

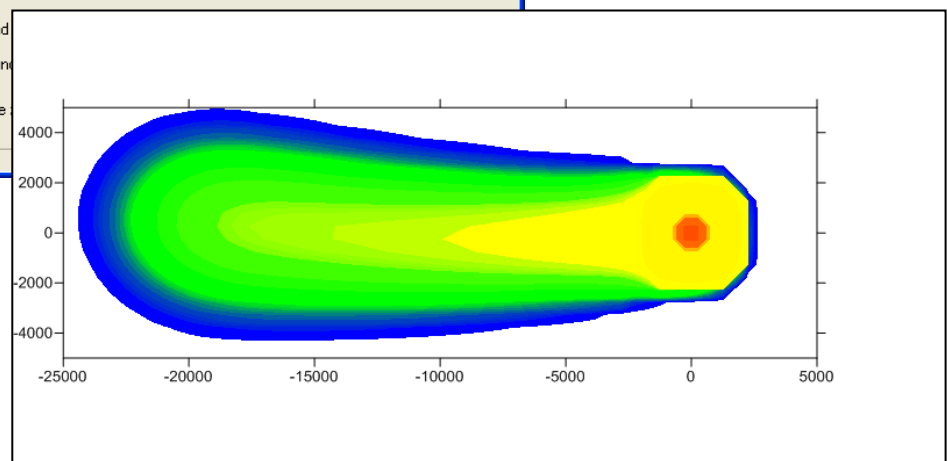
# ADMS-Puff

## *Dense Gas Modelling System*

The screenshot shows the ADMS-Puff software interface. The window title is "ADMS-Puff - (untitled)". The menu bar includes "File", "Run", "Results", and "Help". The left sidebar contains a tree view with the following items: "Complex terrain", "Complex terrain options", "Meteorology", "Output", "Output details", "Setup", and "Setup and source details". The "Meteorology" item is selected. The main panel displays the "Meteorology details" section, which is checked. It includes the following fields and controls:

- Surface roughness (m):** A text box containing the value "0.3".
- Meteorology type:** A dropdown menu set to "Spatially varying".
- Obtain homogeneous met data from:** A dropdown menu.
- Full path to file containing homogeneous met data:** A text box with a browse button ("...").
- Wind speed (m/s):** A text box.
- Wind direction (°):** A text box.
- Air temperature (°C):** A text box.
- Cloud cover (oktas):** A text box.
- Spatially varying meteorology file paths:** A table with a header "Spatially varying meteorology file paths" and a list of paths. The first entry is "Example.nc". There are "Add" and "Delete" buttons next to the table.

At the bottom of the interface, there is a label "Enter the paths of the spatially varying meteorology files".



*User Guide*

CERC



# ADMS-Puff

Dense Gas Modelling System

## User Guide

**Version 1.4**

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## **1. Introduction to ADMS-Puff**

### **1.1 What is ADMS-Puff?**

ADMS-Puff is a Lagrangian dense gas dispersion model developed by CERC. It is ideally suited for modelling accident and emergency response scenarios or investigating site safety involving releases of flammable and/or toxic materials from a variety of industrial accidents.

ADMS-Puff uses a Lagrangian approach to model two types of releases: single instantaneous puffs and continuous plumes. The general philosophy of the dispersion is that an individual puff is dispersed as a dense puff while its Richardson number is above a critical value. Then once the Richardson number goes below this critical value the puff is dispersed using passive algorithms. The concentration is also calculated in different ways depending on the Richardson number, with a weighted solution of the dense and passive calculations being used near the critical Richardson number to ensure a smooth transition in concentration values. The continuous release is modelled as a series of puffs which are dispersed independently, but used collectively in the calculation of the concentration.

Once the release has become passive, its dispersion can continue to be modelled in ADMS-Puff as there is a smooth transition from dense to passive regimes, based on the Richardson number.

