** if already open to create a new input file.

**Step 2** In the **Setup** screen, enter an appropriate **Title** such as "Example 1: Continuous release"

**Step 3** Click **Edit** under **Source material** to bring up the **Material properties** screen. Scroll down the table and double-click on **Propane** to update the **Current material properties** to those of propane. Click **OK** to return to the **Setup** screen.

**Step 4** As we are interested in flammability information, tick the **Calculate flammable output parameters** checkbox under **Model options**. Also tick the **Calculate concentration-time history** checkbox, for reasons that will become apparent in the next section.

Compare your screen to **Figure 6.1** below.

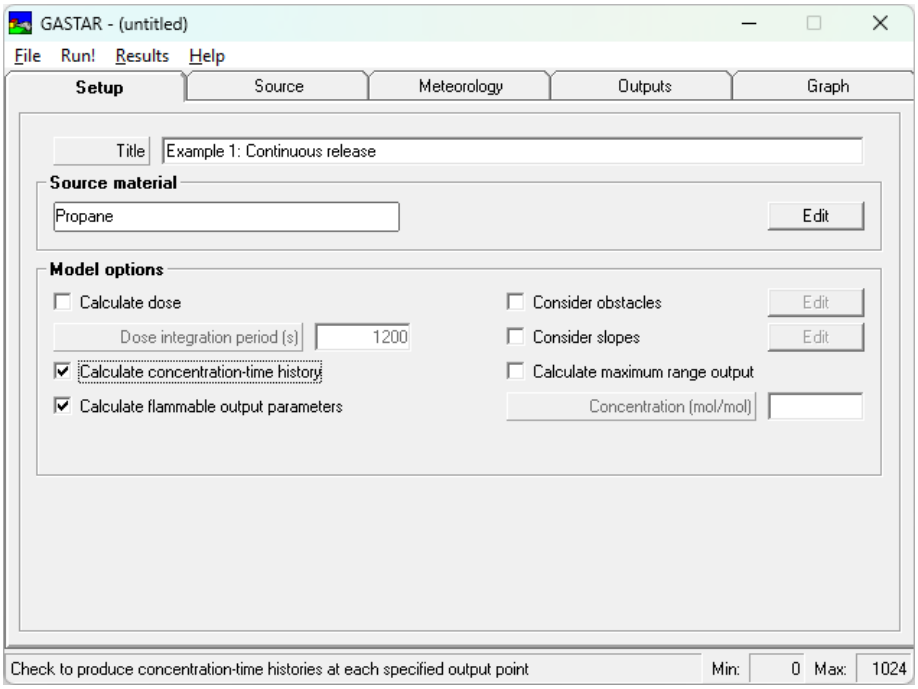



**Figure 6.1** – Example 1: The **Setup** screen.

**Step 5** Move to the **Source** screen. Under **Release type**, select **Continuous**. Leave the **Internally calculate initial plume width** checkbox ticked so that we may enter the physical source width further below. Select **Thermal release** to indicate that the initial temperature of the propane plume is not ambient, but is a single-phase gas (we are modelling the propane plume after boil-off).

**Step 6** Under **Source details**, as this is a fictitious example, leave the **Source Location** and **Release Start** as their defaults (this information is not used by the model other than to include it in the output). Set the **Initial air entrainment** to 0 kg/s, and the **Hazardous fraction** to 1 mol/mol to indicate the plume is initially pure propane. Set the **Physical source width** to 50 m (the width of the bunded area) and the **Mass flux** to 300 kg/s (the known maximum boil-off rate of the propane). Set the **Temperature** to 231 K (the boiling point of propane).

Compare your screen to **Figure 6.2** below.

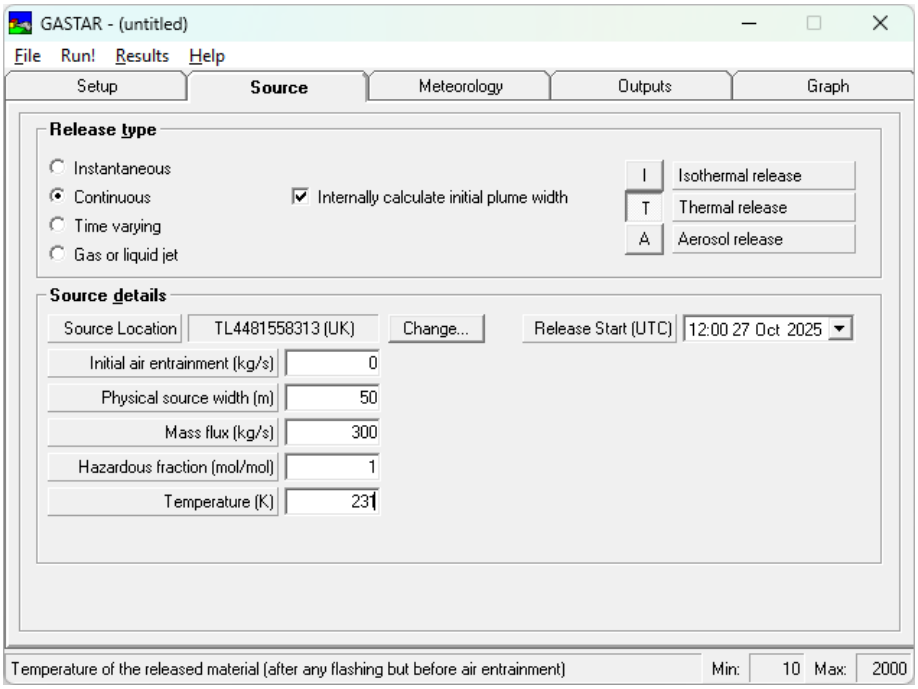



**Figure 6.2** – Example 1: The **Source** screen.

**Step 7** Move to the **Meteorology** screen. Enter the meteorological data from **Table 6.1** into the appropriate fields.

| Parameter | Value |
|---|---|
| Wind speed | 2 m/s |
| Wind speed height | 10 m |
| Wind direction | 270° |
| Roughness length | 0.1 m |
| Air temperature | 288 K |
| Surface temperature | 288 K |
| Atmospheric pressure | 1013 mb |
| Relative humidity | 60 % |

**Table 6.1** – Meteorological data for use with Example 1.

**Step 8** Under **Stability**, select the **Pasquill-Gifford categories** radio button and select category **D** (neutral conditions).

Compare your screen to **Figure 6.3** below.

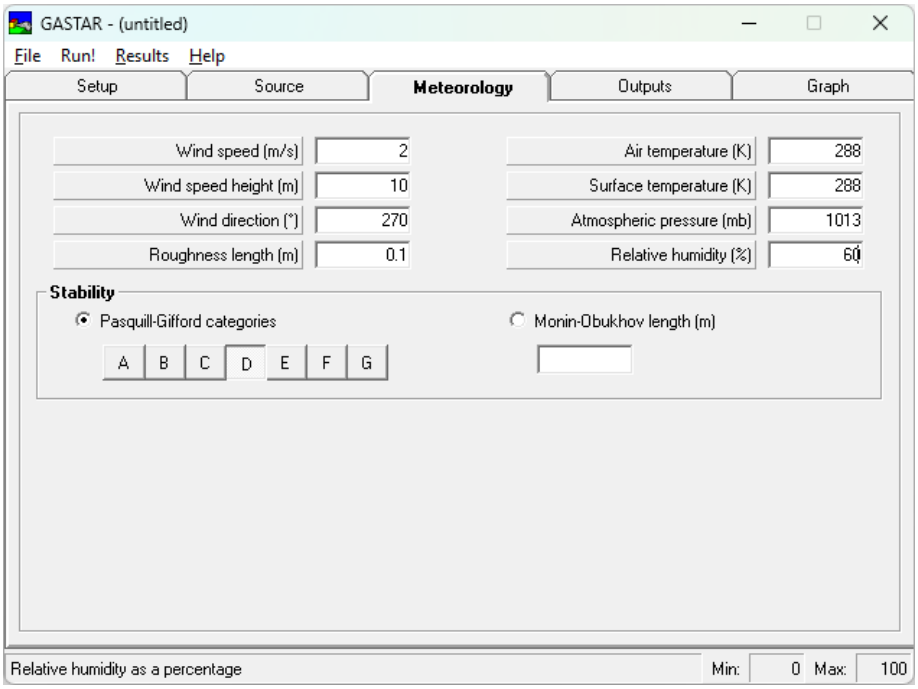



**Figure 6.3** – Example 1: The **Meteorology** screen.

**Step 9** Move to the **Outputs** screen. Enter a **Modelled time** of 1000 s. This is long enough for the plume to reach the receptor of interest without being excessively large. Retain the default **Averaging time** of 20 s.

**Step 10** Tick the **Specified points** checkbox under **Types of output** and then click on **Edit** in the **Specified output points** box to bring up the **Define Specified Output Points** screen. As the sensitive receptor is located 700 m from the source, and specified output points are defined in source-centred wind-aligned coordinates, enter coordinates of (X,Y,Z) = (700,0,0) in the three boxes and click **Add**; if no slopes or obstacles are considered in the run, the worst-case (maximum) concentration at the sensitive receptor will be when the plume advects directly towards the receptor. Click **OK** to return to the **Outputs** screen.

Compare your screen to **Figure 6.4** below.

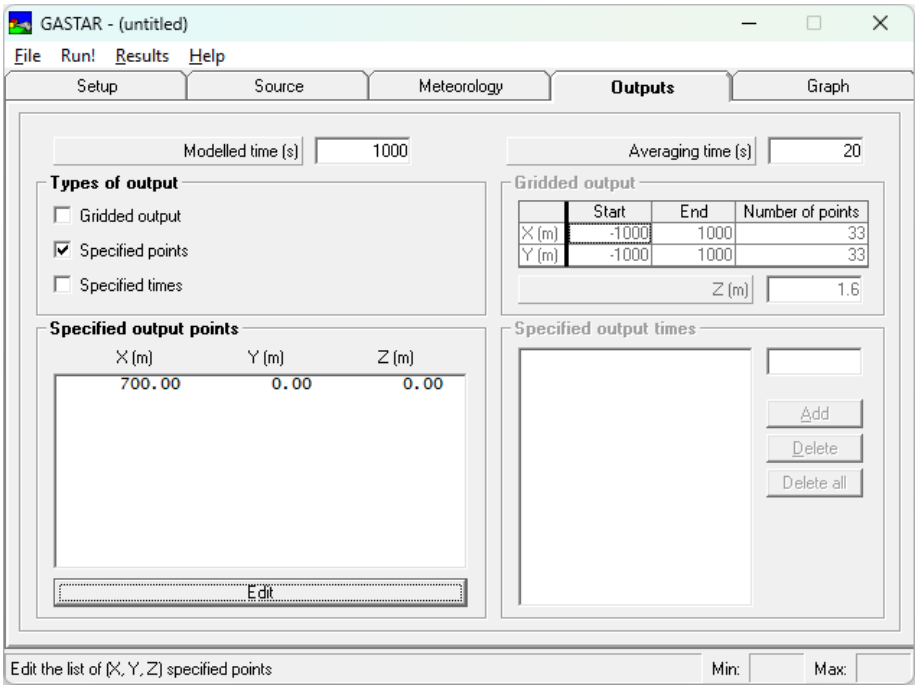



**Figure 6.4** – Example 1: The **Outputs** screen.

**Step 11** Select **File, Save as**... from the menu and save the file as *Example1.gpl* in your working folder.

**Step 12** Click on **Run!** from the menu to run GASTAR. The run will be very quick. A run window similar to **Figure 6.5** will appear.

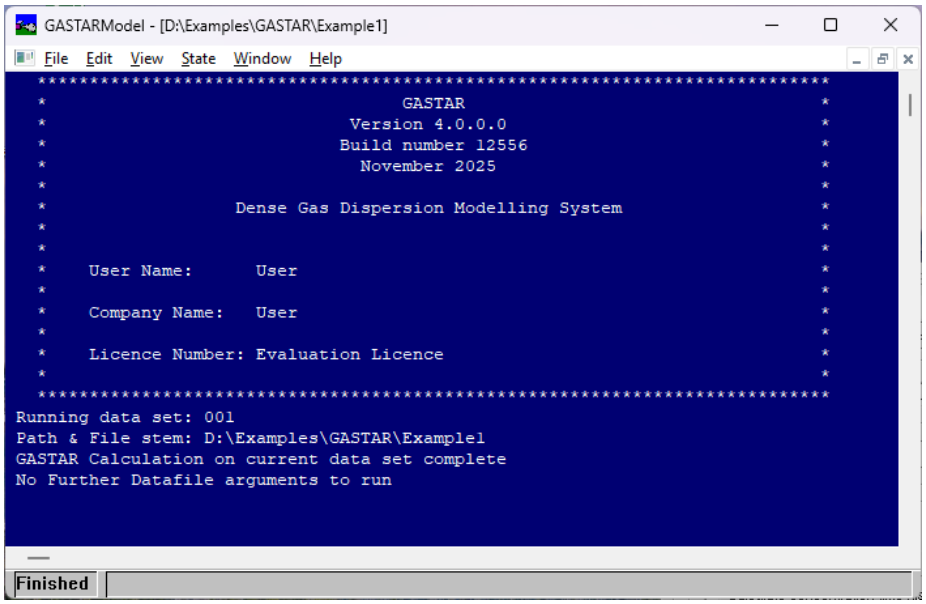



**Figure 6.5** – Example 1: The run window.

At the end of the run, if the **Exit Mode Option** is set to **Normal termination box** (see 'Runtime preferences' under Section 2.5.4), the dialog box shown in **Figure 6.6** will appear. This means that the run has completed successfully.

**Step 13** Click on **Yes** to close the run window.

Alternatively, click on **No** to leave the run window open and view the screen

messages. Close the run window using the close button or by selecting **File, Exit** from the menu bar to return to the main GASTAR interface.

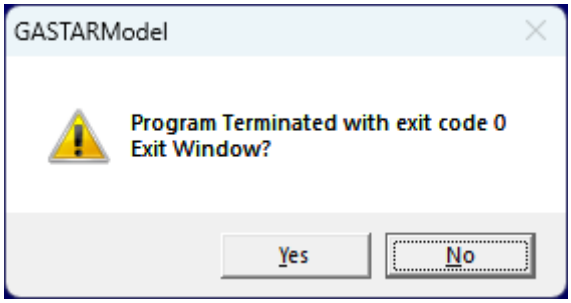



**Figure 6.6** – Example 1: End-of-run dialog box.

### 6.1.2 Viewing numerical output

**Step 14** From the **Results** menu, select **Numerical output**. Browse to select the file *Example1.GOF* and click **Open** to open it in your preferred viewing application (see Section 5.4.1 for how to set this).

**Step 15** Scroll down past the file header and input data summary to the standard results table (labelled 'RESULTS') – it should look similar to the top table shown in **Figure 6.7** (only the first few columns are shown). It is advised to disable 'Word wrap' for clearer viewing.

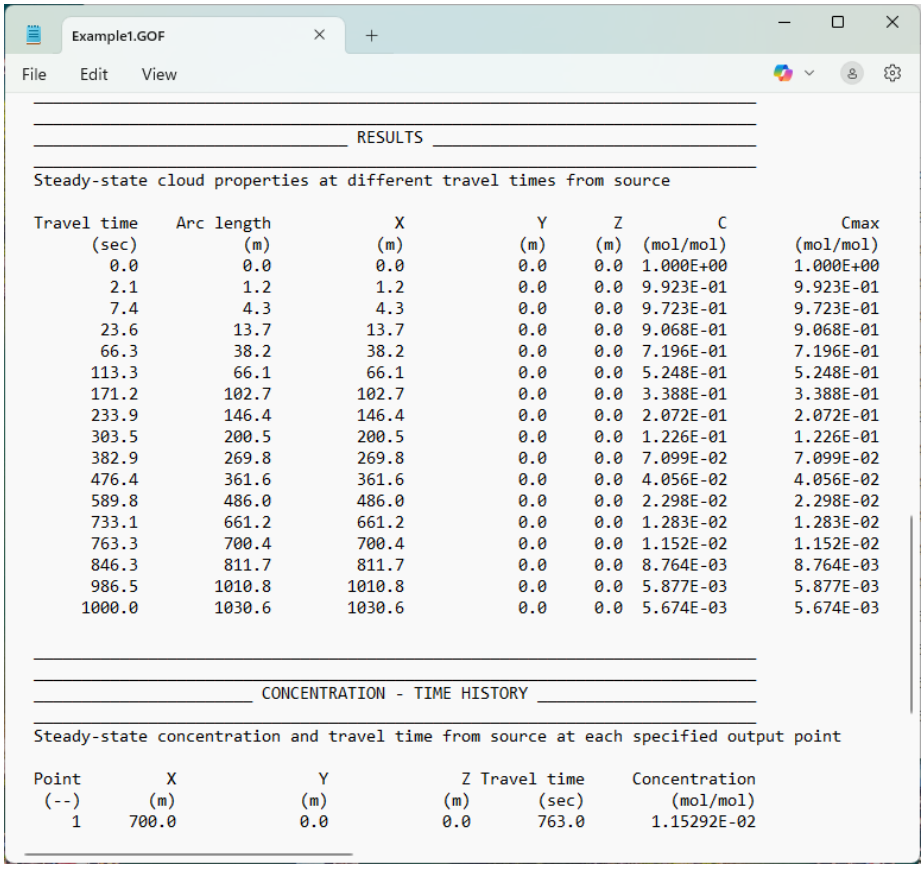



**Figure 6.7** – Results and concentration-time history tables in *Example1.GOF*.

For continuous releases, this table gives the (steady-state) cloud properties at different travel times from the source. The 'Arc length' is the distance

along the plume centreline, in metres, and the (X, Y, Z) values give the location of the plume centreline in source-centred wind-aligned coordinates. The output parameters include the integral concentration (C) and the centreline (maximum) concentration after the crosswind and vertical concentration profiles have been applied (Cmax). Refer to Section 5.1.1 for a full description of all the output parameters in this table.

We are interested in the concentration 700 m downwind of the source. Notice that there is a table entry with (X, Y, Z) coordinates very close to receptor of interest (X = 700.4 in the example above). The centreline concentration (Cmax) for this entry (0.01152 mol/mol in the example above) will therefore be very close to modelled concentration at the sensitive receptor. The table entries in the RESULTS section are all times from the model's integration calculation, which uses an adaptive timestep to try to hit the times where X is equal to the *x*-coordinate of each specified output point; this is only approximate, however, which is why there is no entry with X = 700 m exactly. However, the results in the 'CONCENTRATION – TIME HISTORY' section of the *.gof* file give the concentration at each specified output point exactly. In the example above, the concentration at the receptor of interest is 0.01153 mol/mol.

**Step 16** Scroll further down the *.gof* file to the FLAMMABLES RESULTS section (see **Figure 6.8**).

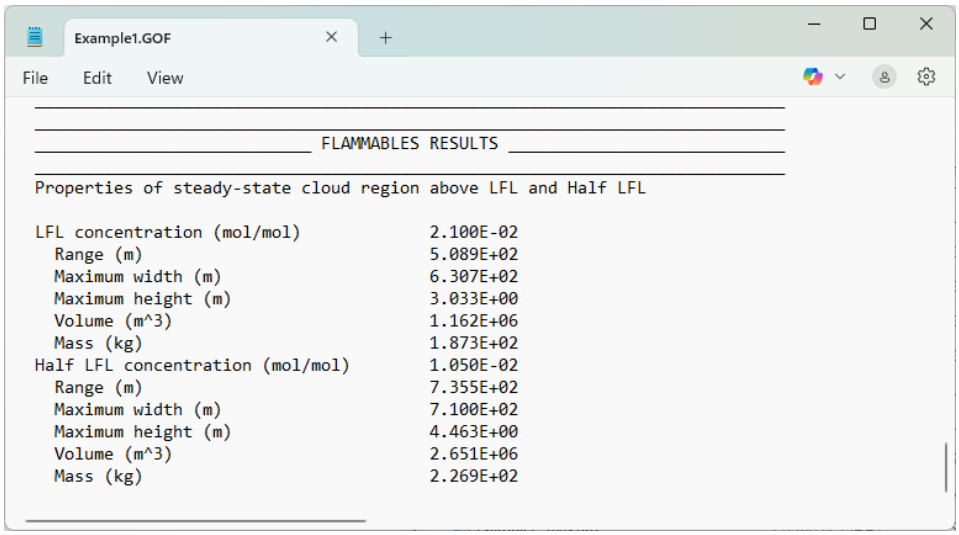



**Figure 6.8** – Flammables results table in *Example1.GOF*.

For continuous releases, properties of the (steady-state) region of the plume within which the concentration is above the Lower Flammability Limit (LFL) and, separately, the half-LFL are given. Looking at the 'Range' values, which give the downwind distance from the source to the LFL and half-LFL concentration contours, it can be deduced that sensitive receptor 700 m downwind of the source lies close to, but within, the half-LFL contour. Given that the "safe" distance is often taken to be the distance to the half-LFL, the flammability risk at the sensitive receptor might therefore be considered significant.

### 6.1.3 Viewing graphical output

**Step 17** Return to the GASTAR interface and move to the **Graph** screen. Use the controls in the **File Details** box to browse to the working folder and select the file *Example1.GPH*.

**Step 18** Ensure that **X-Y line plotting** is selected under **Graph type**. In the **X-Y plotting details** box, use the (circular) radio buttons to select 'Arc length' as the dependent variable (*x*-axis), and the checkboxes to select 'Max profile concentration' as the independent variable (*y*-axis). Finally, click **Plot graph** to display the line plot (see **Figure 6.9**).

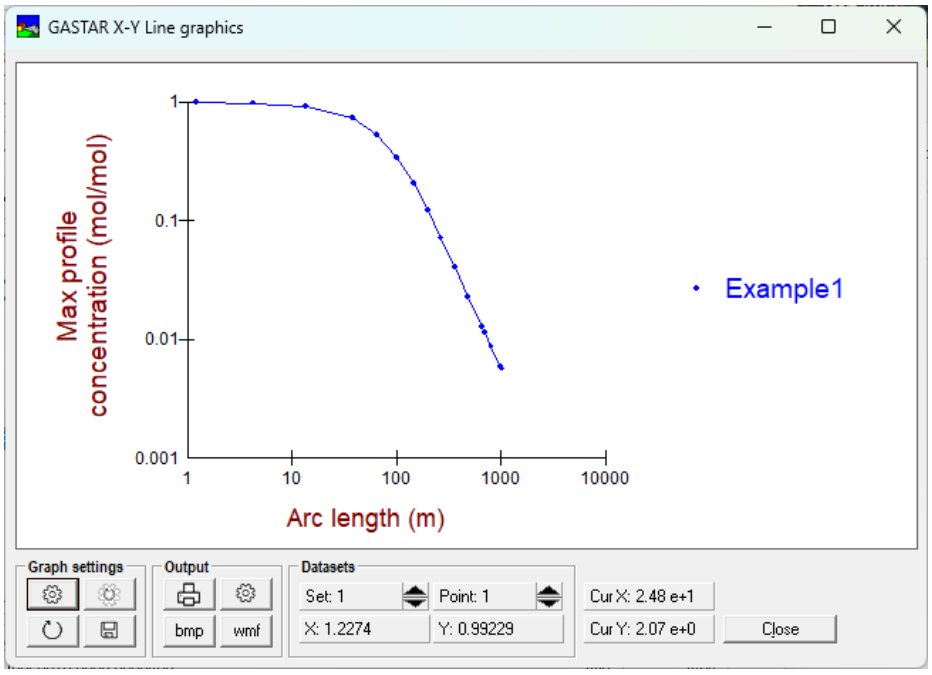



**Figure 6.9** – Example 1: Concentration line plot

**Step 19** By default, the *x*- and *y*-axes use a log scale. Change this by clicking on the  button in the **Graph settings** box below the graph. In the resulting dialog box, untick the **X Axis** and **Y Axis** checkboxes under **Log Data** in the **Style** tab. Click **OK** to return to the plot. The *x*- and *y*-axes should now be on a linear scale. Confirm that concentration at the sensitive receptor 700 m downstream is around 0.0115 mol/mol by clicking on the relevant point on the series and reading from the **Y:** box under **Datasets**.

**Step 20** Try plotting some other output parameters using the checkboxes back on the **Graph** screen of the GASTAR interface. Click **Plot graph** to update the plot each time you make a new selection.

## 6.2 Example 2: Modelling an instantaneous release

In this worked example you will:

- Model an instantaneous dense gas release (puff)
- Model a 'flashing' release
- Determine how the concentration at a sensitive receptor changes as the puff passes by
- Calculate the dose and toxic load at this receptor
- Determine the maximum range to a given concentration
- View gridded results as contour plots using Surfer

### 6.2.1 Setting up the run

This example models the fictitious case of a sudden catastrophic failure of a tank containing pressurised liquid vinyl chloride that 'flashes' to produce a cold, dense aerosol cloud. The concentration history and total dose at two sensitive downwind receptors are of particular interest, along with the maximum range from the source to a specific concentration.

**Step 1** Start GASTAR or click **File, New** if already open to create a new input file.

**Step 2** In the **Setup** screen, enter an appropriate **Title** such as "Example 2: Instantaneous release"

**Step 3** Click **Edit** under **Source material** to bring up the **Material properties** screen. Scroll down the table and double-click on **Vinyl Chloride**. Click **OK** to return to the **Setup** screen.

**Step 4** As we are interested in the dose and concentration-time history at a sensitive receptor, tick the **Calculate dose** and **Calculate concentration-time history** checkboxes under **Model options**.

**Step 5** Also tick the **Calculate maximum range output** checkbox and enter a value of 0.01 mol/mol in the resulting **Concentration** field.

Compare your screen to **Figure 6.10** below.

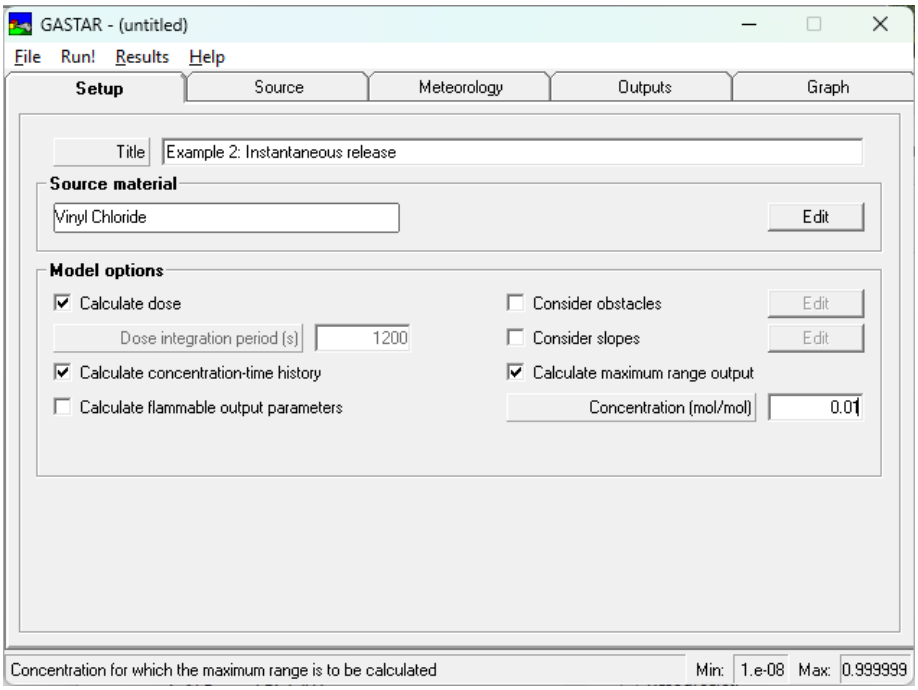



**Figure 6.10** – Example 2: The **Setup** screen.

**Step 6** Move to the **Source** screen. Under **Release type**, select **Instantaneous**. Leave the **Momentum initially well mixed** checkbox ticked to indicate that the initial conditions of the puff momentum are well mixed. Select **Aerosol release** to indicate that the we have a two-phase gas cloud (as a result of flashing).

**Step 7** Under **Source details**, again leave the **Source Location** and **Release Start** as their defaults as this is another fictitious example. Set the **Initial air entrainment** to 50 kg, the initial **Puff diameter** to 8 m, the total **Mass** of the release to 750 kg and the **Hazardous fraction** (which should not include the initial air entrainment) to 1 mol/mol to indicate the release is pure vinyl chloride.

**Step 8** The **Temperature** and **Aerosol fraction** will be calculated using the **Flash calculation** utility. Click on the **Flash** button to bring up the utility. The vinyl chloride was stored in the tank at atmospheric temperature, so enter a value of 280 K in the **Storage temperature** field. Enter an **Atmospheric pressure** of 990 mb. Click **Calculate** to calculate the aerosol fraction and source temperature, followed by the **Use normal** button to close the utility and automatically copy these values back into the **Source** screen.

Compare your screen to **Figure 6.11** below.

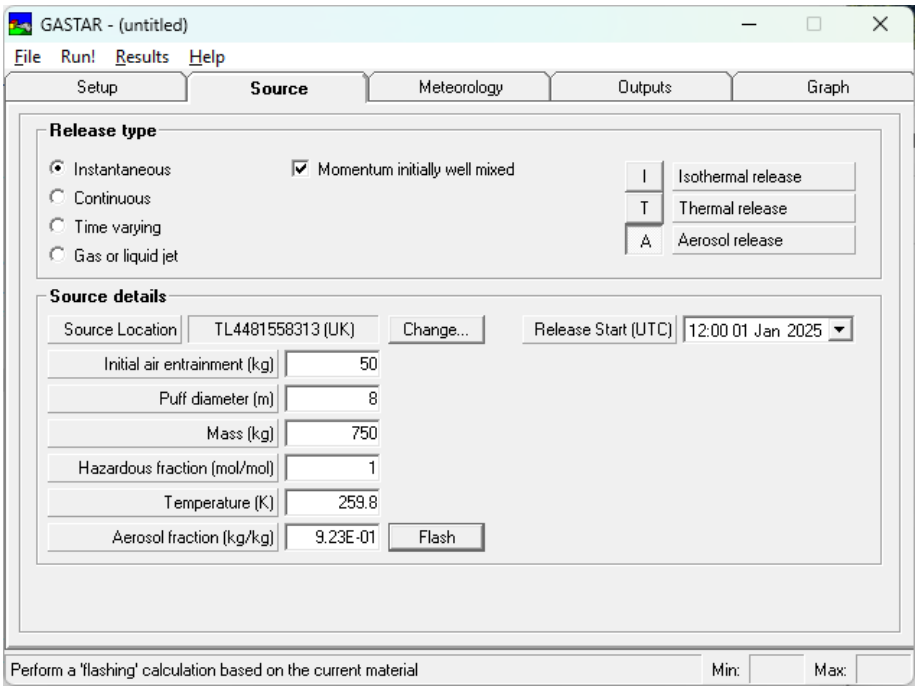



**Figure 6.11** – Example 2: The **Source** screen.

**Step 9** Move to the **Meteorology** screen. Enter the meteorological data from **Table 6.2** into the appropriate fields.

| Parameter | Value |
|---|---|
| Wind speed | 2 m/s |
| Wind speed height | 10 m |
| Wind direction | 0° |
| Roughness length | 0.2 m |
| Air temperature | 280 K |
| Surface temperature | 275 K |
| Atmospheric pressure | 990 mb |
| Relative humidity | 70 % |

**Table 6.2** – Meteorological data for use with Example 2.

**Step 10** Under **Stability**, select the **Pasquill-Gifford categories** radio button and select category **E** (slightly stable conditions).

Compare your screen to **Figure 6.12** below.

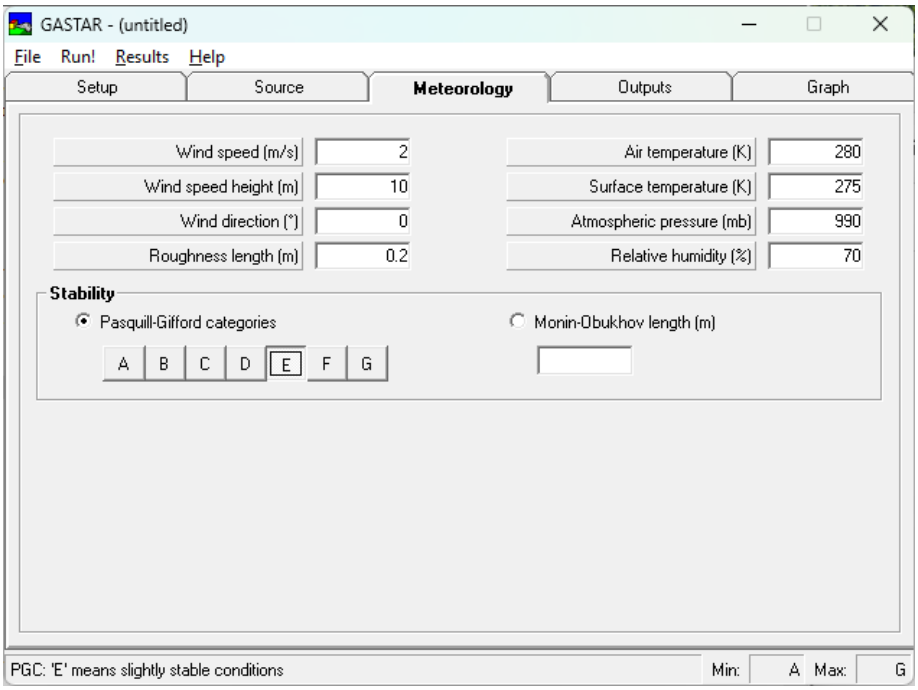



**Figure 6.12** – Example 2: The **Meteorology** screen.

**Step 11** Move to the **Outputs** screen. Enter a **Modelled time** of 2000 s. The **Averaging time** is not editable for instantaneous releases.

**Step 12** In this example, we will generate concentration contour plots at various times since release. Note that this requires the third-party software application Surfer to be installed – if you do not have Surfer installed on your machine, skip this step. Tick the **Gridded output** and **Specified times** checkboxes under **Types of output**. In the **Gridded output** box, change the **Start** and **End** values for **X** to -100 and 1900 respectively, the **Start** and **End** values for **Y** to -1000 and 1000 respectively, the **Number of points** to 33 for both X and Y and the output grid height **Z** to 1.6 m. We will ask for gridded output at 100, 500 and 1000 s after release; **Add** these values to the **Specified output times** box accordingly.

**Step 13** Recall that we have also selected to calculate dose and concentration-time history output for this run, both of which are calculated at specified output points. Thus, also tick the **Specified points** checkbox under **Types of output** and then click on **Edit** in the **Specified output points** box. Use the **Define Specified Output Points** screen to enter two specified output points, one at (X,Y,Z) = (300,100,1.6) and the other at (X,Y,Z) = (1600,-20,1.6), before clicking **OK** to return to the **Outputs** screen.

Compare your screen to **Figure 6.13** below.

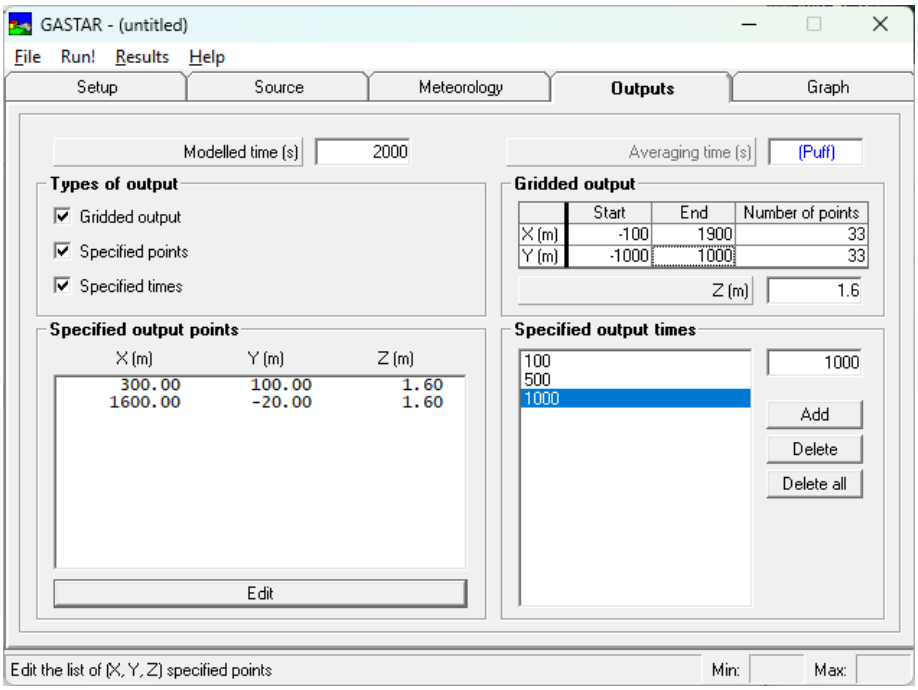



**Figure 6.13** – Example 2: The **Outputs** screen.

**Step 14** Select **File, Save as**... from the menu and save the file as *Example2.gpl* in your working folder.

**Step 15** Click on **Run!** from the menu to run GASTAR.

### 6.2.2 Viewing numerical output

**Step 16** From the **Results** menu, select **Numerical output**. Browse to select the file *Example2.GOF* and click **Open** to open it in your preferred viewing application.

**Step 17** Scroll down to the 'DOSE RESULTS' section (see **Figure 6.14**). For instantaneous releases, the dose values are the dose received over the **Modelled time** (2000 s in this case), which will be equal to the total dose if the puff has fully passed that receptor at the modelled time. We can see that the total dose at the receptor with coordinates (300,100,1.6) is approximately 0.0013 mol/mol min. The table entry for the receptor at (1600,-20,1.6) has the comment 'Still covered', indicating that the cloud is still significantly affecting concentrations at the Modelled time at this receptor; if we want the total dose at this receptor we should therefore increase the Modelled time, rerun GASTAR and check that the 'Still covered' comment has disappeared.

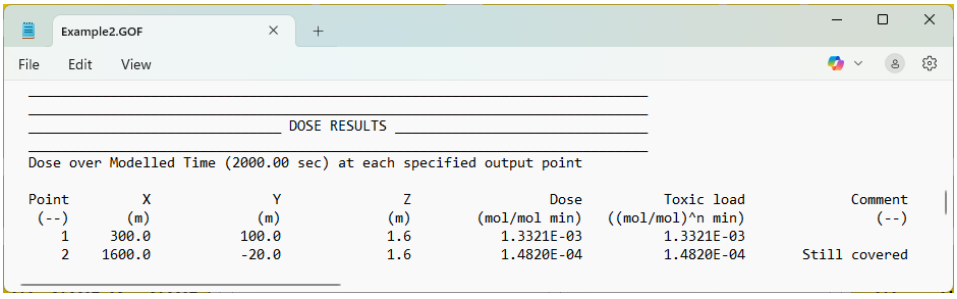
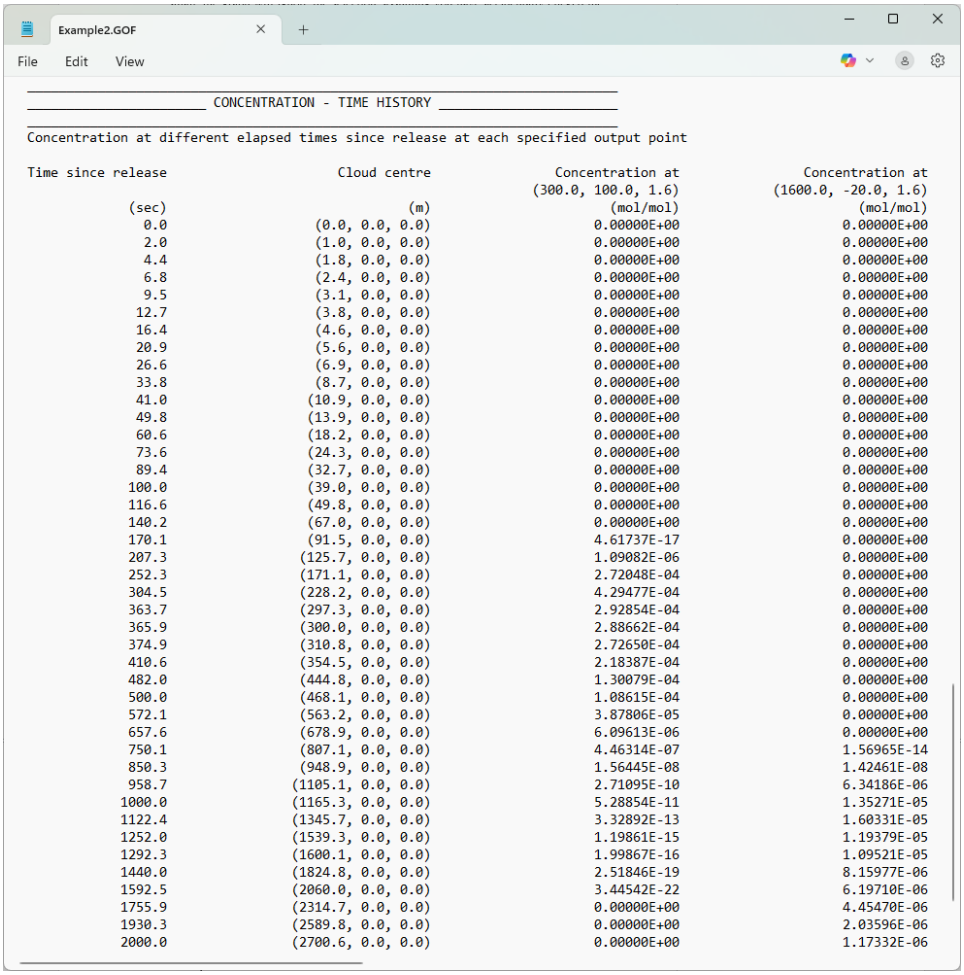