There are two types of meteorological data that can be used in ADMS-Puff: spatially varying meteorology from WRF data; or spatially homogeneous meteorology.

### **1.2 About the User Guide**

The remainder of the user guide is in the following sections. Section 2 outlines how to set up a model run in ADMS-Puff. Section 3 describes the results files produced and the use of the ADMS Contour plotting utility. Worked examples are given in Section 4 and a technical description of the model is provided in Section 5. A list of the permitted materials in ADMS-Puff is given in Appendix A and a glossary of symbols is included in Appendix B. Results from ADMS-Puff are compared to results from GASTAR, a well validated dense gas model, in Appendix C.





## 2. Using ADMS-Puff

To start the ADMS-Puff interface double-click *ADMS-Puff.exe* in the ADMS-Puff installation directory or double-click on the shortcut created during installation. This will launch the ADMS-Puff interface. The ADMS-Puff interface consists of three screens into which the data describing the modelling scenario should be entered. Details of these screens are given in the sections below.

### 2.1 Meteorology screen

The Meteorology screen is shown in Figure 1.

ADMS-Puff - (untitled)

File Run Results Help

Complex terrain  
 Complex terrain options  
 Meteorology  
 Output  
 Output details  
 Setup  
 Setup and source details

☒ **Meteorology details**

Surface roughness (m)

Meteorology type

Obtain homogeneous met data from

Full path to file containing homogeneous met data:  
 ...

Wind speed (m/s)

Wind direction (°)

Air temperature (°C)

Cloud cover (oktas)

Spatially varying meteorology file paths

Spatially varying meteorology file paths

Add  
Delete

Wind vector data height (m)

Boundary layer height

Time zone

This box should always be checked Min:  Max:

Figure 1 – The Meteorology Screen

The information which is required to be entered into the Meteorology Screen is as follows:

- **Surface roughness (m)** – the surface roughness of the site being modelled
- **Meteorology type** – choose one of
  - **Spatially varying** – if you want to model spatial variation of the meteorological data. Spatially-varying meteorological data must be provided in the form of output files from WRF.
  - **Spatially homogeneous** – if you want to run a model with meteorological data that is the same over the entire spatial domain.

The information required in the rest of the screen depends on the type of meteorological data being used. If the meteorology type is **spatially homogeneous** then the following must be provided:

- **Obtain homogeneous met data from** – choose from either
  - **From file** – to specify a file containing a sequence of up to 72 lines of meteorological data.
  - **Define one met condition** – to enter a single meteorological condition.
- **Full path to file containing homogeneous met data** – the path to a meteorological file (only required if **From file** is selected). For details on setting up a meteorological file please see the ADMS 5 User Guide Section 3.3.3<sup>1</sup>.

---

*The meteorological file must contain year/day/hour and must start before the start of the release.*

---

The following parameters are required if **Define one met condition** is selected:

- **Wind speed (m/s)** – the wind speed at 10 m in m/s.
- **Wind direction (°)** – the wind direction at 10 m measured clockwise from North.
- **Air temperature (°C)** – the air temperature at the surface in °C.
- **Cloud cover (oktas)** – the cloud cover in oktas.

If the meteorology type is **spatially varying** then the following information must be provided:

- **Spatially varying meteorology file paths** – click on **Add** to allow the cells in the table to be edited. Then copy and paste the file paths for the WRF files in to the blank cells. Up to 72 WRF files may be added. Use the **Delete** button to delete any cells if necessary.
- **Wind vector data height (m)** – the height in metres at which the wind speed and direction is to be calculated.
- **Boundary layer height** – choose from either

---

<sup>1</sup> [http://www.cerc.co.uk/environmental-software/assets/data/doc\\_userguides/CERC\\_ADMS\\_5\\_User\\_Guide.pdf](http://www.cerc.co.uk/environmental-software/assets/data/doc_userguides/CERC_ADMS_5_User_Guide.pdf)

- **From file(s)** to read in the boundary layer heights from the WRF file.
  - **Calculated** to use the model to calculate the boundary layer heights.
- **Time zone** – enter the time difference between GMT and local time. Enter a positive value for longitudes east of the Greenwich meridian or a negative value for longitudes west of the Greenwich meridian.