**Figure 6.14** – Dose results table in *Example2.GOF*.

**Step 18** Scroll down further to the 'CONCENTRATION – TIME HISTORY' section of the *.gof* file (see **Figure 6.15**).



Example2.GOF

File Edit View

CONCENTRATION - TIME HISTORY

Concentration at different elapsed times since release at each specified output point

| Time since release (sec) | Cloud centre (m) | Concentration at (300.0, 100.0, 1.6) (mol/mol) | Concentration at (1600.0, -20.0, 1.6) (mol/mol) |
|---|---|---|---|
| 0.0 | (0.0, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 2.0 | (1.0, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 4.4 | (1.8, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 6.8 | (2.4, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 9.5 | (3.1, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 12.7 | (3.8, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 16.4 | (4.6, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 20.9 | (5.6, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 26.6 | (6.9, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 33.8 | (8.7, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 41.0 | (10.9, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 49.8 | (13.9, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 60.6 | (18.2, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 73.6 | (24.3, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 89.4 | (32.7, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 100.0 | (39.0, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 116.6 | (49.8, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 140.2 | (67.0, 0.0, 0.0) | 0.00000E+00 | 0.00000E+00 |
| 170.1 | (91.5, 0.0, 0.0) | 4.61737E-17 | 0.00000E+00 |
| 207.3 | (125.7, 0.0, 0.0) | 1.09082E-06 | 0.00000E+00 |
| 252.3 | (171.1, 0.0, 0.0) | 2.72048E-04 | 0.00000E+00 |
| 304.5 | (228.2, 0.0, 0.0) | 4.29477E-04 | 0.00000E+00 |
| 363.7 | (297.3, 0.0, 0.0) | 2.92854E-04 | 0.00000E+00 |
| 365.9 | (300.0, 0.0, 0.0) | 2.88662E-04 | 0.00000E+00 |
| 374.9 | (310.8, 0.0, 0.0) | 2.72650E-04 | 0.00000E+00 |
| 410.6 | (354.5, 0.0, 0.0) | 2.18387E-04 | 0.00000E+00 |
| 482.0 | (444.8, 0.0, 0.0) | 1.30079E-04 | 0.00000E+00 |
| 500.0 | (468.1, 0.0, 0.0) | 1.08615E-04 | 0.00000E+00 |
| 572.1 | (563.2, 0.0, 0.0) | 3.87806E-05 | 0.00000E+00 |
| 657.6 | (678.9, 0.0, 0.0) | 6.09613E-06 | 0.00000E+00 |
| 750.1 | (807.1, 0.0, 0.0) | 4.46314E-07 | 1.56965E-14 |
| 850.3 | (948.9, 0.0, 0.0) | 1.56445E-08 | 1.42461E-08 |
| 958.7 | (1105.1, 0.0, 0.0) | 2.71095E-10 | 6.34186E-06 |
| 1000.0 | (1165.3, 0.0, 0.0) | 5.28854E-11 | 1.35271E-05 |
| 1122.4 | (1345.7, 0.0, 0.0) | 3.32892E-13 | 1.60331E-05 |
| 1252.0 | (1539.3, 0.0, 0.0) | 1.19861E-15 | 1.19379E-05 |
| 1292.3 | (1600.1, 0.0, 0.0) | 1.99867E-16 | 1.09521E-05 |
| 1440.0 | (1824.8, 0.0, 0.0) | 2.51846E-19 | 8.15977E-06 |
| 1592.5 | (2060.0, 0.0, 0.0) | 3.44542E-22 | 6.19710E-06 |
| 1755.9 | (2314.7, 0.0, 0.0) | 0.00000E+00 | 4.45470E-06 |
| 1930.3 | (2589.8, 0.0, 0.0) | 0.00000E+00 | 2.03596E-06 |
| 2000.0 | (2700.6, 0.0, 0.0) | 0.00000E+00 | 1.17332E-06 |

**Figure 6.15** – Concentration-time history results table in *Example2.GOF*.

For instantaneous releases, this table gives the concentration at different elapsed times since release at each specified output point, as well as the coordinates of the cloud (puff) centre at each time since release. This data can be used to create time series plots of the concentration at each receptor, e.g. in Microsoft Excel, as demonstrated in **Figure 6.16**. At each receptor, we can see the concentration increase as the puff approaches that receptor (note the different *y*-axis scales in each sub-plot), before decreasing again as it passes by. At both receptors, the maximum concentration occurs slightly before the time when the cloud centre is nearest to that receptor, highlighting the relative importance of puff spreading (dilution) compared with puff advection in this case. If a more precise maximum concentration at a given receptor is required, additional specified output times around the time of the concentration peak could be added, and GASTAR rerun – these additional times would then appear in the new concentration-time history results table.

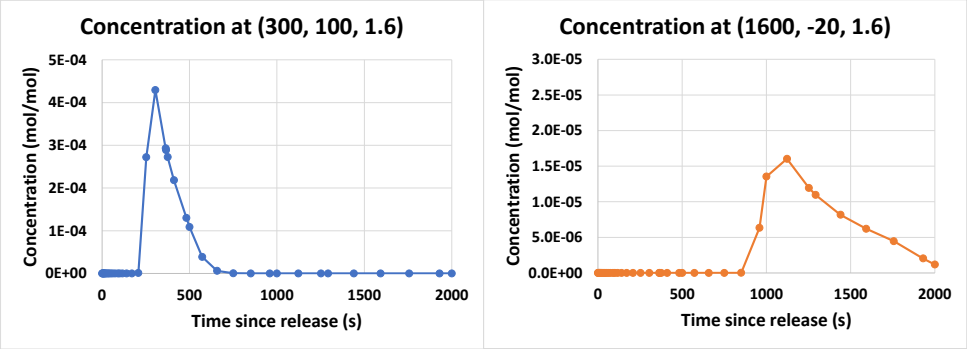



**Figure 6.16** – Example 2: Concentration-time series, plotted in Excel.

**Step 19** Scroll down further to the 'MAXIMUM RANGE RESULTS' section of the *.gof* file (see **Figure 6.17**).

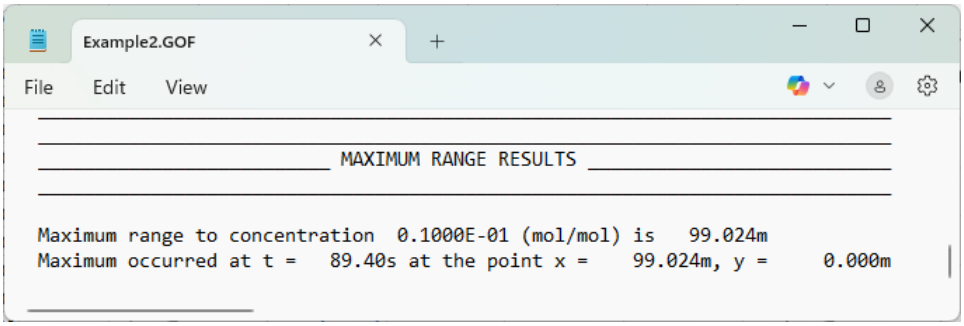



**Figure 6.17** – Maximum range results section in *Example2.GOF*.

Here we are told that the maximum distance from the source to any location where the ground-level concentration was at least 0.1 mol/mol is 99 m. This concentration occurred 89.4 seconds after release, at a point directly under the puff centre (y = 0 m) as might be expected in this case.

### 6.2.3 Contour plotting

This section requires that the third-party software application Surfer is installed on your machine. If this is not the case, it may still be useful for you to read this section.

**Step 20** Select **Contour plot** from the **Results** menu of the GASTAR interface to bring up the **2-D Output Plotter** utility (**Figure 6.18**). In this screen, ensure that **Output type** is set to **Contour**. Set the **File type** to **Time dependent puff** as we are modelling an instantaneous release in this case. Use the boxes on the left to navigate to the working directory in which you saved *Example2.gpl* and select *Example2.GTD*.

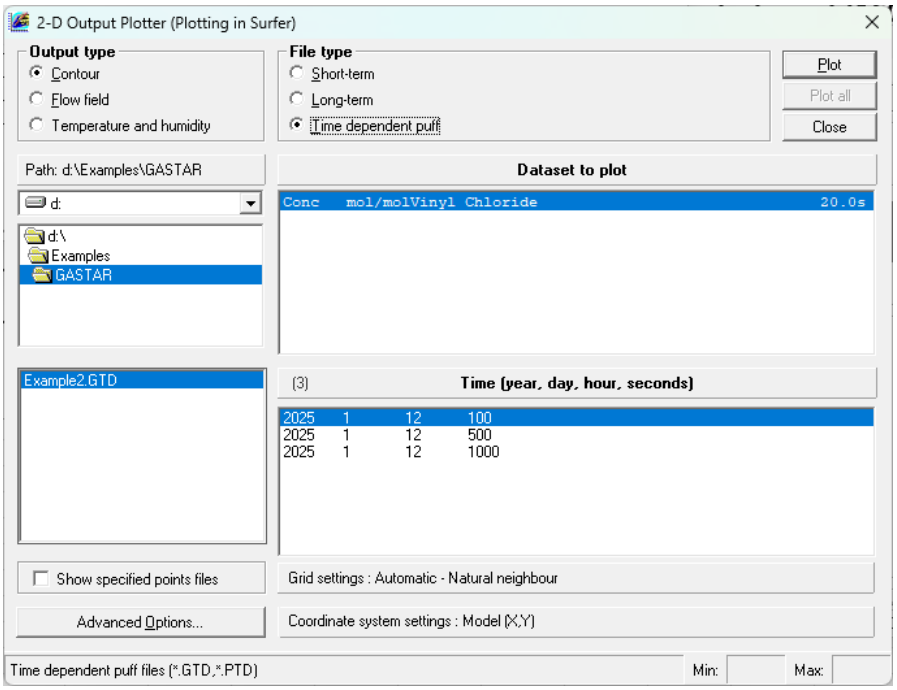



**Figure 6.18** – Example 2: The **2-D Output Plotter** screen.

**Step 21** Select the first time from the **Time (year, day, hour, seconds)** box, which relates to the first specified output time of 100 s since release, and click **Plot**. Choose to save the Surfer grid file in your working directory as *Example2_100s.grd*.

**Step 22** Repeat this for the other two times in the **Time (year, day, hour, seconds)** box, calling the Surfer grid files *Example2_500s.grd* and *Example2_1000s.grd* respectively. You should end up with three separate contour plots, as shown in **Figure 6.19**. Note that these plots have been given a new title etc., and put on the same colour scale – please refer to Surfer's own documentation for guidance on how to do this. The plots show the plume spreading as it advects downwind, via three separate snapshots in time.

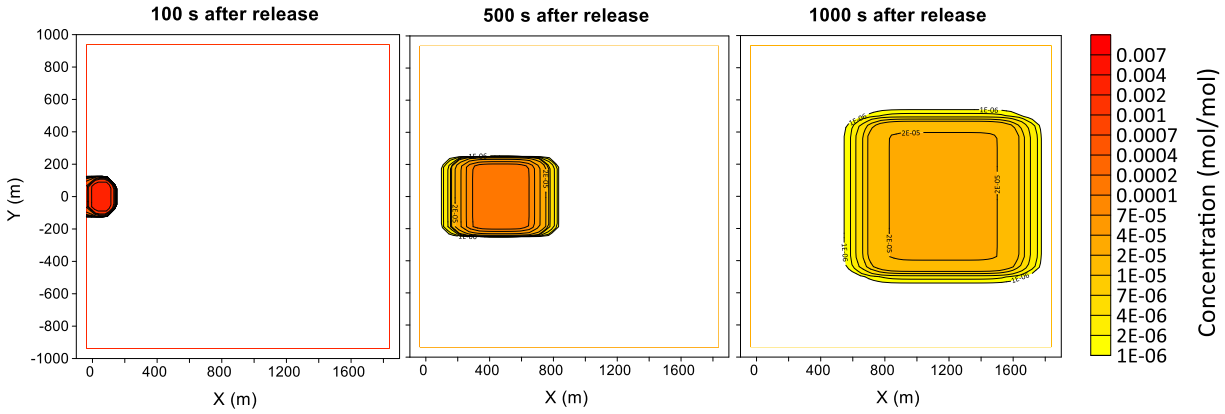



**Figure 6.19** – Example 2: Contour plots in Surfer.

## 6.3 Example 3: Modelling a time varying release

In this worked example you will:

- Model a time varying release from a vaporising pool spill
- Use the Pool Uptake model to calculate the time varying source details
- Look at 'snapshots' of the cloud at different times since release start
- Calculate the dose and concentration-time history at a sensitive receptor

### 6.3.1 Setting up the run

This example revisits the case from Example 1 (Section 6.1) of a propane gas cloud over a vaporising LPG pool spill in a 50 m wide bunded area, but further attempts to account for the reduction in boil-off rate with time as the amount of material available for vaporisation reduces. The total dose at the sensitive receptor located 700 m from the source is also of interest.

**Step 1** In GASTAR, open the input file *Example1.gpl* from Example 1 ('Modelling a continuous release'), select **File**, **Save as**... and save the file as *Example3.gpl*.

**Step 2** In the **Setup** screen, modify the **Title** appropriately e.g. "Example 3: Time varying release". Note the **Source material** is already set appropriately.

**Step 3** Under **Model options**, tick the **Calculate dose** checkbox and untick the **Calculate flammable output parameters** checkbox (not available for time varying releases). Leave the **Calculate concentration-time history** checkbox ticked.

Compare your screen to **Figure 6.20** below.

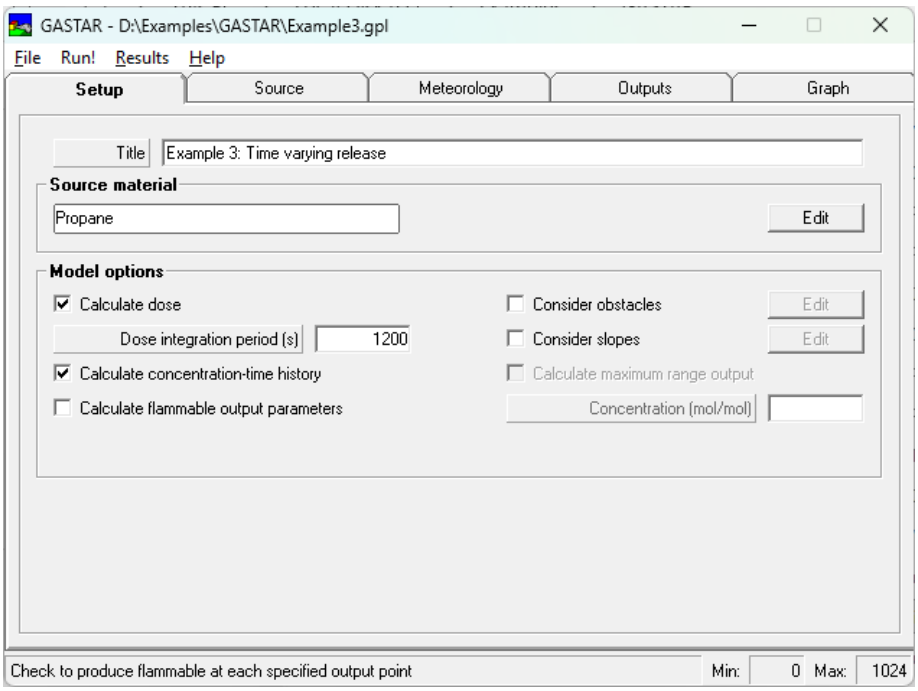



**Figure 6.20** – Example 3: The **Setup** screen.

**Step 4** Move to the **Source** screen. Change the **Release type** to **Time varying**, leaving it as a **Thermal release**.

**Step 5** Click the **Pool Uptake** button to bring up the **Pool uptake source model** screen. Assume that we have already used a liquid spill model (e.g. LSMS) to obtain the following average boil-off rates for five equal-time segments over the lifetime of the pool (**Table 6.3**). Accordingly, in the **Pool details** box of the **Pool** screen, set the pool type to **Time varying** and enter 5 in the **Number of pool segments** field. Then use the **Current segment number** up/down arrows (  ) to enter the data from **Table 6.3** into the **Pool segment duration** and **Mass flux from pool** fields for all five pool segments. Set the **Pool width** to 50 m (the width of the bunded area).

| Segment number | Duration (s) | Average boil-off rate (kg/s) |
|---|---|---|
| 1 | 200 | 100 |
| 2 | 200 | 60 |
| 3 | 200 | 40 |
| 4 | 200 | 30 |
| 5 | 200 | 20 |

**Table 6.3** – Time varying boil-off rates for Example 3.

**Step 6** In the **Initial cloud details** box, enter a **Cloud volume** of 0 $m^3$ to indicate there is no cloud initially. Leave the **Cloud diameter** as 50 m to indicate that vaporisation occurs across the whole pool. Also leave the **Hazardous fraction** as 1 mol/mol and the **Cloud temperature** as 231 K (the boiling point of propane).

**Step 7** Move to the **Meteorology** screen of the Pool Uptake model. The values from the **Meteorology** screen of the main GASTAR interface have been copied over to the Pool Uptake model's **Meteorology** screen; these are appropriate and thus do not need changing.

**Step 8** Move to the **Time varying results** screen of the Pool Uptake model. Leave the **Modelled time** as 1000 s (the lifetime of the pool). Click the **Calculate uptake** button to generate the time varying source data for the cloud above the pool. Click **Use results**; this will to close the Pool Uptake model and copy the calculated data into the **Source details** section of the GASTAR **Source** screen. You can confirm this by checking the **Number of segments** value and using the **Current segment number** up/down arrows (  ) to cycle through the data for each source segment. Note the **Initial air entrainment** is not defined per segment and should be left as 0 kg/s for this example.

Compare your screen to **Figure 6.21** below.

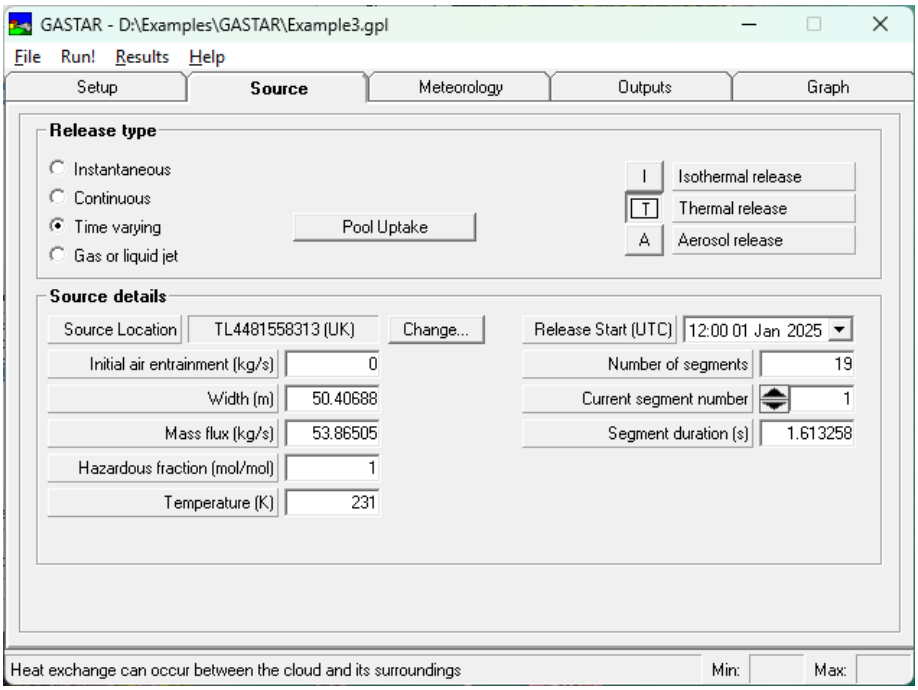



**Figure 6.21** – Example 3: The **Source** screen.

**Step 9** Move to the **Outputs** screen (the **Meteorology** screen can be left as-is). Leave the **Modelled time** and **Averaging time** as 1000 s and 20 s respectively. Retain the specified output point at (X,Y,Z) = (700,0,0), which will be used for the dose and concentration-time history calculations. Additionally, **Add** two **Specified output times** at 100 s and 500 s after ticking the **Specified times** checkbox.

Compare your screen to **Figure 6.22** below.

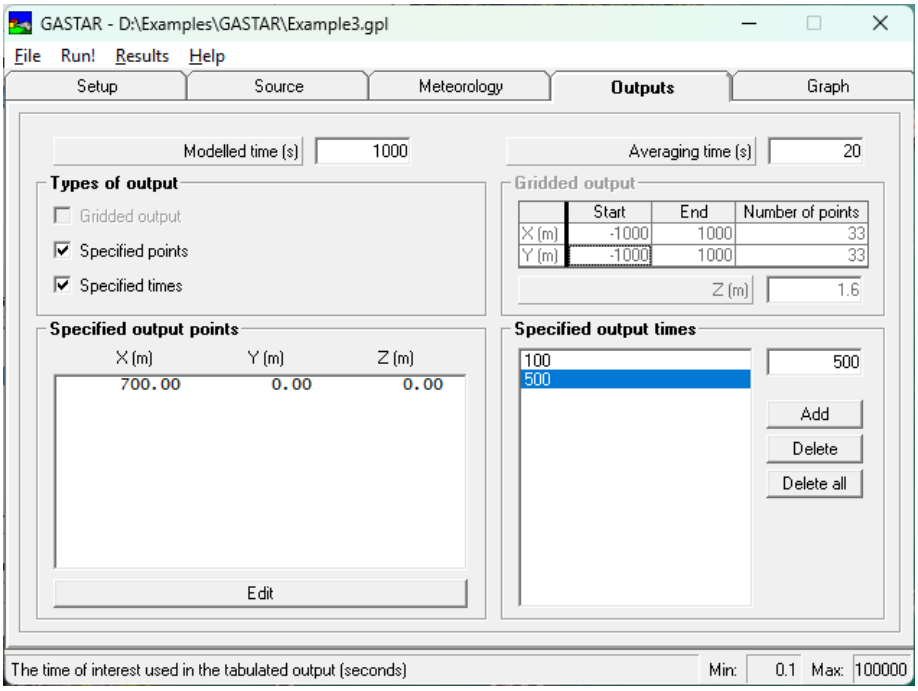



**Figure 6.22** – Example 3: The **Outputs** screen.

**Step 10** Select **File**, **Save** to save the model file, then click on **Run!** to run GASTAR.

### 6.3.2 Viewing numerical output

**Step 11** From the **Results** menu, select **Numerical output.** Browse to select the file *Example3.GOF* and click **Open** to open it in your preferred viewing application.

**Step 12** Scroll down to the 'RESULTS' section. For time varying releases, the first table gives a snapshot of the (multi-segment) cloud properties at the **Modelled time** (1000 s in this case). Under this, there is an additional table for each specified output time, giving a snapshot of the cloud at that time. Note that at 1000 s after release start, all source segments will have been emitted (just), while at e.g. 100 s, only the first few segments will have been emitted.

**Step 13** Scroll down to the 'DOSE RESULTS' section. For time varying releases, the dose at a given output point represents the total dose over all time, i.e. the dose after the final source segment has passed beyond that output point. Here we can see that the total dose at the sensitive receptor 700 m downwind of the source is approximately 0.035 mol/mol.

**Step 14** Scroll down to the 'CONCENTRATION-TIME HISTORY' section. For time varying releases, this table gives, at each specified output point, the arrival time of each segment at that output point and the (steady-state) concentration while that segment was passing that output point. We can see that the first segment took around 670 s after release start to reach the sensitive receptor 700 m downwind of the source, while the last segment arrived around 1400 s after release start (and thus will have passed beyond the receptor at around 1600 s after release start, given it has a segment duration of 200 s). We can also see that the highest concentration at this receptor (around 0.0039 mol/mol) occurred while the middle part of the cloud (segment numbers 8-15) was passing it – see **Figure 6.23**, where Microsoft Excel has been used to plot concentration versus arrival time for all segments at this receptor. This corresponds to those segments for which the Uptake Model calculated the mass flux as ≈ 100 kg/s. Note the maximum concentration is less than that calculated in Example 1 because in that example the maximum instantaneous boil-off rate (300 kg/s) was used, while in this example time-averaged boil-off rates were used (this acts to 'smooth out' extreme values). This could be improved by including more shorter-duration segments in the time varying run, particularly near the release start time.

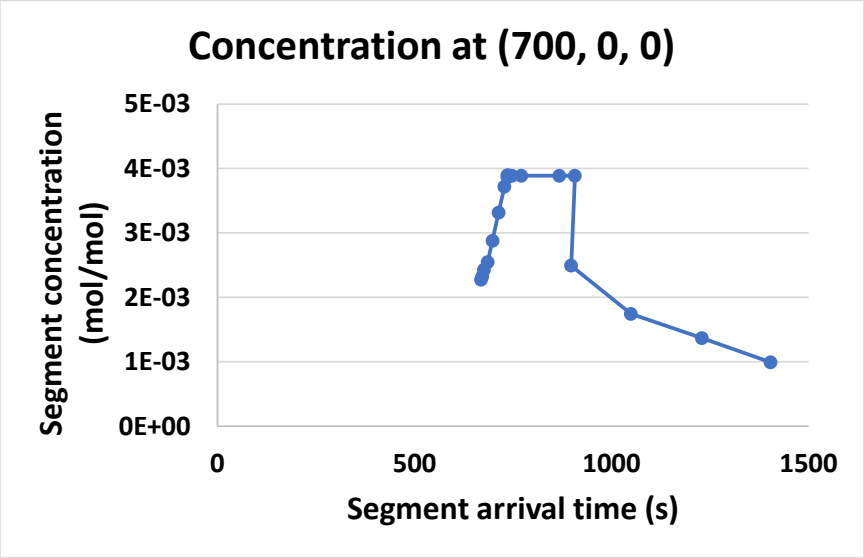



**Figure 6.23** – Example 3: Segment concentration vs arrival time, plotted in Excel.

### 6.3.3 Viewing graphical output

**Step 15** Return to the GASTAR interface and move to the **Graph** screen. Use the controls in the **File Details** box to browse to the working folder and select the file *Example3.GPH*.

**Step 16** Ensure that **X-Y line plotting** is selected under **Graph type**. In the **X-Y plotting details** box, use the (circular) radio buttons to select 'Downwind coordinate' as the dependent variable (*x*-axis), and the checkboxes to select 'Max profile concentration' as the independent variable (*y*-axis). Finally, click **Plot graph** to display the line plot (see **Figure 6.24**). As this is a time varying release, this plot is showing a snapshot of the concentration field at the **Modelled time** at different downwind distances from the source.

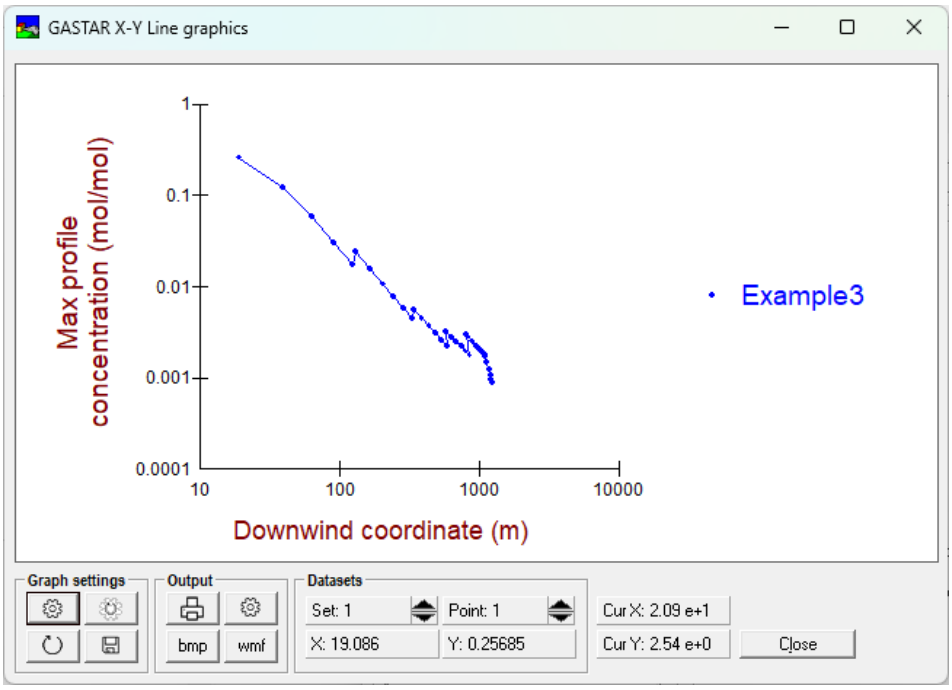



**Figure 6.24** – Example 3: Concentration line plot

# SECTION 7 Technical Summary

## 7.1 Dense gas dispersion theory

Public concern over the risks posed by the use of hazardous materials has grown markedly over the past few decades. The dioxin release in Seveso (Italy) in 1976, that of methyl isocynanate in Bhopal (India) in 1984, the liquefied petroleum gas explosions in Mexico City in the same year and the chlorine spill at the Port of Aqaba (Jordan) in 2022 emphasised the possible scale of the tragedies that may accompany activities involving hazardous materials.

The development of appropriate regulatory measures to achieve an acceptable balance between economic benefit and potential harm accompanying such activities requires quantitative assessment of the consequences of the accidental release of material into the environment.

It is commonly the case that both flammable and toxic hazardous industrial materials produce a cloud that is denser than the environment upon release into the atmosphere.

Knowledge of dense gas dispersion has been outlined in reviews by Britter and McQuaid (1988), Britter (1989a), Britter (1995a) and Hanna and Drivas (1987, 1997).

The information on dense gas dispersion that is of interest to the hazards analyst is contained in the distribution of concentration as a function of the spatial coordinates and time. Very often, this information is required only in summary form, such as:

- the distance to a given concentration (for example, the lower flammability limit);
- the size, composition, and shape of the cloud. These are needed for thermal radiation estimates in the event of burning or as input to methods of estimating explosion propagation;
- the mass of gas in the cloud between the upper and lower flammability limits. This is often regarded as the appropriate mass to be used in estimating the TNT-equivalence of a flammable cloud; and
- the concentration and its time history at a given distance, needed to define toxic effects on human and non-human biota.

### 7.1.1 Formation of dense gas clouds

The density of the cloud[1] results not only from the properties of the material released, but also from the methods of storage and of release. Most cases of interest are covered by the following broad categories:

- material with a high molecular weight compared with that of air (e.g. chlorine);
- materials with low molecular weight that may be at a low temperature (e.g. cold methane evolving from the boiling of refrigerated liquefied natural gas (LNG) following a spill onto a warmer surface);

[1] "Cloud" is used here as a general descriptive term: "plume" refers to a continuous release, whereas "puff" refers to an instantaneous release.

- materials with low molecular weight and whose vapour at the boiling temperature is less dense than the environment, but which, as a result of the release type, produce a cloud including liquid droplets. The cloud-borne droplets increase the cloud density, as does the cooling resulting from their subsequent evaporation, e.g. ammonia (see Griffiths & Kaiser 1982); and
- materials in which a chemical transformation takes place as a result of reaction with water vapour in the ambient atmosphere, e.g. nitrogen tetroxide, $N_2O_4$, hydrogen fluoride, HF (see Clough *et al.* 1987).

Storage and release conditions have been discussed by Fryer & Kaiser (1979). The releases may be broadly classified as instantaneous (e.g. catastrophic release), continuous (e.g. pipe break) or time varying. The release may also be classified as either pressurised or non-pressurised depending on the type of containment. Source term models have been reviewed by Hanna & Drivas (1987).

The quantitative assessment of the dispersion of dense gases is quite different to conventional dispersion problems for the following reasons:

- unlike chimney emissions, the modes of release are very diverse in terms of geometry and source specification;
- because the released material is typically stored in a liquid phase, the volumes of gas released may be very large;
- the release may be a gas/liquid mixture;
- the release is usually transient;
- the formation of the gas cloud typically involves phase changes; and there may be heat and/or mass transfer with the underlying surface.

In addition, the dispersing gas forms a low-level cloud that is sensitive to the effects of both man-made and natural obstructions and topography.

These complications indicate that the task of predicting the consequences of an accident will not be simple. Further, the rapid development of the field has restricted specific study of the various, relevant fluid-mechanical phenomena.

### 7.1.2 Physical processes in dense gas clouds

The density difference between the released material and its environment introduces four major effects with regard to dispersion problems:

- The velocity field produced by the horizontal density difference, in a gravitational field, is an additional transport mechanism to that provided by the ambient flow. This self-generated flow produces a cloud with an increased horizontal, and reduced vertical, extent when compared with a similar release having no density difference. In addition, the self-generated component of the motion is predominantly deterministic, not random; as a result, profiles of concentration in the lateral direction are frequently quite uniform.
- The velocity shear introduced by this velocity field may lead to a gross intermingling of the two fluids and eventually to turbulence generation and consequential turbulent mixing and cloud dilution. This mechanism of dilution is of primary importance when

the self-generated velocities are large compared with the mean ambient velocity. In addition, turbulence generated from this flow near rigid boundaries provides a mechanism for cloud dilution.

- Frequently it is the ambient turbulence that is responsible for cloud dilution, be it locally generated or advected from upstream. The variation of density in the vertical direction will, in a gravitational field, be stably stratified, and turbulence and turbulent mixing can be significantly reduced or entirely inhibited (Turner 1973). This effect can extend to the atmospheric turbulence in the wind flow over the cloud, as well as to the cloud itself.
- The inertia of the released material is directly dependent upon the density of the material. However, when the density difference is small compared with either density, the influence of the *density difference* on the inertia is small and may be neglected. This may not be valid close to the source, but cloud dilution will eventually allow this assumption. Under these conditions, the density difference frequently appears as $g' = g[(\rho - \rho_a)/\rho_a]$, where $g$ is the acceleration due to gravity and $\rho$ and $\rho_a$ are the density of the cloud and of the ambient fluid, respectively.

These effects emphasise the difference between the dense gas dispersion and the dispersion of non-dense, or "passive", pollutants. It is obvious that the density difference is not the sole variable determining whether the release behaves as a dense gas. A very small release or release rate into a strong wind, or alternatively a release over a large source area, may be considered effectively passive. A continuous source of volume flow rate $q_0$, with source density difference characterised by $g_0'$, may be considered effectively passive when

$$(g_0' q_0/D)^{1/3}/U \leq 0.15, \tag{7.1}$$

where $D$ is the source dimension and $U$ is the ambient velocity (Britter & McQuaid 1988).

For an instantaneous source of release volume $Q_0$ and implied source dimension $Q_0^{1/3}$, the criterion becomes

$$\left(g_0' Q_0^{1/3}\right)^{1/2}/U \leq 0.2. \tag{7.2}$$

The form of these criteria emphasises the importance of the ambient velocity in describing the flow. In the latter criterion, a halving of the wind speed is equivalent to a 64-fold increase in $Q_0$.

In addition, there may be thermodynamic or chemical processes depending on the nature of the material and the release conditions. Eventually the dispersion of the cloud becomes *passive* due to dilution.

### 7.1.3 Dispersion models

There are probably in excess of 100 analytical or numerical models currently available that purport to describe the dispersion of dense gases. Reviews by Blackmore *et al.* (1980), Wheatley & Webber (1985) and Hanna & Drivas (1987, 1997) describe some of these models. Modifications of the conventional Gaussian dispersion models have been shown to be inadequate, leading to errors of as much as two orders of magnitude (Havens 1980).

There have been two distinct approaches in dense gas dispersion models:

- The first approach, three-dimensional models, uses Reynolds-averaged, three-dimensional, time-dependent conservation equations. The most common of these use K-theory for turbulent closure. Havens *et al.* (1987) compared four models. There are still considerable difficulties in applying this type of model.
- The second approach, an integral formulation, integrates out vertical and horizontal variations in the cloud or plume, and later reincorporates these through empirically determined profiles. These models, referred to as box models, have a small number of adjustable constants whose effect may be easily interpreted physically. These models are effective and computationally inexpensive. Hanna & Drivas (1987) list over 40 models.

Integral models incorporate three specific effects:

- the cloud spreads horizontally under its own negative buoyancy
- there is a dilution of the cloud by mixing with the ambient flow
- the cloud is advected by the ambient flow

### 7.1.4 Instantaneous releases

The near-instantaneous release of material giving rise to a dense cloud may result from the catastrophic failure of a storage vessel. This produces a rapidly expanding, entraining cloud whose description and quantification are still unclear.

Shortly after release, this self-generated motion weakens and the cloud collapses toward the surface and spreads horizontally while being advected and diluted by the ambient flow. This latter collapse and subsequent motion has been extensively studied. The initial geometrical configuration is typically an aspect ratio (height to diameter) of about 1.

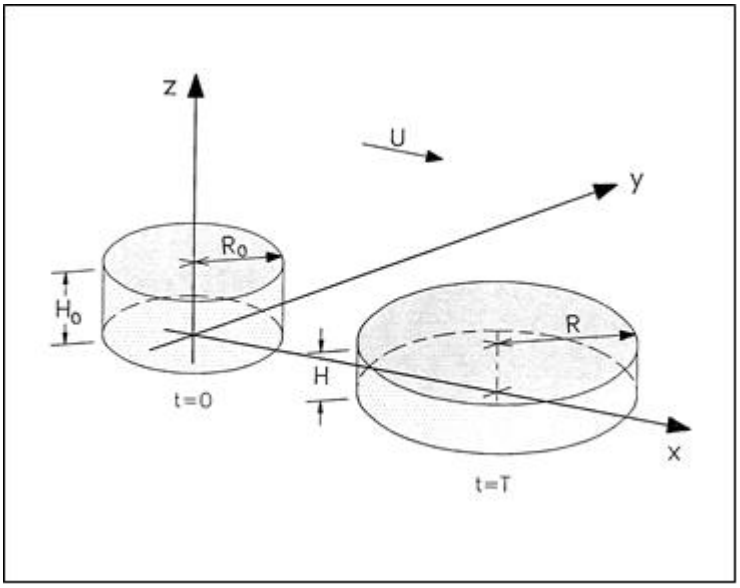



**Figure 7.1** – Box model representation of a puff release.

Observations (Spicer & Havens 1985) show that after the cloud collapse, much of the cloud material is contained within a toroidal vortex formed from the roll-up of the vorticity generated

by the nonvertical density gradient at the cloud edge. This horizontally propagating vortex ring is stabilized by vortex stretching and produces intense mixing of the cloud with the environment. Some of the mixed fluid is left behind the advancing vortex to provide a substantially diluted cloud. Eventually the leading edge vortex weakens and adopts the classical gravity head form. It is only at this stage that similarity theory can be valid.

A very substantial dilution of the cloud is observed in the laboratory (Spicer & Havens 1985) and field experiments (Brighton & Prince 1987). The cloud dilution is a direct consequence of the strong leading-edge vortex and is nearly an order of magnitude larger than the mixing associated with the gravity current head (Puttock 1988).

Releases in ambient flows, both in the laboratory and in the field, show a cloud spreading under its own buoyancy and being advected downwind. Multipoint data from large-scale field experiments (Brighton *et al.* 1985) confirm that the growth rates of cloud area are similar to those in calm conditions. The clouds are slightly longer than they are wide as a result of longitudinal dispersion. The movement downwind results from mixing between the cloud and the ambient flow (Rottman *et al.* 1985) rather than from any form drag.

Britter and McQuaid (1988) summarised available data from laboratory and field experiments.

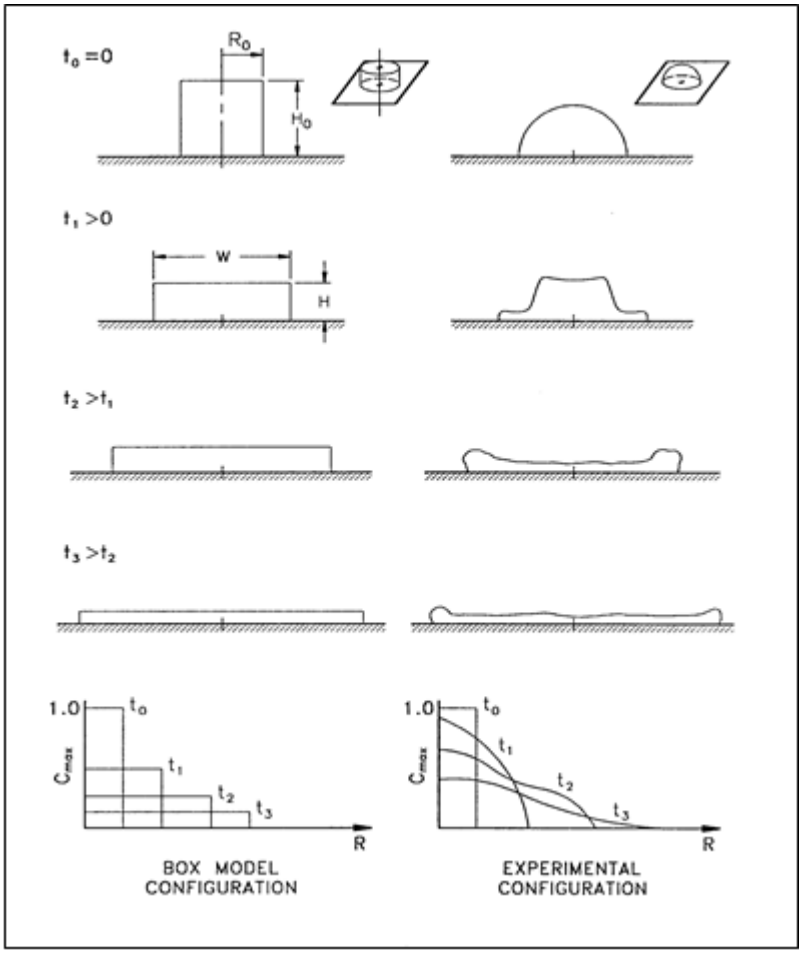



**Figure 7.2** – Model and experimental puff development.

### 7.1.5 Continuous releases

Continuous releases from ground-level sources or near-ground-level sources have been the subject of many studies. Britter & McQuaid (1988) summarized available data from laboratory experiments using idealized area sources with low momentum. More complicated source configurations will eventually lead to a dense plume at ground level to which these idealized source experiments may be relevant (Meroney 1982). Field experiments have also considered more realistic, less idealized sources.