## 2.2 Output details screen

The Output details screen is shown in Figure 2.

ADMS-Puff - (untitled)

File Run Results Help

Complex terrain

Complex terrain options

Meteorology

**Meteorology**

Output

**Output details**

Setup

Setup and source details

☒ **Output details**

Grid side length (km)

Number of grid lines

Receptor points

X, Y

Add Delete

☐ Receptor points file

Receptor points file path  ...

Output dates and times

DD MM YYYY, HH MM

Add Delete

☐ Instantaneous health limit contour output

Instantaneous health limits

Limit (g/m3)

Add Delete

☐ Time-integrated health limit contour output

Time-integrated health limits

Limit (gs/m3)

Add Delete

☐ Flammability limit contour output

This box should always be checked

Min:  Max:

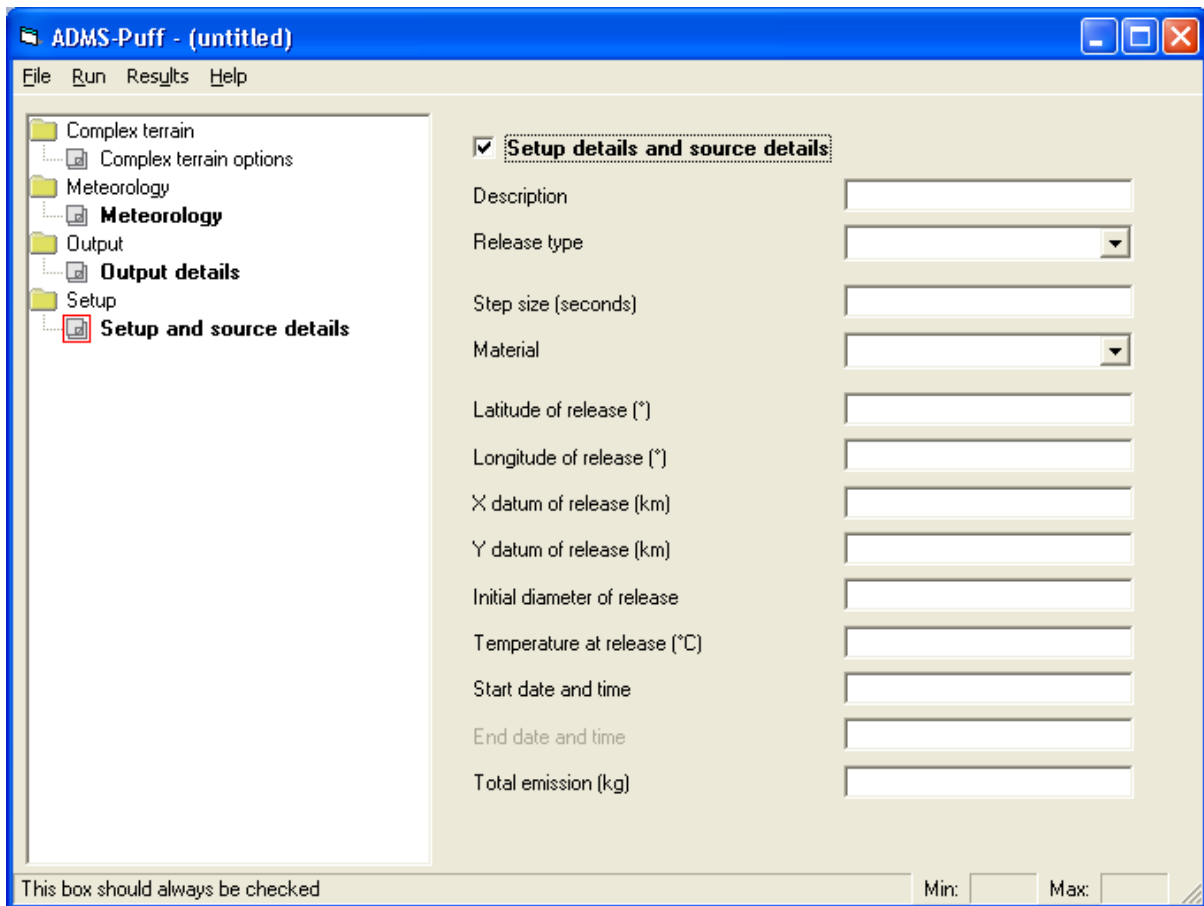
Figure 2 - The Output details screen

The information which is required to be entered into the output details screen is as follows:

- **Grid side length (km)** – the size of the output grid in km. The output grid is square and centred on the source.
- **Number of grid lines** – the number of grid points in the x direction and the y direction.
- **Receptor points** – enter the locations of receptor points as locations relative to the source, in metres. Click **Add** to add a new receptor point and then enter the required location in the format: X, Y e.g. for a point 100 m to the east and 200 m north of the source enter '100, 200'.
- **Receptor points file** – check this box if you wish to enter receptor points from an additional receptor points file, which is a comma-separated text file with the extension \*.arp that contains a line of data for every extra receptor point required. Each line contains the X coordinate and the Y coordinate in that order, in metres.
- **Output dates and times** – enter the dates and times at which output is required in local time. Instantaneous values of concentration are calculated at each output time along with the time integrated concentration between the start of the release and the final output time. The dates and times should be entered in the format – DD MM YYYY, HH MM i.e. day of month, month, year, hour and minutes. For example 10:23 on the 22<sup>nd</sup> May 2011 should be entered as '22 05 2011, 10 23'. The spaces and comma are important in entering data in the correct format.
- **Instantaneous health limit contour output** – check this box if you want health limit contour output for the instantaneous output dates and times entered above. This option will provide contour levels in the gridded output file. Click **Add** to add a new health limit value and then enter the required health limit value, in g/m<sup>3</sup>. A maximum of 5 limit values may be entered.
- **Time-integrated health limit contour output** – check this box if you want health limit contour output integrated over the model run, from the start date and time of the release to the final output date and time. This option will provide contour levels in the gridded output file. Click **Add** to add a new health limit value and then enter the required time-integrated health limit value, in gs/m<sup>3</sup>. A maximum of 5 limit values may be entered.
- **Flammability limit output** – check this box if you want flammability limit output for the instantaneous output dates and times entered above. This option will provide an indication when concentrations exceed the lower and upper flammability limits, in the output file.

### 2.3 Setup and source details screen

The Setup and source details screen is shown in Figure 3.