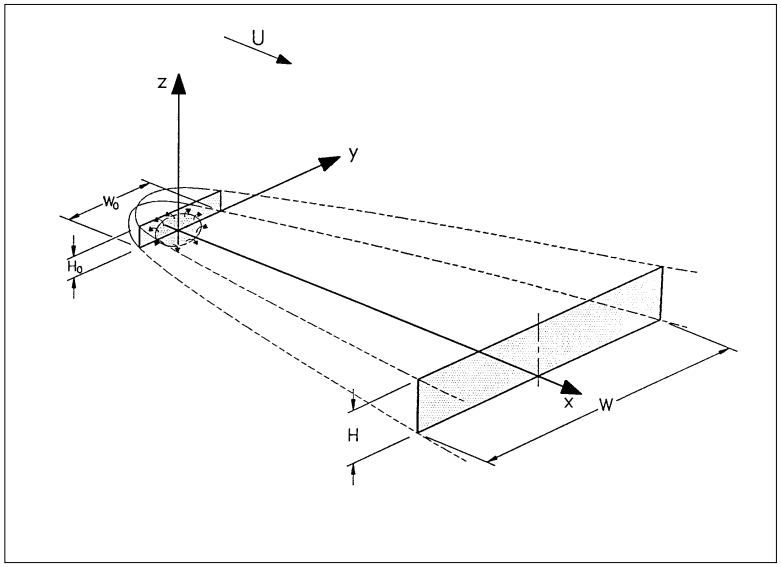



**Figure 7.3** – Box model representation of a plume release.

Britter (1979) considered a release in calm conditions. An imposed ambient flow will limit the upwind spreading and ensure that all the source material is eventually carried downwind. The mechanism by which this flow reversal is attained is uncertain. For a uniform flow, the flow reversal may occur solely through an inertial, nonmixing process. The flow interaction is less clear when the ambient flow is a turbulent boundary layer.

For a gravity current spreading under a turbulent flow, the near source region may involve both an inertial interaction and a scouring or detrainment of the fluid near the source by the ambient flow. Observation of laboratory experiments would favour the latter of these mechanisms.

One or both of these mechanisms allow the plume to travel upwind and laterally at the source prior to being advected downwind.

If the plume is considered downwind from the source, the plume width increases as a result of the lateral buoyancy driven motion and atmospheric diffusion, whereas the cloud depth decreases as a result of lateral spreading and increases as a result of diffusion by atmospheric and self-generated turbulence.

In contradiction to the often-made assumption, there is no evidence in laboratory or field experiments that dense gas plumes appear as a well-mixed layer surmounted by a sharp density interface. In fact, quite the opposite is observed, with the vertical profiles of mean concentration having a near-exponential variation. The height of the plume centroid is substantially reduced when the plume is dense, which is a result of the buoyancy-driven flow and reduced vertical mixing.

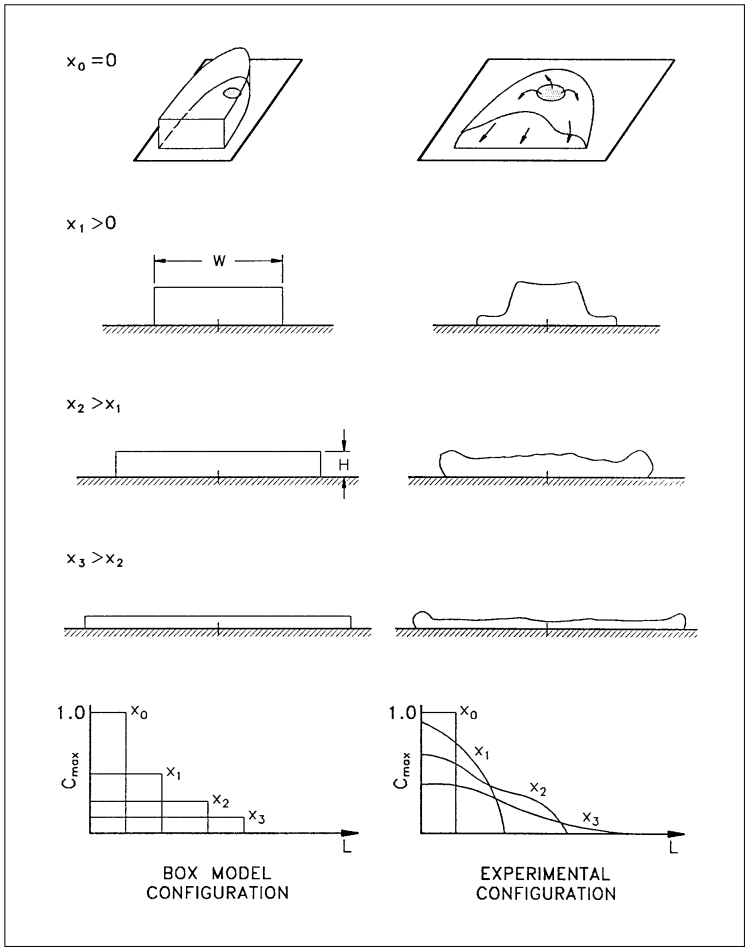



**Figure 7.4** – Model and experimental plume development.

Density differences reduce the mixing between the plume and the environment, but the large surface area of the plume across which mixing takes place will enhance dilution. Observations from Britter & Snyder (1988) show that these two effects can often produce a decay of the maximum ground-level concentration very similar to that for neutrally buoyant passive plumes. Other laboratory studies, e.g. Meroney (1982), have also found that the ground-level concentration is not as strongly influenced by the density difference as is the plume shape.

### 7.1.6 Time varying releases

In many situations the release is neither instantaneous nor continuous, but varies with time. For example, consider a pool of a boiling liquid cryogen, or a rupture of a pressurised line or vessel. In the former case, the pool can spread over the ground providing an increasing area for the transfer of heat from the underlying surface; and in the latter, as the stored material slowly depressurises, the mass flow rate through the rupture will reduce.

These are typically treated by replacing the time varying release as a finite number of discrete release rates. Segments of the solution for each of these release rates are combined to form a segmented plume solution. Longitudinal diffusion/ dispersion may be added to smooth between the segments or to treat the leading and trailing segments.

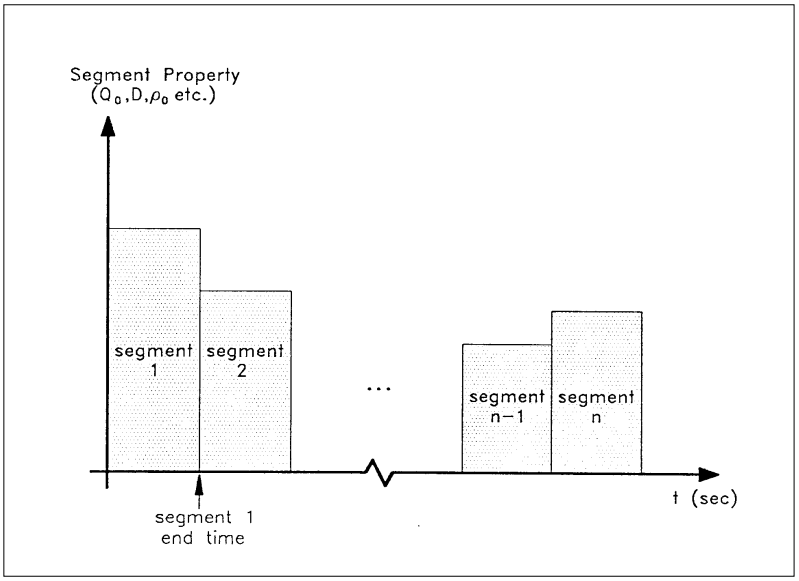



**Figure 7.5** – Time varying release.

It might be noted here, and will be considered further in Section 7.12, that not all the released airborne material need be taken up by the ambient flow passing over the source position. If this is the case, the cloud over the source position will expand with time to produce a secondary source or 'vapour blanket'. This will continue to expand until the material taken up by the ambient flow matches the material emanating from the primary source.

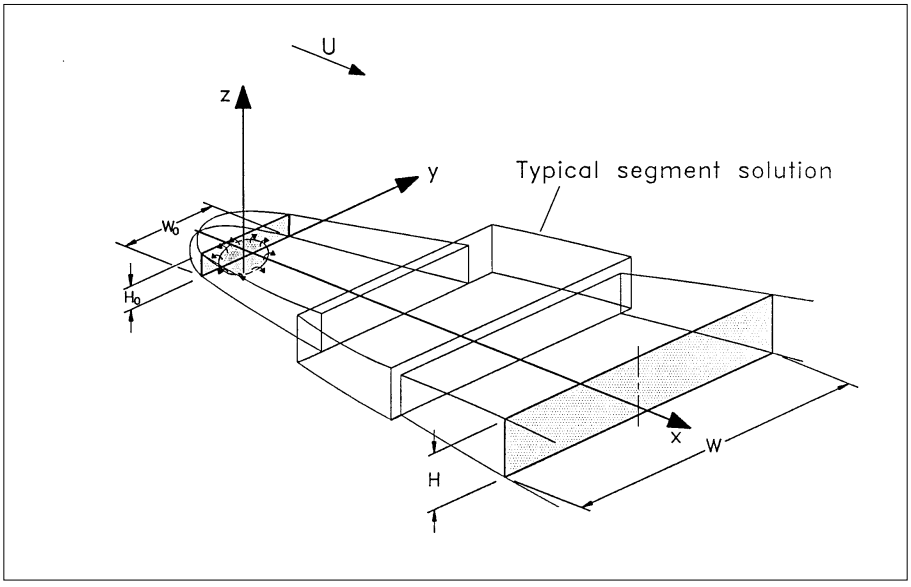



**Figure 7.6** – Box model representation of a time varying release.

## 7.2 GASTAR dispersion model

A specific description of the overall GASTAR model is best addressed by considering the dispersion module first.

The model is a similarity model in that similar shapes are assumed for various parts of the model, thus reducing the basic equations of motion to simpler ordinary differential equations. These equations are written in bulk (or box model) form; then modified to re-introduce the assumed profile. This technique is common in the study of buoyancy or density influenced flows (Turner 1973). The dynamics of the flow influence the motion of the "similar shape".

The bulk characteristic dimensions of the puff or plume, the radius or width and the height, are then the mean radius ($R$) or width ($w$) and the height of the puff or plume ($h$).

The rate at which a puff or plume spreads horizontally under its own negative buoyancy is given by a gravity current head formula.

### 7.2.1 Horizontal spreading

Horizontal spreading of a plume is modelled with a gravity current head formula

(7.3) $$u_f = C_e(g'h)^{1/2},$$

where

(7.4) $$g' = g\left(\frac{\rho-\rho_a}{\rho_a}\right)$$

and $C_e$ is near unity, $\rho$ is the (uniform) density within the modelled puff or plume and $\rho_a$ is the ambient density. The velocity $u_f$ is the horizontal velocity of the edge of the plume.

Thus

(7.5) $$\frac{dR}{dt} \text{ or } \frac{dw/2}{dt} = C_e(g'h)^{1/2}.$$

In the case of an instantaneous (puff) release a more complicated algorithm is used in the model to account for the initial radial acceleration, although this rapidly asymptotes to the above form.

Atmospheric turbulence acts to reduce $C_e$ (see Linden & Simpson 1988) and this effect is modelled by the empirical form

(7.6) $$C_e = C_{e0}\left(1 - \frac{1}{Ri_*}\right),$$

where the Richardson number $Ri_*$ is a measure of the puff or plume stability

(7.7) $$Ri_* = g\left(\frac{\rho-\rho_a}{\rho_a}\right)\frac{h}{u_*^2} = \frac{g'h}{u_*^2},$$

in which $u_*$ is the friction velocity of the undisturbed flow, and is a measure of the

atmospheric turbulence.

### 7.2.2 Dilution of the cloud

The dilution of the cloud is modelled using an entrainment velocity approach, i.e. the cloud mass $m$ evolves according to

(7.8) $$\frac{dm}{dt} = \rho_a(u_e A_e + u_t A_t),$$

where $u_e$ and $u_t$ are edge and top entrainment velocities and are determined by appeal to correlations based on experiments. $A_e$ and $A_t$ are edge and top entraining areas respectively.

The puff or plume is diluted by mechanisms associated with the advancing leading edge (edge entrainment) and the downwind advection by the ambient wind field (top entrainment). These are modelled using entrainment velocities. The edge entrainment velocity $u_e$ is modelled by

(7.9) $$u_e = 0.6u_f,$$

where $u_f$ is the leading edge velocity. For instantaneous releases a further factor $h_0/R$ accounts for the initial aspect ratio of the release.

The top entrainment velocity $u_t$ is modelled by

(7.10) $$u_t = \frac{0.4u_*}{(1+0.125Ri_*)}$$

after an appeal to the results of McQuaid (1976) as analysed by Britter (1980) and further experimental results by Stretch (1986) and others.

Top entrainment due to thermal convection in the cloud is incorporated using a model based on penetrative convection. This reduces essentially to the incorporation of the conventional convection velocity $w_*$ in addition to $u_*$.

### 7.2.3 Advection by the wind

The modelling of the cloud movement downwind is based on either entrained momentum or, more simply (and valid away from the source), on the ambient wind speed at a height representative of the cloud height. Referred to as the advection velocity, it is given by

(7.11) $$U_a = U(z_{\text{eff}}),$$

where $U(z)$ is the wind speed profile and $z_{\text{eff}} = 0.56h$. The coefficient is taken after appeal to *passive* puff results e.g. Lagrangian similarity results of Batchelor (1952) or Chatwin (1968).

This result is obtained from a consideration of a neutrally stratified boundary layer. It is not considered worthwhile to modify this for any explicit influence of atmospheric

stability.

However, a dense puff or plume does not travel with the ambient wind velocity: the puff or plume perturbs the ambient flow. This effect has been accounted for by using a multiplicative factor to adjust the advection velocity, given by

(7.12) $$0.8 + \frac{0.2}{(1+Ri_*)}.$$

The puff is assumed to adopt an advection velocity determined by the ambient velocity profile. However, for an unmixed release, e.g. the field tests at Thorney Island, the puff advection is solely by momentum added to the puff by subsequent mixing with ambient fluid (as a result of atmospheric turbulence and the flow generated by the negative buoyancy).

## 7.3 Meteorology

The required meteorological information for the model is that of:

- wind speed profile
- atmospheric stability, and
- the dependent friction velocity, $u_*$

The atmospheric stability may be characterised by the Pasquill-Gifford stability category (PSC), or more objectively, the Monin-Obukhov length, denoted here and elsewhere in Section 7 by $L$. The user may input either the Pasquill-Gifford stability category or the Monin-Obukhov length, and the surface roughness length, $z_0$. When required, the non-specified descriptor is calculated from the relationships given in **Table 7.1**.

| Pasquill-Gifford Stability Category | Monin-Obukhov Length (m) |
|---|---|
| A | $-8.81z_0^{0.1025}$ |
| B | $-26z_0^{0.1710}$ |
| C | $-123.5z_0^{0.3045}$ |
| D | 4 |
| E | $123.5z_0^{0.3045}$ |
| F | $26z_0^{0.1710}$ |
| G | $8.81z_0^{0.1025}$ |

**Table 7.1** – Relation between Pasquill-Gifford Categories and Monin-Obukhov Lengths.

The mean wind velocity profiles are given by

$$\frac{U_w}{u_*} = \frac{1}{k}\left[\ln\left(\frac{h}{z_0}+1\right) - \Psi\right], \tag{7.13}$$

where $u_*$ is the friction velocity (m/s), $k$ is the von Karman constant, $h$ is the height (m) at which the wind speed is to be calculated, $z_0$ is the roughness length (m) and $\psi$ is dependent on the atmospheric stability, .e.g. the Monin-Obukhov length $L$.

For stable atmospheric conditions

$$\psi = -4.7\frac{h_w}{L} \qquad L > 0 \tag{7.14}$$

and for unstable atmospheric conditions

$$\psi = 2\ln\left(\frac{1+\zeta}{2}\right) + \left(\frac{1+\zeta^2}{2}\right) - 2\arctan(\zeta) + \frac{\pi}{2} \qquad L < 0, \tag{7.15}$$

where $h_w$ is the height at which the wind speed is measured and with

$$\zeta = \left(1 - \frac{15h_w}{L}\right)^{1/4}. \tag{7.16}$$

The friction velocity is obtained by inverting the mean velocity equation.

## 7.4 Thermal effects

Heat transfer to or from the ground is based on conventional forced and free convection heat transfer correlations. Phase changes of the released material or water vapour in the atmosphere are based on an assumption of homogeneous thermodynamic equilibrium.

The thermal codes use an enthalpy balance with surface heat transfer inputs given by the maximum of the forced and free convection heat transfer coefficients multiplied by the relevant surface area.

The heat transfer coefficients used are

(7.17) $$h_{\text{free}} = 0.19\left(\frac{gk^3}{\nu\alpha T}\right)^{1/2}\Delta T^{1/3}$$

and

(7.18) $$h_{\text{forced}} = \rho C_p U_r \left(\frac{C_f}{2}\right)\left(\frac{\nu}{\alpha}\right)^{-2/3},$$

where $k$ is the thermal conductivity, $\nu$ the kinematic viscosity, $\alpha$ the thermal diffusivity, $C_p$ the specific heat at constant pressure, $C_f$ the surface skin friction coefficient, $T$ the cloud temperature, $\Delta T$ the surface-cloud temperature difference and $U_r$ the reference velocity given by

(7.19) $$U_r = \left(U_a^2 + aU_f^2\right)^{1/2},$$

where $U_a$ is the advection velocity of the cloud and $U_f$ is the front velocity due to the negative buoyancy of the cloud. The constant $a$ is 2/3 for puff releases and 1/2 for plume releases.

## 7.5 Thermodynamics

The aerosol model is a homogeneous equilibrium model which assumes that the liquid droplets are in thermodynamic equilibrium with the (uniform) concentration puff or plume cross section. That is, the cloud with a given enthalpy flux (based on source conditions and any subsequent ground heating) adopts a temperature, $T$, and an aerosol mass fraction such that the partial pressure of the released vapour, $p_v$, satisfies the equation

(7.20) $$\log_{10} p_v = A - \frac{B}{T+C},$$

where $A$, $B$, $C$ are constants, namely the Antoine coefficients.

The model allows for atmospheric water vapour to condense to liquid.

## 7.6 Passive dispersion

The dispersion of the release in the atmosphere may be passive from the source if the release has a density the same as the atmospheric density, or may become effectively passive when the density difference (characterised through the Richardson number, $Ri_*$) becomes small.

Under these conditions, the dispersion should be similar to that from conventional dispersion formulae. The lateral growth of the plume is automatically accounted for by the use of $\sigma_y$ in the lateral concentration profile. The $\sigma_y$ values used are taken from Briggs (1973) as outlined below for open country conditions. The form of $\sigma_y$ remains unchanged,

(7.21) $$\sigma_y = \frac{C_1 x}{\sqrt{1+0.0001x}},$$

where $C_1$ is a coefficient taken from **Table 7.2** and $x$ is the downwind distance (the modulus is used to allow for negative $x$ with slopes).

| PSC | $C_1$ |
|---|---|
| A | 0.22 |
| B | 0.16 |
| C | 0.11 |
| D | 0.08 |
| E | 0.06 |
| F | 0.04 |
| G | 0.04 |

**Table 7.2** – Coefficients used in expression for the lateral diffusion term $\sigma_y$.

The vertical growth of the release when effectively passive is based on the extended Lagrangian similarity theory and uses a modification to the vertical entrainment velocities, e.g. see Hanna, Briggs and Hosker (1982); Wheatley (1988). Specifically

(7.22) $$\frac{u_e}{u_*} = k\left(1 - 9\frac{h}{L}\right)^{1/2}$$

for unstable conditions and

(7.23) $$\frac{u_e}{u_*} = k\left(1 - 6.3\frac{h}{L}\right)$$

for stable conditions, which have the limit of

(7.24) $$\frac{u_e}{u_*} = k$$

For neutral conditions; $k$ is the von Karman constant.