**Figure 3 - The Setup and source details screen**

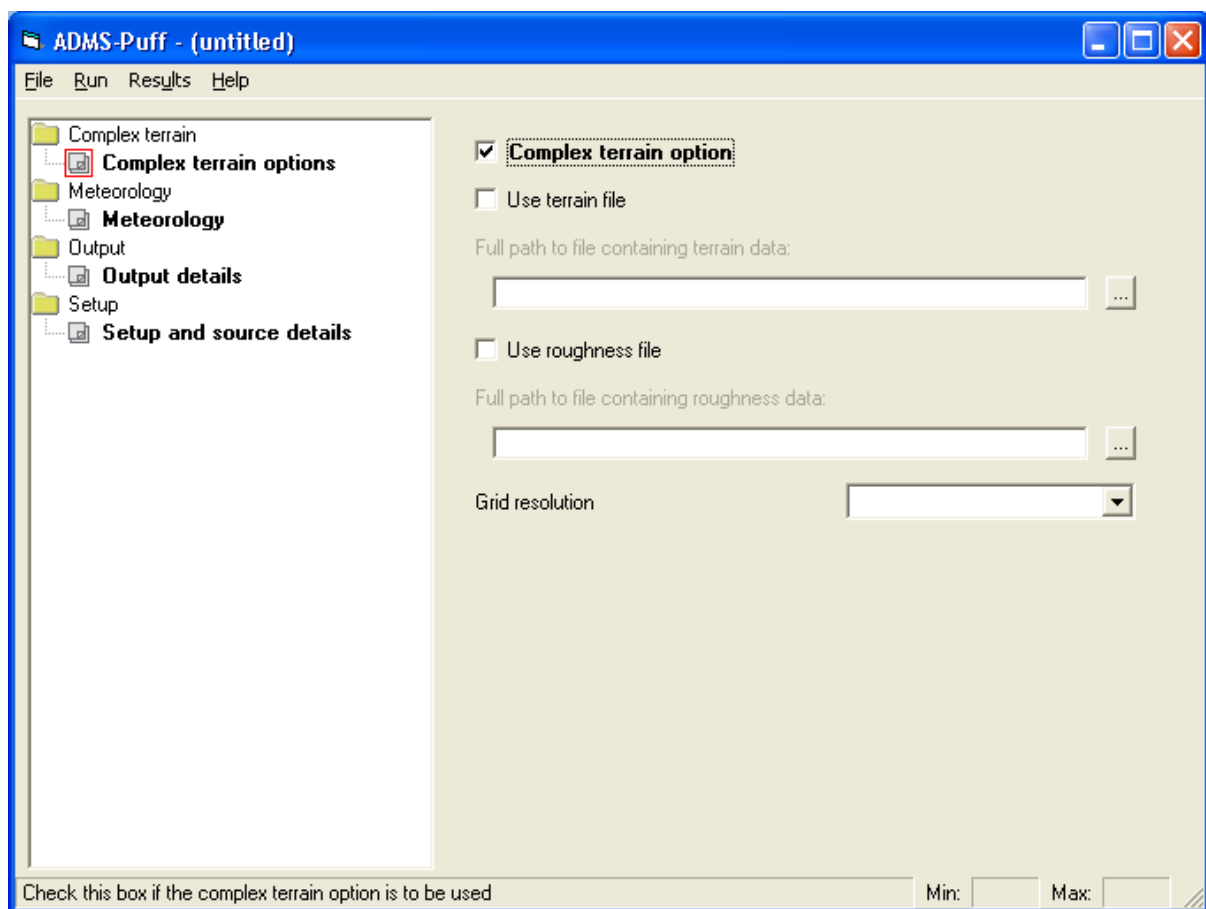
The information which is required to be entered into the Setup and source details screen is as follows:

- **Description** – enter a description of the modelling run, up to 80 characters
- **Release type** – select from either
  - **Instantaneous** – for an instantaneous release
  - **Continuous** – for a finite duration release
- **Step size (seconds)** – enter the calculation time step size to be used by the model. Decreasing the step size will improve the resolution of the model but will also increase the run time, particularly for continuous releases.
- **Material** – select the material which is being released
- **Latitude of release** – enter the latitude of the source
- **Longitude of release** – enter the longitude of the source
- **X datum of release (km)** – enter the X datum of the source on a local Cartesian grid, in kilometres
- **Y datum of release (km)** – enter the Y datum of the source on a local Cartesian grid, in kilometres
- **Initial diameter of release** – enter the initial diameter of the release in metres

- **Temperature of release (°C)** – enter the initial temperature of the release in °C
- **Start date and time** – enter the date and time of the start of the release in local time. The date and time should be entered in the format – DD MM YYYY, HH MM i.e. day of month, month, year, hour and minutes. For example 10:23 on the 22<sup>nd</sup> May 2011 should be entered as '22 05 2011, 10 23'. The spaces and comma are important in entering data in the correct format.
- **End date and time** – for a continuous release enter the date and time of the end of the release in local time. See Start date and time for the format required.
- **Total emission (kg)** – enter the total mass of material emitted in kg

## 2.4 Complex terrain screen

The Complex terrain screen is shown in Figure 4.