These formulations are used when the cloud Richardson number, $Ri_*$, falls below 1.1. For puff releases, where necessary, the along-wind turbulent diffusion, characterised by $\sigma_x$, is equated with $\sigma_y$.

## 7.7 Longitudinal shear dispersion

For ground-based puff releases in particular, the variation of the mean velocity with height leads to the cloud being stretched longitudinally, i.e. the upper parts move faster than the lower parts, while there is also vertical mixing. This process is known as shear dispersion. This will produce a characteristic longitudinal $\sigma_s$.

Many empirical formulae are available for $\sigma_s$, but those are traditionally based on passive releases and written in terms of the downwind distance. Instead, we have reinterpreted such formulae (e.g. Wheatley 1988) in terms of development with the cloud height, $h$, this being the region which is undergoing shear dispersion. We have then argued that this approach, based on cloud height, will not be influenced by whether the cloud is passive or dense.

The algorithms used are

- For neutral stratification (category D),

(7.25) $$\sigma_s = 4.5h$$

- for stable ambient stratification (categories E-G),

(7.26) $$\sigma_s = 4.5h^p$$

where

(7.27) $$p = \left(1 - \frac{8}{L}\right)^{-1}$$

- for unstable ambient stratification (categories A-C),

(7.28) $$\sigma_s = 2h^p$$

There is a small interpolation region such that

(7.29) $$\sigma_s = \left(4.5 - \frac{250}{L}\right) h^p$$

if $0 \geq 1/L \geq -0.01$. In equations (7.27) and (7.29), $L$ is the Monin-Obukhov length.

The overall characteristic longitudinal scale of the puff is

(7.30) $$(\sigma_x^2 + \sigma_s^2)^{1/2}$$

## 7.8 Concentration profiles

The 'uniform' puff or plume concentration is determined from a mass balance.

The assumed profiles in the horizontal are a uniform concentration with error function edges in order to represent a puff or plume with a central uniform concentration being eroded at the edges by ambient turbulence. When the two eroding edges eventually overlap substantially, the merged error functions produce the conventional Gaussian distribution.

The edge erosion is modelled by appeal to conventional passive dispersion results. Currently the formulation proposed by Hanna, Briggs & Hosker (1982) is used.

The vertical concentration profile for ground level sources in passive plumes is typically of the form $\exp(-z^{1.5})$ (*not* $\exp(-z^2)$, though this is commonly employed as a useful approximation in Gaussian plume theory). There is no evidence that the concentration profile is $\exp(-z^{1+\alpha})$ where $\alpha$ is the power law exponent in the mean velocity profile.

The model uses observations from the field and laboratory to justify the vertical concentration profile of the form $\exp(-z)$ when the puff or plume is exhibiting dense gas effects.

## 7.9 Averaging time

An averaging time option is available for plumes and this accounts for meander. This has a minimum default value, to be consistent with puff dispersion parameters.

The use of smaller averaging times is not justified for determining 'peak' puff or plume concentrations. A separate concentration fluctuation model is required for this.

## 7.10 Current model limitations

The general philosophy behind the modelling has been to ensure that the model is physically correct and as simple (transparent) as possible. Certain physical effects have not been included where it is felt that their inclusion produces a vastly more complicated model with no commensurate improvement in model performance. We believe that it is essential for there to be strong experimental evidence that demands a change to the model before any alteration is considered.

Listed below are some known limitations/uncertainties of the current model:

- Along-wind shear dispersion has been included for instantaneous releases but not for the time varying releases.
- The vertical concentration profiles will change with cloud stability, being nearly top-hat when $Ri_*$ is large and the buoyancy driven flows are larger than the ambient flows, with a negative experimental coefficient of 1.5 when $Ri_*$ is of order unity or less and with a negative experimental coefficient of 1.0 over the extensive range of $Ri_*$. The current model only allows for a value of unity. This could be changed if enough evidence is available that this is necessary.
- The near-source description in this model for very negatively buoyant releases is

thought to be more correctly based than in other models, however, this complicated region may require more attention. There is, in fact, very limited experimental data available on which to base a more sophisticated model of this region.

- The influence of surface roughness and atmospheric stability on the dispersion code enters, essentially, through the effect on $u_*$. There is little evidence available to confirm or negate this approach.

# 7.11 Source input algorithms

## 7.11.1 Instantaneous release

The instantaneous source is modelled as a right-cylinder with user-specified dimensions. Two options are available:

1. in which the cloud and ambient momentum are well-mixed, such as might result from a catastrophic release and subsequent cloud expansion and mixing. This cloud adopts the ambient velocity from the initiation time.

2. in which the cloud and ambient momentum are not well-mixed, such as might result from idealised laboratory or field tests e.g. Thorney Island. In this case cloud acceleration results solely from subsequent mixing between the cloud and the ambient fluid.

## 7.11.2 Continuous release with no significant momentum

It is observed in experiments in the laboratory and field that a continuous plume may travel upwind from the source and can be far wider at the source position than the physical dimension of the source. This has been interpreted as the formation of a vapour blanket over the physical source.

The continuous release source module provides plume widths and heights at the source position in terms of ambient conditions, the plume density and release rate and the physical size of the source region. If the release rate is small and the source dimension large there will be dilution of the plume at the source position. If this is the case the effective source density and concentration will be less than that from the source.

The algorithms used here address the *detrainment* of the source material by the ambient flow, a balance being met when the effective source is large enough to allow complete detrainment of source volume flux, $q_0$. Note that this is not an entrainment problem and thus the use of the entrainment relationships is not valid. Some conventional codes use such entrainment relationships and then utilise the experiments of Britter (1980) on near-source dimensions of dense gas clouds to calibrate an uptake model. A simplified version of such a calibrated model, appeal to the original experiments, appeal to the correlation provided by Britter (1980) and analysis based on detrainment due to a buoyancy limited Kelvin-Helmholtz instability all suggest that the plume depth above any gas blanket and just downstream of the source will scale on $u_*^2/g_0'$ with a coefficient of about 100.

From experience we use a plume depth of $200\,u_*^2/g_0'$ but apply a minimum restriction of 0.20 m based on pragmatic, physical grounds. We had considered setting this minimum as some multiple of the surface roughness length $z_0$ but found no evidence that this would be preferable.

The width of the source, $w$, is determined from

(7.31) $$q_0 = wh_{\text{out}}U(z = 0.56h_{\text{out}})$$

where $q_0$ is the continuous volume release rate.

If the source width so calculated is smaller than the physical source width, obviously the more appropriate physical source width is selected.

There must be an upper limit on the plume height at the source input to the dispersion model as the density difference becomes small ie. $u_*^2/g_0'$ increases without limit. The passive limit will be an upper limit and will, approximately, have a linear plume growth over the downstream distance of the physical source size or, possibly, over the vapour blanket. We use, as an upper limit of the plume thickness to input to the dispersion model, $0.05D$ where $D$ is the along-wind dimension of either the physical source or the vapour blanket if one exists, the along-wind dimension being equated to the cross-wind dimension in the current version.

Under these circumstances, such as the dispersion from a large pool of evaporating petrol, the initial concentration of the plume will be less than the concentration from the source.

Finally, we note that a difficulty can arise when the release is near passive (thus not allowing any significant vapour blanket formation) but with a large vapour flux. Under these circumstances the plume depth $H$ is determined solely by the kinematic mass conservation requirements that

(7.32) $$\dot{m}_{\text{src}} = DHU(z = 0.56H)$$

where $D$ is the width of the physical source.

### 7.11.3 Continuous release alternative

This source allows completely user-specified initial width for input to the continuous release code. This option is applicable if, for example, the releases scenario imposes externally a specific dimension on the plume at the source position.

## 7.12 Uptake model

A continuous release, starting from time $t = 0$ will take some time to establish steady-state near source conditions. Initially, due to the small source width, only a fraction of released material is taken up by the ambient flow and carried downstream to form a plume. The remaining fraction will spread radially as a "vapour blanket"; eventually the blanket width is adequate to allow all the released material to be taken up by the ambient flow and advected downstream, corresponding to steady state conditions.

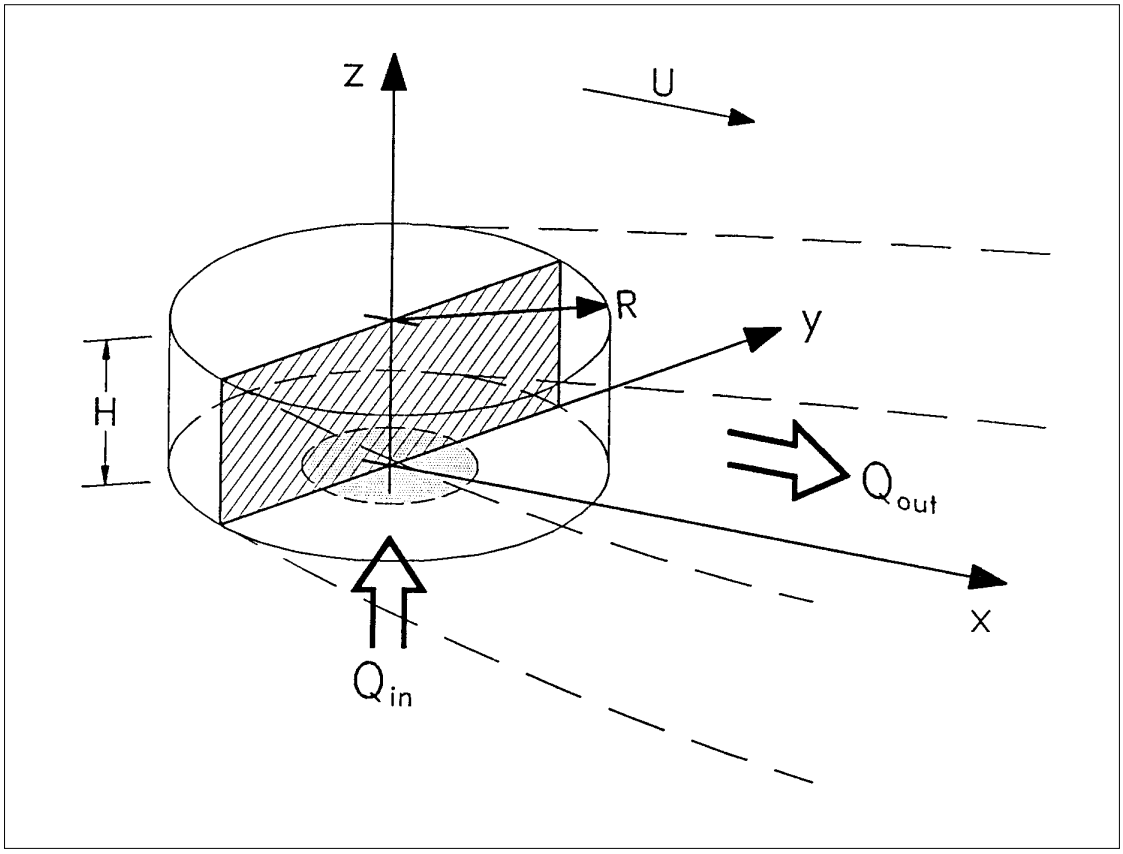



**Figure 7.7** – Uptake of material and cloud development over a liquid pool.

The vapour blanket is modelled as a radially growing cloud following the general approach of Britter (1979). The height $H$, and radius $R$ of the vapour blanket are determined by the conservation expression

$$\frac{d}{dt}(\pi R^2 H) = Q_{\text{in}} - Q_{\text{out}}, \tag{7.33}$$

where $Q_{\text{in}}$ and $Q_{\text{out}}$ are the volume fluxes of the released material from the source and advected downstream by the ambient wind, respectively, and an equation for the leading edge motion

$$\frac{dR}{dt} = C_{\text{E}}(g'H)^{1/2}, \tag{7.34}$$

which is consistent with the formulation of the instantaneous release algorithms. The calculation is normally commenced with an initial radius reflecting the area of the physical source, although GASTAR users can choose any initial radius. The radial growth is stopped whenever $Q_{\text{in}}$ equals or falls below $Q_{\text{out}}$.

The volume flux out of the vapour blanket follows the argument in Section 7.11.2 where

(7.35) $$h_{\text{out}} = \frac{200u_*^2}{g_0'}$$

and

(7.36) $$Q_{\text{out}} = 2Rh_{\text{out}}U(z = 0.56h_{\text{out}}).$$

The width of the source is taken to be $W = 2R$.

As outlined in Section 7.11.2, a vapour blanket need not exist if the physical source size is large or the mass release rate at the source is small e.g. the evaporation from a large pool of petrol. Thus, at time $t = 0$, the calculated $Q_{\text{out}}$ is larger than $Q_{\text{in}}$. Under these conditions, the source flow rate must be $Q_{\text{in}}$ and the source width must be the physical source width. Also, the plume depth is the smaller of $200\,u_*^2/g_0'$ and $0.05D$. It will be apparent that the initial plume concentration will then be smaller than the source concentration as expected. These calculations are performed by GASTAR.

In general, output of the model provides the source width, source flow rate, density and concentration as a function of time. This output is segmented and automatically placed into the main GASTAR interface for subsequent running of the time varying release code.

For a release of constant mass flux starting at time $t = 0$, and stopping at a much later time, the mass flux in the plume and the width of the plume at the source will grow to their steady state values and, after the release stops, these values are maintained as the vapour blanket is removed and $H$ decreases to zero.

For a release in which the mass flux increases with time the plume mass flux and source width will increase monotonically with time to a maximum when $Q_{\text{out}}$ becomes equal to $Q_{\text{in}}$. Thereafter the width is maintained until the vapour blanket is removed. After that, $Q_{\text{out}}$ is set equal to $Q_{\text{in}}$ and the steady state relationships are used to determine the plume width at the source.

# 7.13 Jet model

The jet model is a conventional integral jet model which broadly follows the approach used in Cleaver and Edwards (1990) with extensions e.g. from a single-phase two-dimensional model to a single or two-phase three-dimensional model. The model assumes that the jet is at atmospheric pressure and, consequently, high pressure releases require a separate release model to reduce under-expanded jets down to atmospheric pressure.

The model is applicable to single and two-phase (aerosol) jets released at any direction to the ambient wind. The equations are written in terms of the mass, momentum and enthalpy fluxes of the jet.

The jet centreline trajectory is written in natural coordinates $(s, \theta, \phi)$ where $s$ is the distance along the trajectory. The ambient wind is along the $x$ axis with $(x, y, z)$ forming a right-handed system. Thus $\theta = 90°$, $\phi = 0°$ is the $y$ axis and $\phi = 90°$ is the $z$ axis.

The jet is given a similarity shape which is circular while not in contact with the underlying surface. Thus the jet has radius $R_j$, velocity (actually speed along the $s$ coordinate) $u$ and density $\rho$ which is different to the ambient density of $\rho_a$. The ambient density and ambient temperature, $T_a$, in the model are assumed constant and independent of height.

## 7.13.1 Fundamental equations

The scalar mass flux in the jet is

(7.37) $$\dot{m} = \pi R_j^2 u \rho,$$

the vector momentum flux is

(7.38) $$\underline{M} = \dot{m}\underline{u} = \left(M_x, M_y, M_z\right),$$

and the scalar enthalpy flux is

(7.39) $$H = \dot{m}h,$$

where $h$ is the specific enthalpy of the jet material.

The fundamental differential equations are

(7.40) $$\frac{d\dot{m}}{ds} = E,$$

where $E$ is referred to as the mass entrainment rate,

(7.41) $$\frac{dM_x}{ds} = EU(z),$$

(7.42) $$\frac{dM_y}{ds} = 0,$$

(7.43) $$\frac{dM_z}{ds} = g(\rho - \rho_a)\pi R_j^2,$$

(7.44) $$\frac{dx}{ds} = \cos\phi\,\cos\theta,$$

(7.45) $$\frac{dy}{ds} = \cos\phi\,\sin\theta$$

and

(7.46) $$\frac{dZ}{ds} = \sin\phi.$$

Similarly, if $M$ denotes the magnitude of the momentum flux then the momentum components are

(7.47) $$M_x = M\,\cos\phi\,\cos\theta,$$

(7.48) $$M_y = M\,\cos\phi\,\sin\theta,$$

and

(7.49) $$M_z = M\,\sin\phi.$$

Two further equations are those for enthalpy flux

(7.50) $$\frac{d}{ds}\dot{m}h = Eh_\infty,$$

and species concentration, $C$

(7.51) $$\frac{d}{ds}\dot{m}C = EC_\infty,$$

where $h_\infty$ and $C_\infty$ refer to ambient enthalpy flux and species concentration respectively

To simplify the calculations the enthalpy is referenced to the ambient enthalpy, and so $h_\infty = 0$. Similarly, the species concentration in the ambient air is taken as zero. Thus, the equations simplify to

(7.52) $$\frac{d}{ds}\dot{m}h = 0,$$

and

(7.53) $$\frac{d}{ds}\dot{m}C = 0,$$

The mass flux consists of released material and air, with mass fractions of $m_f$ and $(1 - m_f)$ respectively. The released material may be in gaseous or liquid (aerosol) forms with mass fractions $(m_f - a_f)$ and $a_f$ respectively.

The specific enthalpy of the cloud at temperature $T$ (K) is then

(7.54) $$h = C_{pa}(T - T_a)(1 - m_f) + C_{pg}(T - T_a)(m_f)$$

if there is complete evaporation, or

(7.55) $$h = C_{pa}(T - T_a)\left(1 - m_f\right) + C_{pg}(T - T_a)\left(m_f - a_f\right) + \cdots$$
$$\ldots C_{pl}(T - T_{BP})\left(a_f\right) + C_{pg}(T_{BP} - T_a)\left(a_f\right) - H_{lg}\left(a_f\right)$$

otherwise. Here, $T_{BP}$ is the boiling point (K) of the released material, $T_a$ is the air temperature (K), $C_{pg}$ is the specific heat capacity (kJ/K.kg) of the material vapour, $C_{pa}$ is the specific heat capacity (kJ/K.kg) of the air, $C_{pl}$ is the specific heat capacity (kJ/K.kg) of the material liquid and $H_{lg}$ is the heat of vaporisation (kJ/kg) of the released material. In particular, at release there is no ambient air and the specific enthalpy at the source is given by

(7.56) $$h = C_{pg}(T_0 - T_a)\left(1 - a_f\right) + C_{pl}(T_0 - T_{BP})\left(a_f\right) + \cdots$$
$$\ldots C_{pg}(T_{BP} - T_a)\left(a_f\right) - H_{lg}\left(a_f\right)$$

The crucial empirical input to integral jet models is the parameterisation of the entrainment. This is typically represented in terms of a product of an entraining area/unit jet length (i.e. $2\pi R_j$), the ambient air density and an entrainment velocity. There are three different contributions to the entrainment velocity. The first relates to an entrainment due to the differing velocities in the along-jet direction ($s$) between the jet and the environment, i.e.

(7.57) $$\alpha_1 |u^2 - (U_a \cos\phi\, \cos\theta)^2|^{1/2}.$$

The value of the coefficient $\alpha_1$ is taken to be 0.07 (Cleaver & Edwards, 1990).

The second term relates to the velocity of the ambient wind normal to the jet trajectory

(7.58) $$\alpha_2 U_a (\sin^2\theta + \sin^2\phi\, \cos^2\theta)^{1/2}.$$

The value of the coefficient $\alpha_2$ is taken to be 0.7 (Cleaver & Edwards, 1990).

Two factors are introduced to reduce the entrainment close to the source. A factor $f_1$ given by

(7.59) $$f_1 = \min\left(1, \frac{U_0}{3.7U}\right)$$

is incorporated into the first entrainment velocity term (equation (7.57)) to account, in part, for a region of flow establishment. The second entrainment velocity term (equation (7.58)) will not be significant when the jet momentum is dominant, and so a factor

(7.60) $$f_2 = \min\left(1, \max\left(0, \frac{s/L - 0.4}{0.6}\right)\right)$$

is introduced. In the equation, $L$ is a length scale over which momentum is dominant, i.e.

(7.61) $$L = D\left(\frac{\rho_0 U_0^2}{\rho_a U_a^2}\right),$$

where $D$ is the source diameter and the subscript '0' refers to source conditions. Finally,

both entrainment velocity terms are multiplied by a factor $(\rho/\rho_a)^{1/2}$ to reflect increased entrainment due to dynamic rather than solely kinematic effects.