**Figure 4 - The Complex terrain screen**

Modelling complex terrain is optional. If you want to model complex terrain, check the **Complex terrain option** box. If this box is checked you must provide the following information in the complex terrain screen:

- Terrain / roughness – choose one or both of:
  - **Use terrain file** – if you want to model spatially-varying terrain.

- **Use roughness file** – if you want to model spatially-varying surface roughness.
- **Grid resolution** – if the complex terrain option box is checked, you must select a grid resolution for the complex terrain calculations from the drop-down box. Choose one of:
  - **16 x 16** grid resolution
  - **32 x 32** grid resolution
  - **64 x 64** grid resolution, this is the default resolution in ADMS 5
  - **128 x 128** grid resolution
  - **256 x 256** grid resolution

If the **Use terrain file** option is selected, then the following must be provided:

- **Full path to file containing terrain data** – the path to a \*.ter terrain file. For details on setting up a terrain file please see the ADMS 5 User Guide Section 4.10.1<sup>1</sup>.

If the **Use roughness file** option is selected, then the following must be provided:

- **Full path to file containing roughness data** – the path to a \*.ruf surface roughness file. For details on setting up a terrain file please see the ADMS 5 User Guide Section 4.10.1<sup>1</sup>.

---

*The terrain and/or roughness file must be comma separated and the maximum number of data points that may be included in each file is 66,000*

---

## 2.5 Running ADMS-Puff

Once information has been entered in all three screens of the ADMS-Puff interface the data file can be saved and then run. To save a model file select **Save** or **Save As** from the **File** menu. The file should be saved with the extension .ppl. To run the model select **Model** from the **Run** menu. This will launch the model and run the current file. Once the run has completed the model window will close. Details of the output files produced by the model are given in the next section.



### 3. ADMS-Puff output

#### 3.1 ADMS-Puff output files

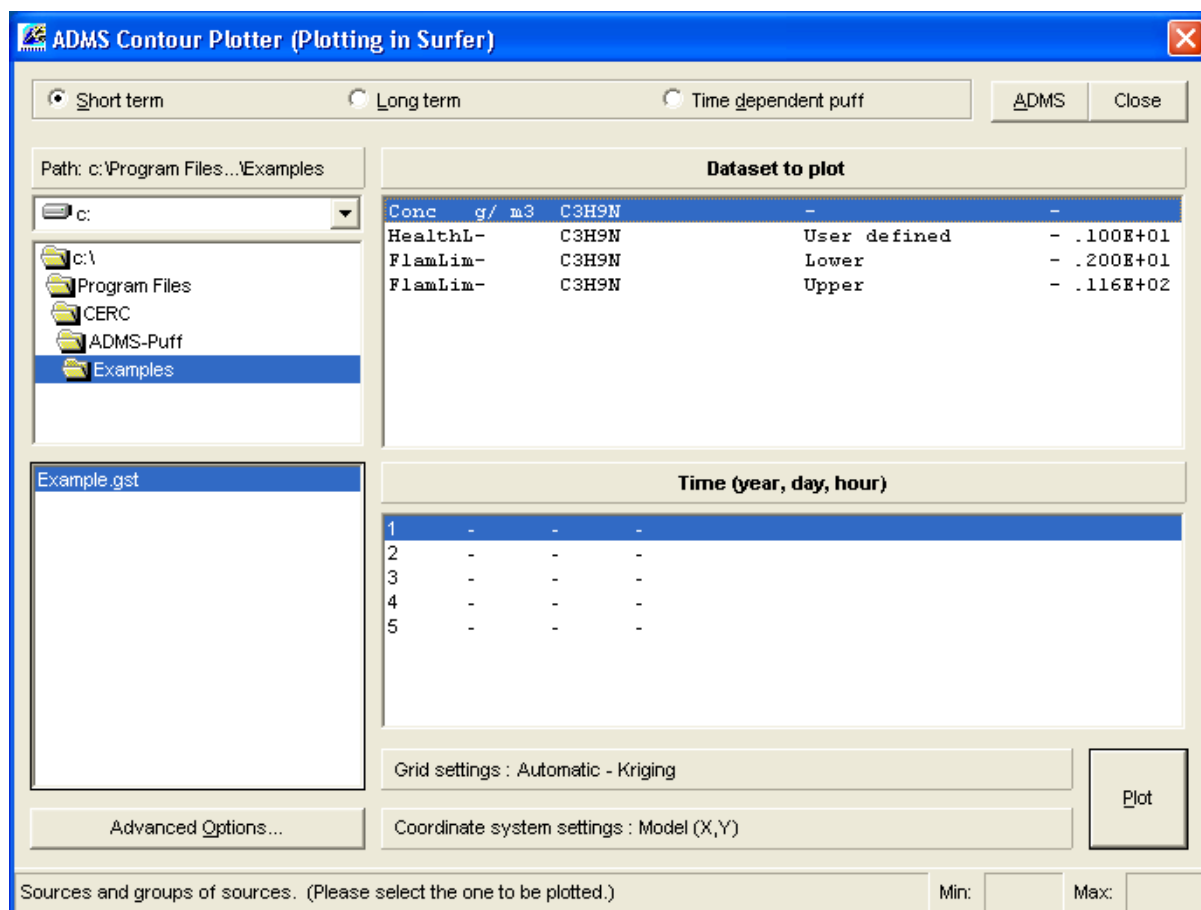
During an ADMS-Puff run a series of output files is created. These files contain the results of the run and are stored in the same directory as the corresponding *.ppl* file. All output files for a model run have the same file stem as the *.ppl* file and are associated with a different extension that indicates the type of output data contained in the file:

- **.log** – contains a log of the model run including any error or warning messages if there are problems with the model setup.
- **.gst** – contains instantaneous snapshots of concentration for all gridded output points at each of the output times, in  $\text{g/m}^3$ . When the **instantaneous health limit contour output** option is selected, this file will also contain columns of the instantaneous concentration divided by the user-defined health limit values. When the **flammability limit output** option is selected, this file will also contain columns of the instantaneous concentration divided by the lower and upper flammability limits of the material released.
- **.pst** – contains instantaneous snapshots of concentration for all specified receptor points at each of the output times, in  $\text{g/m}^3$ . When the **flammability limit output** option is selected, this file will also contain columns of the instantaneous concentration divided by the lower and upper flammability limits of the material released.
- **.glt** – contains the time integrated concentration, up to the last output time, for all the gridded output points, in  $\text{gs/m}^3$ . When the **time integrated health limit contour output** option is selected, this file will also contain columns of the time integrated concentration divided by the user-defined health limit values.
- **.plt** – contains the time integrated concentration, up to the last output time, for all the specified receptor points, in  $\text{gs/m}^3$ .

All the numerical output files are in comma separated variable format and so can easily be viewed in a variety of software packages.

#### 3.2 Contour plotting in Surfer

If Surfer is installed, contour plots of the gridded output can be produced using the ADMS Contour Plotter. To launch the ADMS contour plotter select **Contour plot in Surfer** from the **Results** menu of the ADMS-Puff interface. This will launch the ADMS Contour Plotter, Figure 5.



**Figure 5: The ADMS Contour Plotter**

The ADMS Contour Plotter allows for both the instantaneous snapshots of concentration (**Short term**) and time integrated concentration (**Long term**) to be plotted. Firstly, select the type of file to be plotted and the browse to the appropriate directory and select the file. Then select the dataset to plot. Choose from the concentration (**Conc**) or when selected, the health limit contour output (**HealthL**) or flammability limit output (**FlamLim**). For instantaneous concentrations then select the output time to be plotted (**1** corresponds to the first output time entered in the interface, **2** to the second etc.). Then click **Plot** to create the contour plot in Surfer. Some of the parameters used in creating the plot can be altered by clicking **Advanced Options** and setting the values as required.