The third entrainment term accounts for the effect of ambient turbulence and this will be more significant as the influences of momentum and buoyancy decline away from the source. The intent is to smoothly link the model into the conventional ambient turbulence dispersion curves by Briggs (1973). Rather than switch from an active to a passive description with the attendant difficulties of the selection of a transition criterion, we have differentiated the Briggs curves and introduced the differential curves into the entrainment formulation. This requires a third entrainment term of the form

(7.62) $$4\pi\rho_a \frac{d(\sigma_y\sigma_z)}{dx} U_a(z=10).$$

### 7.13.2 Interaction with the ground

When the jet reaches the ground the $z$ momentum is turned off, and the cross-sectional shape is changed from circular to semi-circular but maintaining the jet area. The jet 'touchdown' occurs when the centroid height reaches $R_j/2$. The code also calculates when both the jet edge (i.e. the radial edge) and the centroid intersect the ground.

After the jet reaches the ground it may still develop in the horizontal plane subject to the ambient wind. However, as the jet axis (but not the centroid) is now on the ground, the velocity of the entrained ambient fluid is taken to be at a fraction of the jet radius, namely

(7.63) $$z_e = 0.56R_j.$$

### 7.13.3 Transition to the dense gas model

The jet model calculation is halted when the jet velocity reduces to some predetermined level and the jet has attained the touchdown criterion.

The jet velocity must asymptote towards the ambient velocity, so the criterion for transition must be in terms of $(u - U_a)$ and this should be referenced to buoyancy-generated velocities, which will scale on $\left(g'R_j\right)^{1/2}$. We use, as an indicator of transition, the criterion

(7.64) $$(u - U_a) = \frac{1}{2}\left[g'\left(\frac{\pi R_j^2}{4}\right)^{1/2}\right]^{1/2}.$$

At this point, transition to the dense gas model occurs with an initial width of

(7.65) $$2\left(\frac{\pi R_j^2}{4}\right)^{1/2}$$

and a height determined by a mass balance calculation in the usual manner for plumes.

### 7.13.4 Positively buoyant jets

The model can address the problem of a positively buoyant jet although the development is based solely on the vertical buoyancy force giving rise to an increasing vertical momentum and consequent jet rise.

### 7.13.5 Underexpanded jets

High pressure gaseous releases can lead to underexpanded jets in which the pressure at the release exit is in excess of the ambient pressure. For perfect gases this is the case when the upstream (stagnation) pressure, $P_0$, is greater than

(7.66) $$\left(\frac{\gamma+1}{2}\right)^{\frac{\gamma}{\gamma-1}} P_a,$$

where $\gamma$ is the ratio of specific heat at constant volume to the specific heat at constant pressure, $C_v/C_p$. Under these conditions the exit pressure will be

(7.67) $$P_e = \left(\frac{2}{\gamma+1}\right)^{\frac{\gamma}{\gamma-1}} P_0$$

However, the jet model, like most integral jet models, is based on ambient pressure throughout. The underexpanded jet undergoes various shocks and expansions close to the release to drop the jet pressure to ambient pressure. During this process the momentum flux of the jet increases. The momentum flux of the jet is the *dominant* parameter describing the development and dilution of a jet. Thus, the correct momentum flux must be determined (Britter 1994, 1995b).

Although the complex processes close to the source will also involve entrainment of ambient air, it is convenient to keep these processes distinct.

For a release with pressure $P_e$, density $\rho_e$, velocity $U_e$ and area $A_e$, the appropriate input condition to a jet model is one with a velocity of

(7.68) $$U = U_e + \frac{A_e}{\dot{m}}(P_e - P_a)$$

where $\dot{m} = \rho_e A_e U_e$ and $P_a$ is the atmospheric pressure, i.e.

(7.69) $$U = \frac{\dot{m}}{\rho_e A_e} + \frac{A_e}{\dot{m}}(P_e - P_a).$$

The appropriate input area is determined from $\dot{m}$, $U$ and the appropriate density. The density may be obtained from the jet temperature, which in turn may be determined by application of the enthalpy equation.

### 7.13.6 Flashing releases

Pressurised liquids which flash upon release to the atmosphere require calculation of the flash fraction i.e. the proportion of the release changing to gas; the remaining material is assumed to be suspended aerosol. No allowance for rainout is made.

The correlation used for the aerosol (or "flash") fraction is

$$\text{Aerosol Fraction} = 1 - \left(C_{pl}\frac{T_{\text{storage}} - T_{BP}}{H_{LG}}\right). \tag{7.70}$$

where $T_{\text{storage}}$ is the storage temperature of the liquid, $T_{BP}$ is the boiling point of the released material, $H_{LG}$ is the specific heat of vaporisation of the released material and $C_{pl}$ is the specific heat capacity of the released liquid.

Obviously, a rainout allowance may be introduced manually following the flash fraction calculation and prior to running the jet model. The previous comments on determination of the correct momentum flux to input into the jet model also apply here. Frequently the exit pressure for flashing releases is the saturation pressure of the material at the storage (stagnation) temperature. The excess above ambient pressure will also lead to an increase in the jet momentum.

# 7.14 Obstacles

The arguments and algorithms below are based on work in Britter (1982), Britter and McQuaid (1988), Britter (1989a), Britter (1989b), Britter, Cleaver and Cooper (1991) and Brighton *et al.* (1993). Some of the original algorithms developed by Britter were implemented in GASTAR version 2.24. They have been extended (particularly with appropriate interpolation formulae), implemented within a dense gas model and compared favourably with experiments by Cleaver *et al.* (1995). The interpolated algorithms have been incorporated into GASTAR since version 3.0.

## 7.14.1 Releases near individual obstacles

Denser-than-air clouds may be significantly affected by the interaction of the cloud with solid (or porous) obstacles such as buildings, tanks or pipe arrays or the source structure itself.

Our approach is to consider a small number of relevant and commonly occurring situations and to seek to provide models for those cases. Within the spirit of integral models we look for algorithms that will reflect the influence of obstacles on advection (speed and direction), dilution and, for time varying or instantaneous releases, the fluid 'hold-up' near the obstacle.

Studies by Britter (1982), König (1987) and Britter (1989b) provide a basis for algorithm development. In addition, there are many studies, both field and laboratory, which can be used for model assessment. Most of the available experiments have been reviewed by Brighton *et al.* (1993).

The model algorithms are not intended to describe complex flow processes near an obstacle but to quantify the net change in cloud features as the cloud interacts with the obstacle, thereby providing a step adjustment to the cloud variables at the obstacle position. This may be used to estimate the concentrations of the cloud approaching the front face or leaving the rear face of the obstacle, although care would be required in assessing the concentrations in the immediate neighbourhood of the obstacle.

There are three types of obstacle that can be modelled in the current version of GASTAR:

- Two-dimensional fence, at any angle to the ambient flow;
- Rectangular building, solid or porous, at any angle to the ambient flow;
- Circular building, solid or porous.

For the case of a two-dimensional fence normal to the flow, the relevant dimensionless parameters are

(7.71) $$\frac{U^2}{g'h}$$

in the absence of the fence, and

(7.72) $$\frac{h}{H}$$

otherwise, where $H$ is the fence height, $U$ is the cloud advection speed, $h$ is the height of the cloud centroid and $g'$ is the reduced gravity.

The reduced gravity is defined as

$$g' = g\left(\frac{\rho_m}{\rho_a} - 1\right), \tag{7.73}$$

where $\rho_m$ is the maximum ground-level density within the cloud and $\rho_a$ is the density of the ambient air. Observations from Britter (1989b), based on continuous plume experiments, indicate that the effect of the fence is to widen the plume upstream of the fence and to dilute the plume in the lee. Britter argued that the ratio of plume width with a fence, $w_f$, to that without the fence, $w_{nf}$, was such that

$$\frac{w_f}{w_{nf}} = f\left(\frac{U^2}{g'h}, \frac{h}{H}\right). \tag{7.74}$$

An empirical fit[1] to the data which is currently used is

$$\frac{w_f}{w_{nf}} - 1 = (1)\left[\frac{H}{h}\right]\left[\frac{g'h}{U^2}\right]^{1/3}. \tag{7.75}$$

The dilution in the lee of the fence is such that the bulk plume concentration can be expressed as

$$C = (1)\frac{C_0 q_0}{U(z=\beta H) H w_f}, \tag{7.76}$$

where $C_0 q_0$ is the mass flux of pollutant at the source and $U(z = \beta H)$ is the plume advection velocity, i.e. the ambient velocity at a specified fraction $\beta$ of the plume height.

The change in variables from Britter (1989b) to those used here produces coefficients whose values are near unity. Given further data, it is possible that more precise values could be assigned to these coefficients and improved algorithms could be developed. In the absence of this definitive data coefficients of unity have been used.

In addition, the following constraints are imposed on the solution:

- the cloud depth cannot be decreased by the fence;
- the cloud concentration cannot be increased by the fence.

The same approach can be applied to instantaneous releases (puffs), with the same correlation for increased puff width and the puff depth being determined in a consistent manner.

### 7.14.2 Hold up

Hold up of material in the front and in the lee of the fence will occur due to altered advection velocities and the recirculating flow in the regions of flow separation. The regions of flow separation will appear as an effective longitudinal diffusion. The work

[1] The curve fit given here is a corrected version of that appearing in Britter (1989b).

of Vincent (1979) suggests that the retention of material in wakes can be modelled as an effective longitudinal diffusion $\sigma_x$ of about $10H$.

The altered advection velocity will appear as a net time delay as the cloud is slowed ahead of the fence and accelerated over it. There has been the "drift" function introduced by Lighthill (1956). The time delay must be proportional to $H/U$ and depend upon $h/H$ in the absence of buoyancy effects. Currently, our model includes an empirical description of this time delay function that is independent of buoyancy effects.

Thus, the model includes algorithms for:

- cloud widening
- cloud dilution
- cloud hold-up, i.e. longitudinal diffusion, and
- cloud time delay

These algorithms are based on an appropriate description of the physical phenomena involved and semi-empirical or empirical quantification.

Turning now to the case of an individual building, the same type of arguments can be applied when seeking to model the cloud widening, cloud dilution etc.

The plume width downstream of an obstacle of width[1] $W$ is taken to be the larger of

- the obstacle width and
- the plume width in the absence of the obstacle plus half the obstacle width.

These rules have the pragmatically correct limits i.e.

- if the plume is much wider than the obstacle there is relatively little effect on the plume width.
- if the plume is much narrower than the obstacle then the plume width becomes equal to the obstacle width.
- If the plume width is equal to the obstacle width then the plume width is increased by some fraction of the obstacle width (here taken as half). This uncomplicated algorithm should cover situations when the plume and obstacle are co-linear and when their overlap is only slight; alternatively, the algorithm has spread any error across the possible scenarios.

Britter (1982) argued that the turbulent kinetic energy created in the lee of an obstacle was able to raise the potential energy of the dense gas plume by an amount that could be characterised by a height increase $\Delta h$, proportional to

$$C_D \frac{U^2}{g'h} H, \tag{7.77}$$

The coefficient of proportionality $C_D$ is typically of order 0.1 and this value has been

[1] The width $W$ is actually the effective width in a direction normal to plume trajectory.

used in the model.

Of course, the increased height should not lead to a cloud height greatly in excess of the obstacle height $H$; the limit chosen in the model is $H$.

The increased depth only occurs over the region in which the plume interacts with the obstacle; however consistent with the use of an integral model, the increased height is spread (averaged) over the complete plume width.

### 7.14.3 Model implementation

Cleaver *et al.* (1995) have combined the algorithms for fences and buildings into a common algorithm.

A fence (normal to the flow direction) has unlimited width and a height $H$ while a building has a width $W$ and height $H$.

Three cases are considered:

| | |
|---|---|
| $h \leq H$ | a strong interaction regime, |
| $H < h < 3H$ | an intermediate regime, |
| $h \geq 3H$ | a no-interaction regime, |

where $h$ is the cloud depth prior to obstacle.

The model requires a conversion of the cloud dimensions $w$, $h$ prior to the obstacle to $w'$, $h'$ following the obstacle. These, together with the standard advection velocity formulation[1], will determine the cloud concentration.

#### *Strong interaction regime*

In the first of these three cases the cloud width is given by:

$$w' = \min\left(w_f', w_b'\right), \tag{7.78}$$

where $w_f'$ is the width after implementing the fence algorithm and $w_b'$ is the width after implementing the building algorithm.

The new width due to a fence is found from

$$\frac{w_f'}{w} - 1 = \frac{H}{h} Ri^{1/3}, \tag{7.79}$$

where $w$ is the width of the cloud before the interaction and $Ri$, the Richardson number, is defined by

[1] That is, the advection velocities determined from the ambient velocity at a fixed fraction of the cloud depth (together with any slope induced velocity).

(7.80) $$Ri = \frac{g'h}{U^2},$$

where $U$ is the advection velocity prior to the interaction (c.f. $Ri_*$ based on the friction velocity $u_*$).

The new width due to a building is found from

(7.81) $$w_b' = \max(W, w + 0.5W),$$

These results are applied to instantaneous, continuous and time varying releases. For the instantaneous release, $W$ is replaced by $D$, the puff diameter.

The height conversion is given by

(7.82) $$h_b = \max(h_0', h),$$

where

(7.83) $$h_0' = \left(\frac{w}{w'}\right)^n h + R_{\text{overlap}} dh.$$

The 'overlap' parameter, $R_{\text{overlap}}$, is given by

(7.84) $$\frac{w_1'}{w'}$$

for the continuous and time varying cases where $w_1'$, is the length of the overlap region and by

(7.85) $$\frac{A_1'}{(\pi/4)w'^2}$$

for instantaneous releases, where $A_1'$ is the overlap area.

The first term just spreads the upstream cloud depth over the new cloud width. The exponent $n$ is unity for continuous and time varying releases and two for instantaneous releases. The height rise $dh$ is given by a mixture of expressions for fences and buildings: the expression for a fence is

(7.86) $$dh_f = H - h\left(\frac{w}{w'}\right)^n$$

and that for a building is

(7.87) $$dh_b = \min\left(\frac{0.1H}{Ri}, H - h\left(\frac{w}{w'}\right)^n, 5h\right)$$

so that

(7.88) $$dh = F\, dh_f + (1 - F) dh_b,$$

where $F$ is a factor used to combine the two results:

- When $w_f' > 2w_b'$, the interaction will be that for a building, in that the cloud can

go around as well as over the building. Thus $F = 0$.

- When $w_f' < w_b'/2$, the building will look more like a fence and the cloud must go over the building. Thus $F = 1$.

Between the cases an interpolation is used, namely

(7.89) $$F = \frac{1}{2} + \frac{3}{2}\left(\frac{w_b' - w_f'}{w_b' + w_f'}\right).$$

***Intermediate regime***

For the intermediate region an interpolation is provided between the interaction when $h = H$ and the no-interaction case when $h = 3H$ using an interpolation parameter

(7.90) $$G = \frac{3H - h}{2H},$$

which runs from unity to zero as the cloud depth increases from $H$ to $3H$.

The cloud width conversion is

(7.91) $$w' = G w_H' + (1 - G) w,$$

where $w_H'$ is calculated as before in equation (7.78), but with $h = H$.

The cloud height conversion is

(7.92) $$dh' = G\, dh_H,$$

where $dh_H$ is calculated as before in equation (7.82), but with $h = H$.

The previous calculation in cloud height increase has not taken into account that in some scenarios the cloud after the obstacle can extend beyond the obstacle; however only the cloud in the lee of the obstacle can be diluted by the lee turbulence. Again, consistent with the integral model formulation being developed, this increase is spread (averaged) over the complete cloud. This is handled by the parameter $R_{\text{overlap}}$.

### 7.14.4 Releases near individual obstacles

Another scenario for which current models are not directly applicable is an accidental release into a complex array of obstacles occurring on site.

Brighton *et al.* (1993) in his review notes "Although some other data exists on dispersion on models of industrial sites it seems clear that arrays of roughness elements are the type of obstacle most in need of investigation both into passive flow and dispersion characteristics and into heavy-gas effects".

Our objective is to develop and validate a set of algorithms within the context of integral modelling that allow for dispersion through such an obstacle array. It is our intention to treat any site in a broad statistical manner in the first instance, rather than with a detailed description of its individual component elements on the site.

As before we address the effects of the obstacle arrays on

- advection
- horizontal spreading due to buoyancy
- dilution of the plume, and
- plume hold-up, which is particularly important for transient releases.

We have examined the available experimental data summarised in Brighton *et al.* (1993) and the further data given in Petersen and Ratcliff (1989). We conclude that

1. There is support for the view that an industrial site may be modelled as an equivalent uniform roughness. Care must be taken to ensure that no isolated large structures require separate treatment. It should be noted that within this approach the accuracy of the predictions of the model are limited to scales which are larger than those of the isolated structures.

2. For homogeneous arrays there is evidence that the advection velocity should be treated in the same manner as for smooth or small roughness surfaces i.e. dependent upon the plume depth. The most appropriate velocity profile within the roughness array is, however, still uncertain.

3. The presence of many distributed obstacles has two effects on the cloud. The obstacles lead to an increase in the turbulence levels in the flow and this by itself will tend to increase horizontal diffusion of the cloud. This can be parameterised by an increased value of the ground friction velocity, $u_*$. However, as Linden and Simpson (1988) have shown, increased turbulence levels may also break down the organised frontal motions associated with the gravitational spreading and hence lead to reduced cloud widths.

4. The influence of the surface roughness on vertical entrainment is still uncertain. However, it appears that conventional entrainment correlations may be used without serious loss of accuracy.

5. The evidence in Melia and Britter (1990) suggests that the retention time of dense gas plumes in the wakes of individual roughness elements might best be modelled by the incorporation of a longitudinal diffusion, with $\sigma_x \propto u_* t$ where $t$ is the travel time within the array.

A model based on these arguments has been developed and does reproduce the existing data base satisfactorily. For example, it accommodates the effect of turbulence on gravity spreading by reducing the buoyancy-spreading velocity asymptotically to zero as $g'h/u_*^2$ approaches a critical value. We have extended this approach, with the same consistent critical value, from cases where the plume is larger than the obstacles to cases where the plume may be smaller than the obstacles. More definitive data is required to confirm the correctness of this extension. The model is unable to predict the detail of the concentration distribution within the congested region. That is, the lower limit on the spatial resolution is of the same order as the largest obstacles within the obstructed area.

### 7.14.5 Further effects

#### *Fence at angle to the ambient wind*

For a fence at an angle to the ambient wind we note that, as far as turbulence generation by the fence is concerned, the length of the fence interacting with the cloud increases but the ambient velocity normal to the fence decreases. These two opposing (though not exactly equal) effects suggest that in the case of an oblique fence the model should just consider the fence as being effectively normal to the wind. Arguments can also be presented for mechanisms to increase or decrease the cloud width caused by the fence as the angle changes. In the absence of definitive information, it is assumed that the "effectively normal" fence is adequate, this also being consistent with the treatment of buildings.

#### *Fence or building solidity*

There is obviously an interest in modelling porous structures e.g. pipe racks, forests etc. This is initially approached by noting that some of the correlations for cloud depth increase are implicitly based on an assumed drag coefficient of unity. Consequently, we consider solidity in terms of the drag coefficient. We expect that decreased solidity will inhibit both the width and height increases.

The simple approach we have adopted is to include the solidity $S$ in the following algorithms (cf. equations (7.79), (7.81), (7.86) and (7.87)):

(7.93) $$\frac{w_f'}{w} - 1 = S\frac{H}{h}Ri^{1/3},$$

(7.94) $$w_b' = \max(WS, w + 0.5WS),$$

(7.95) $$dh_f = \left[H - h\left(\frac{w}{w'}\right)^n\right]S,$$

(7.96) $$dh_b = \min\left(\frac{0.1H}{Ri}S, \left[H - h\left(\frac{w}{w'}\right)^n\right]S, 5h\right).$$

#### *Multiple Fences and Buildings*

The code allows for multiple fences and buildings of arbitrary orientation. If the buildings and fences are in close proximity their diluting effects will not be additive. Consequently, buildings within $2H$ of a given building will be completely or partially discounted depending upon the extent of overlap in the direction of the cloud trajectory. The proximity distance $2H$ was selected as representative of the extent of the recirculation region for three-dimensional, surface mounted obstacles.

#### *Buildings upwind of the source*

Sources that are within the recirculating region downstream of an obstacle will be influenced significantly by the obstacle. Initially quite complex algorithms were considered in order to allow for this scenario. However, after some experience a simpler alternative has been adopted, namely for any building within $2H$ upwind of the source the standard obstacle interaction calculation is performed.

### *Time and Position Steps*

For computational reasons the new solution downstream of the obstacle is started at a position $H/10$ downstream.

There will be a hold up of the cloud as it encounters the obstacle. This time delay is modelled with

(7.97) $$\Delta t = S\frac{H}{U_a}\min\left(1, \frac{w_1}{w'}\right).$$

### *Passive or Near-Passive Releases*

There will obviously be a temptation to use this modelling approach for passive or near-passive releases and it would be attractive if this were possible. The only significant difficulty is that for passive releases the box model plume or puff will not grow in the non-vertical directions, the influence of the ambient turbulence being incorporated later through $\sigma$, a measure of cloud spread. Thus, the occurrence of any interactions may be underestimated with the present approach. The least disruptive way to deal with such cases is to check for any interaction using the effective or total cloud extent. For a puff, this would mean replacing the diameter, $D$, by $2R_{\text{tot}}$ where

(7.98) $$R_{\text{tot}} = R(1 + 3\sigma^2/R^2).$$

For a plume, the width, $w$, would be replaced by $w_{\text{tot}}$, where

(7.99) $$w_{\text{tot}} = \frac{w}{2}\left[1 + \frac{3\sigma^2}{(w/2)^2}\right].$$

In order to conserve mass, the reduced gravity term must also be replaced. Thus, for puffs we use

(7.100) $$g'_{\text{tot}} = g'(1 + 3\sigma^2/R^2)^{-1}$$

and for plumes

(7.101) $$g'_{\text{tot}} = g'\left(1 + \frac{3\sigma^2}{(W/2)^2}\right)^{-1}.$$

If an interaction does occur the previous algorithms are used.

### *Blocking*

A difficulty may arise with the combined slopes and obstacles code with scenarios in which the ambient wind is zero or much smaller than slope driven velocities. The kinetic energy in the cloud itself may be considerably less than that in the atmospheric wind. This is obvious when considering a solely slope driven flow encountering a fence: whereas an ambient wind driven flow will eventually surmount the fence a slope driven flow may just pool in front of the fence. A satisfactory treatment of this scenario is still under development.

## 7.15 Slopes

Variations in the elevation of the underlying surface will influence the buoyancy driven motion of the dense gas. Topography, whether in the form of a general slope, isolated hills or more complex terrain, will alter or divert the cloud or plume. The topography may enhance plume dilution and divert the plume away from regions of elevated terrain. Alternatively, the dense plume may be channelled into valleys or low-lying areas and then be protected from the diluting influence of the ambient flow. There is extensive treatment of the interaction of topography with buoyancy influenced flows in the geophysical literature, but little use has been made of this information source.

Topographic features that are small compared with the size of the release may be considered in much the same way as buildings or structures but without any substantial flow separation unless the topography is very abrupt.

When the topographic feature is large compared with the scale of the release, the topography reduces to the local slope. Somewhat surprisingly, the downslope velocity of a dense fluid released on a slope under calm conditions is not a strong function of the slope. Hopfinger (1983) summarises results of instantaneous, continuous and starting two-dimensional flows and finds that the flow has velocities such that $U/(g'h)^{1/2}$ is typically between 1 and 2 for slopes between $0^o$ and $90^o$. Larger slopes lead to increased entrainment and dilution, with the entrained fluid acting as an effective drag on the downslope flow.

Little information is available concerning three dimensional flows under calm conditions. Unlike two dimensional flows, the release is able to spread across the slope, and the Reynolds number of the flow, based on the flow depth, may increase with distance from the source (Fietz & Wood 1967). As a consequence, these flows in the laboratory are frequently influenced by viscosity, which reduces the downslope velocity, the width and the dilution. Picknett (1981) found that instantaneous releases under non-calm conditions on a slope of 1/13 were influenced by the slope for very low wind speed conditions. Hall *et al.* (1974) observed that slopes of 1/12 and 1/50, respectively, altered their continuous plume results.

Broadly, three characteristic velocities are relevant:

- the ambient wind velocity
- the buoyancy generated velocity found on flat terrain
- the buoyancy generated velocity found on slopes (downslope)

The latter two velocities both scale on $(g'h)^{1/2}$. As the coefficient in the expression for the slope flow is only a weak function of slope, the slope will have an effect on the clouds for which buoyancy-generated velocities are relevant. However, the flow development times may differ. For example, the instantaneous release might initially spread radially, then develop a bulk downslope flow, before finally being diluted and swept upslope by an ambient flow.

When the wind is upslope, the cloud widens and its dilution is enhanced. When the wind is downslope, the cloud is narrower and the dilution is decreased. The variation of the lateral growth of the plume results from the effective summation of the wind and the buoyancy induced motion down the slope. The entrainment is influenced by the velocity shear and will therefore be enhanced by an upslope wind and reduced by a downslope wind. The ambient velocity required to reverse a downslope flow of a plume or cloud is a weak function of a slope and is

typically twice the downslope flow under calm conditions (Turner 1973). In the case of cross winds, Hall *et al.* (1982) found that the dilution is not greatly affected, although their conclusion is based on a single wind tunnel experiment. Further discussion of these points is available in Britter (1982).

A distinctly different topographic influence occurs when the topography alters the velocity field within which the cloud is dispersing. Britter & Snyder (1988) found this to be more important than the direct effect of the slope on the cloud.

Koopman *et al.* (1982) provide results of field experiments showing the effect of more complicated topography, with the plume moving to low lying areas.

The scouring of gases from low lying areas by the ambient flow has been addressed by Bell and Thompson (1980), and Briggs *et al.* (1990).

### 7.15.1 Uniform slopes

Here we consider the influence of slopes on the dispersion of denser-than-air gas clouds i.e. where the cloud size is small compared to the scale over which the topography is changing. This work follows that of Britter (1982), Britter (1989a), Britter (1989b) and Britter, Cleaver and Cooper (1991). We will later allow the slope to change in the advection direction of the clouds.

Many authors have considered the effects of slopes and, in particular, Ellison and Turner (1959), Britter and Linden (1980) and Beghin *et al.* (1981) have studied two-dimensional buoyancy-driven flows on slopes using entrainment theory. In cases of releases into still air, observations support the predictions that entrainment into the plume and subsequent plume dilution increases with slope in a manner so as to ensure that the plume velocity is independent of distance down the slope and very nearly independent of the gradient of the slope. Similar results also hold for the 'starting plume', and the downslope velocities $U$ are generally about $U \sim (g'h)^{1/2}$. Point or area source releases on slopes have received less attention, but unpublished work by Britter suggests that a similar analysis may be appropriate.

In its simplest form, for the two-dimensional problem, the cloud growth rate on a slope of angle $\theta$ is given by an entrainment function.

(7.102) $$E = \frac{dh}{dx} \approx Ri_n \tan\theta,$$

where

(7.103) $$Ri_n \approx \frac{g'h}{U_d^2} \cos\theta$$

and $U_d$ is the downslope cloud velocity.

Further progress requires the use of experimental information linking two of $E$, $Ri_n$ and $\theta$. Although correlations between $E$ and $Ri_n$ are more fundamental, a correlation between $E$ and $\theta$ is often used, e.g. $E = 0.0012\theta$ (see Petersen, 1980). Note that this produces a downslope cloud velocity with a weak dependence on the slope angle $\theta$ in the form of $\sin\theta/\theta$. More complicated expressions provide more rigour and allow the

introduction of the surface drag coefficient which is important at small slopes.

An ambient flow can be incorporated in the two-dimensional case. This can be achieved through the inclusion of a momentum equation. However, following Ellison and Turner (1959), a satisfactory approximation to this results from summing the velocities produced by the slope and the ambient flow. The entrainment due to surface-generated turbulence is based on the resulting absolute velocity, whilst that due to interfacial shear-generated turbulence is based on the velocity difference.

This general approach can be extended to point or area sources and to cases where the wind and slope are not aligned, and to puff or time varying releases.

The predictions obtained using such algorithms are generally consistent with the field data from Picknett (1981) and the relevant laboratory experiments of Hall *et al.* (1974), Britter and Snyder (1988), Knudsen and Krogstad (1986) and Jindal (1989). **Figure 7.8** and **Figure 7.9** show a prediction for the radius and concentration of an instantaneous release dispersing over level terrain compared with predictions for dispersion up and down a small slope. The level terrain case corresponds with conditions experienced during Trial 15 of the Thorney Island Phase 1 tests, and the predictions of the model are in agreement with the experimental data for that trial. The effect of the slope is seen in that a narrow faster moving cloud is produced when the wind is blowing down the slope. In contrast, the centroid of the cloud initially moves in an upwind direction in the case when the wind is blowing up the slope. Having experienced some dilution there, the cloud then moves off in a downwind direction (up the slope), giving the lower concentrations seen in **Figure 7.9**.

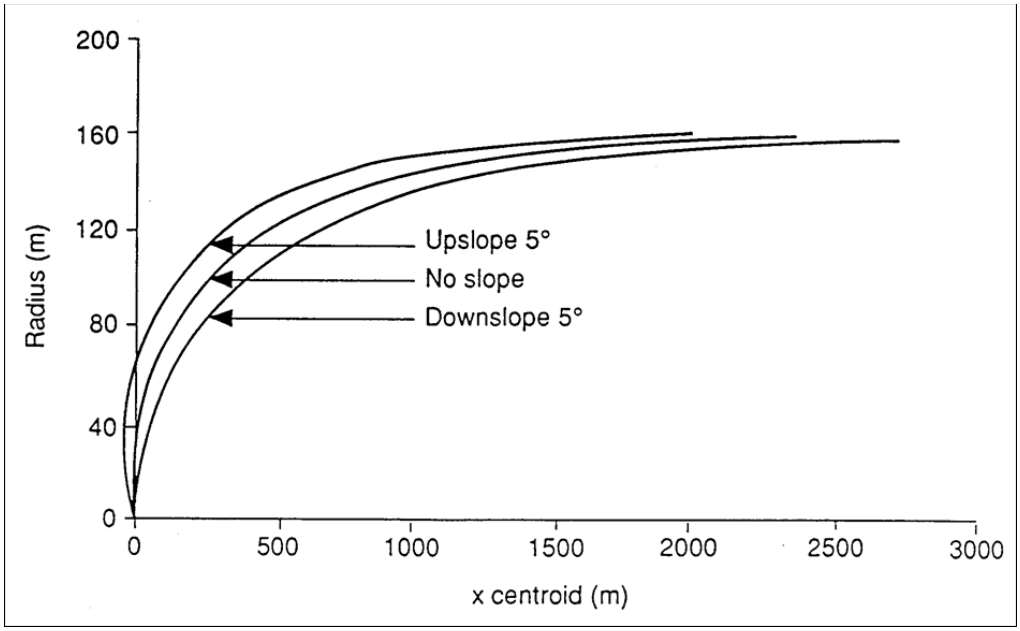



**Figure 7.8** – Effect of Slope on Cloud Radius. The $x$ coordinate is in the direction of the wind.

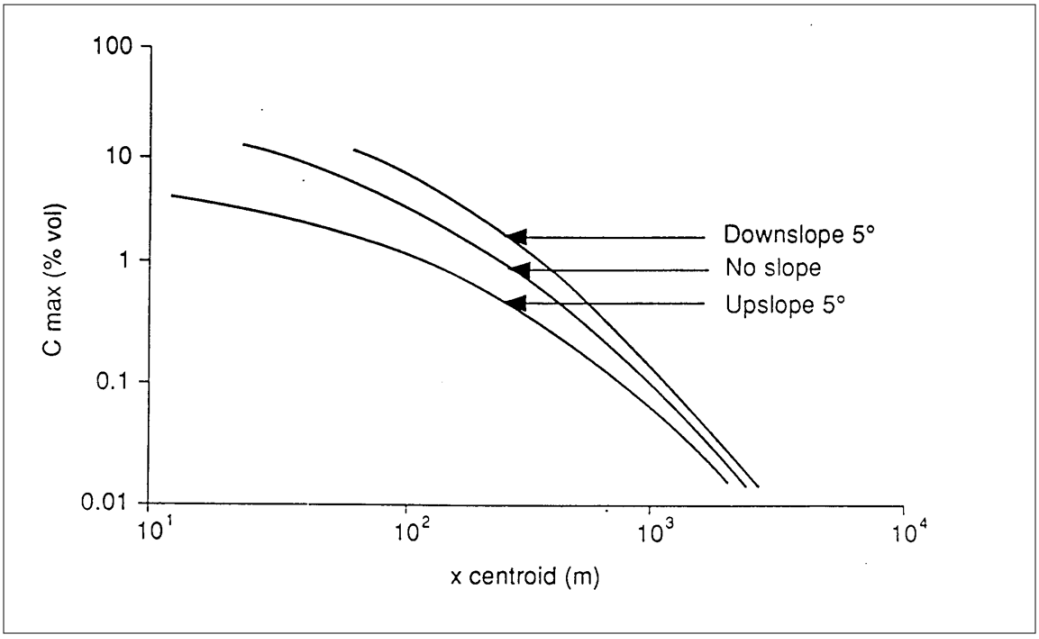



**Figure 7.9** – Effect of Slope on Centreline concentration. The $x$ coordinate is in the direction of the wind.

The above development for modelling the release of dense gas on slopes assumes that the ambient velocity field is known. Thus, we must consider the influence of the slope on the wind field. Extensive on-site field measurements could provide this separately; alternatively, three other approaches could be considered:

a) Estimation of maximum and minimum changes from analysis and experiment, for example Britter (1982), Britter, Hunt and Richards (1984) and others.

b) Use of specific codes for wind fields in complex terrain.

c) Specific codes might be used for a number of standard cases, e.g. plateau to slope, plateau to slope to plateau etc., and a simple library formulated.

As an interim measure the use of case (a) has been found to provide output consistent with available data.

### 7.15.2 Basis for code development

Previous simple analyses which are of an integral type provide support for the possibility of incorporating slope effects into integral models for dense gas dispersion. Of course, the analyses have only been developed for somewhat idealised situations. Nevertheless, the limited field and laboratory data available are quite consistent with the simple analyses. Thus, such analyses or a simplified interpretation of their outcome are used.

We assume that the ambient velocity field has been separately specified in terms of a friction velocity and a velocity profile which may vary in space. Initially we consider only a uni-directional flow.

### 7.15.3 Advection velocity

Analysis and experimental observation indicate that the advection velocity (for the

cloud) $U_{ad}$ be modelled as

(7.104) $$U_{ad} = U_{am} + U_d = U_{am} + C(g'_m \bar{z})^{1/2},$$

where $U_{am}$ is the ambient wind, $C$ is a function of slope and the last term is the downslope velocity. The coefficient $C$ is near unity and is a weak function of slope. It may be obtained from experimental results in the absence of any ambient wind. In these cases, the flows adopt a constant value of $C$ due to a local balance between a downslope force and a retardation due to skin friction and/or entrainment.

In the current version of the code the coefficient $C$ has been set to 1 reflecting the approximations pervading the approach. More refinement may be appropriate following extensive model usage.

### 7.15.4 Lateral plume spreading

No modification is made to the radial or lateral plume spreading to account for slopes. This implies that the velocity, in particular the downslope component, for both the uphill and downhill edges remains unchanged by the presence of the slope and there is symmetric spreading about the cloud centreline. Any modification would have involved a velocity scaling on $(g'h)^{1/2}$ – the same scaling used for the downslope flow and, typically, for the cloud edge velocity.

### 7.15.5 Entrainment

In dealing with the entrainment we note two effects:

- entrainment due to the difference in velocity between the 'buoyant' downslope motion and the ambient motion which is considered as an interfacial mixing flow; and
- entrainment due to surface generated turbulence – this might be expected to depend on the advection velocity over the ground.

For the first effect we note that the difference in velocity is just $C(g'h)^{1/2}$. We appeal here to the basic entrainment relation from Ellison and Turner (1959) and others that an additional entrainment velocity

(7.105) $$u_t = 1.2 \times 10^{-3} \theta C (g'h)^{1/2}$$

should be included for plumes. A similar result is applied for instantaneous releases but with a coefficient of $4 \times 10^{-3}\theta$, the coefficient reflecting the growth rate of the leading edge of gravity currents (Britter and Linden, 1980) which is similar to the flow resulting from instantaneous releases (Beghin *et al.*, 1981).

The approach used here is to model the second effect (surface generated turbulence) by using the standard entrainment correlation for flow over flat terrain but with the friction velocity adjusted from $u_*$ to

(7.106) $$u_* \left| \frac{U_{ad}}{U_{am}} \right|.$$

The correlation based directly on slope has, effectively, included this second effect, albeit in an approximate way. Consequently we select the larger of the two entrainment estimates[1].

### 7.15.6 Reversing flows

#### *Instantaneous releases*

These could move downslope (under gravity) and then upslope (due to the ambient wind). This is directly handled by the previous algorithms.

#### *Continuous/time varying releases*

These are also directly handled to allow the reversing of the plume; however, we note that after the plume has been reversed it will be riding over the downslope plume.

### 7.15.7 Ambient wind not parallel to the slope

The model breaks the downslope velocity into "along-wind" and "cross-wind" components. The along-wind component is added to the usual advection velocity while the cross-wind component provides a normal velocity, the relative magnitudes providing the cloud trajectory direction. Entrainment is treated in two parts as previously: an increased surface-generated turbulence and an explicit slope-dependent part (but see also footnote, Section 7.15.5 regarding the former).

### 7.15.8 Change of slope

The current version of the model allows changes of slope up to a predefined maximum (see Section 4.5.3). The line of maximum slope for all slope sections lies along a single vector, which itself can be oriented in any direction. The only restriction is that we must consider the puff or a representative plume cross section to always be on only one slope. This is not a very severe constraint.

### 7.15.9 Experiences and developments

A difficulty was found in the implementation of the code when a plume, after initially flowing downslope, attempts to reverse. As the plume advection velocity decreases towards zero, the calculated plume depth increases to satisfy mass conservation. The increased depth produces a larger downslope velocity and, consequently, the plume does not reverse.

The difficulty has been overcome by forcing $U_{ad} = 0.3U_{am}$ if $|U_{ad}| \leq 0.3U_{am}$. Such a modification is probably a better reflection of the physics of plume turning than the simple velocity addition anyway (see Turner, 1973).

Note that in his analyses and experiments, Turner paid little attention to the velocity

[1] Incorporation of the second entrainment term introduced some complications with no significant change in model performance. This was subsequently omitted but will be reinstated if model performance indicates that its lack is of consequence.

profile of the ambient flow; the ambient velocity would be substantially larger than the ambient velocity used in our model.

Attempts to reduce the above coefficient from 0.3 to 0.1 dramatically increased the execution time and output was not always obtained.

For reversing flows of plumes on a slope it had been intended to determine the point of maximum downslope extent and commence a new calculation from there. Upon further consideration this seemed unwise.

Currently the code calculates the plume development as it descends the slope and as it is blown back up the slope. This is obviously appropriate for all cases except when the ambient wind is directly up the slope. However we shall apply the result to all cases, including the directly upslope wind, until experimental results show this to be unsatisfactory.

The code allows for plume or puff development over a series of slopes with no limit on the number of changes. Relevant ambient velocities and surface roughness must be entered by the user for each slope change.

A case often encountered is when a cloud on horizontal ground is advected on to an uphill slope. Depending upon the magnitude of this slope the cloud may then have an advection velocity back down the slope towards the horizontal ground. In practice it is expected that a cloud (puff or plume segment) would linger there broadening and diluting until the cloud was able to travel up the slope. The code mimics this behaviour by allowing the cloud to make very small time steps on and off the upward slope until the density is such that the ambient wind will take the cloud up the slope. Thus, there may be two cloud conditions at the base of the slope, one corresponding to the cloud's arrival there and one corresponding to its departure from there up the slope.

The downslope velocity will asymptote towards zero with time.

The slope entrainment term for the instantaneous release has been taken from still air experiments on slopes. It is apparent that this will include (to some extent) the edge entrainment velocity of conventional box models. There is then the possibility of double counting. Consequently, the direct slope entrainment term is only used when it exceeds the sum of all other entrainment terms.

A possible defect of the model for instantaneous releases is the assumed similarity shape, essentially based on a flat circular cylinder, which may be less appropriate for situations with significant slopes. Of course, this does not mean that the predictions may not be very useful, only that there exists an avenue for model improvement if this was found necessary.

# APPENDIX A Useful Contacts

## A.1 GASTAR Helpdesk

Tel: (01223) 357 773 – ask for GASTAR Helpdesk
Email: help@cerc.co.uk Website: www.cerc.co.uk

This service is available to those with valid support contracts (see below) between the hours of 9.30am and 5.00pm (UK local time), Monday to Friday (excluding UK public holiday periods and the period 25th December to 1st January).

## A.2 Support contract

A valid support contract entitles the user to

- use of the GASTAR Helpdesk;
- model upgrades;
- access to further technical advice and downloads on the User Area of the CERC website www.cerc.co.uk/UserArea

All period licence holders are entitled to support during the period of the licence. Permanent licence holders receive free support for one year, after which an annual support contract should be purchased.

## A.3 Scope of the GASTAR Helpdesk service

The scope of the GASTAR Helpdesk Service is to provide answers to specific questions about using GASTAR, such as *"How do I define my own source material?"*, to respond to any reported error messages that occur while running the model, and to record and report on any issues found. Where appropriate, CERC staff can also provide advice on setting up particular modelling scenarios and advice on interpreting the results.

Any Surfer problems should be directed to Golden Software (www.goldensoftware.com).

# APPENDIX B References

In the following list of references a letter in square brackets at the end of the reference denotes that it appears in a particular section, namely [J] = jet model (Section 7.13), [O] = obstacles (Section 7.14) and [S] = slopes (Section 7.15).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