## 4. Worked Examples

This section contains worked examples. The first shows how to set up and run a model of an instantaneous release using spatially homogeneous meteorological data. The second shows how to setup and run a model of a continuous release using spatially-varying meteorological data.

### 4.1 Example 1

This example shows how to set up and run a model of an instantaneous release when using spatially homogeneous meteorological data.

1. To start ADMS-Puff, double click on the AdmsPuff.exe file in your install directory. The initial screen is as shown in Figure 6.

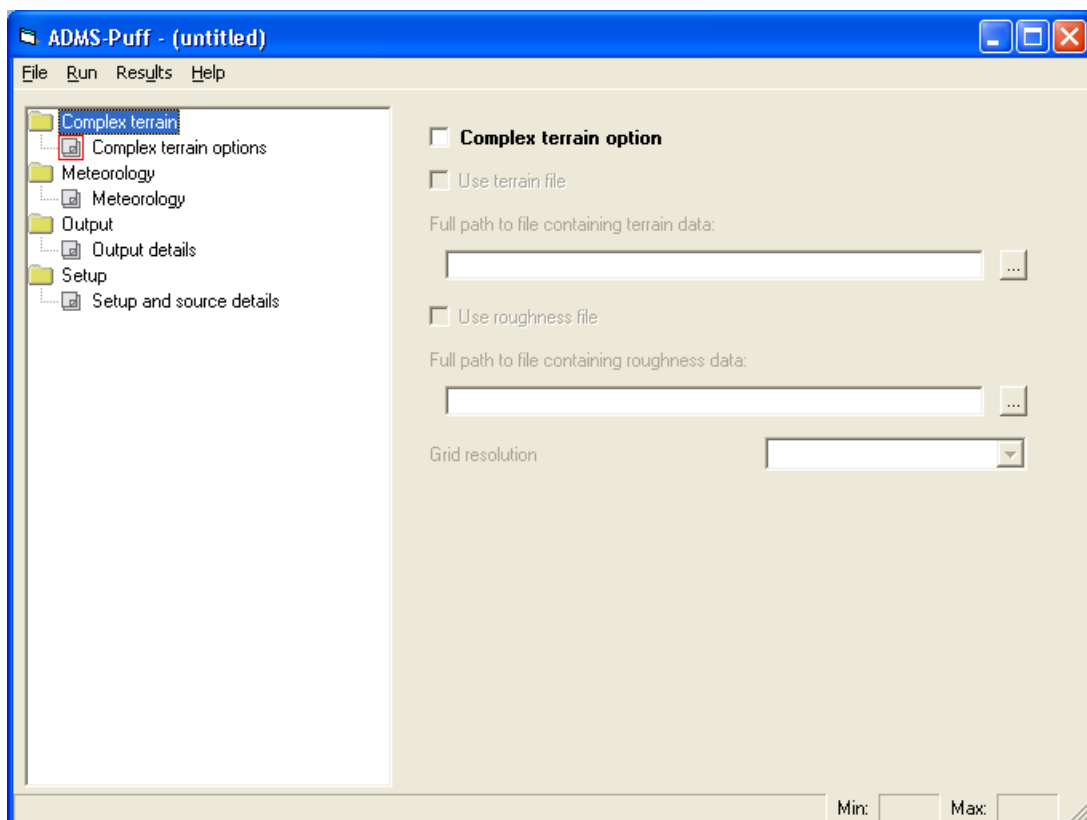


Figure 6: The initial screen after starting ADMS-Puff.

2. To enter the meteorological data first click on the phrase **Meteorology** in the menu on the left and click in the box next to **Meteorology details**. The **Surface roughness (m)** and **Meteorology type** are no longer greyed out and in the menu on the left **Meteorology** is now shown in bold. See Figure 7.

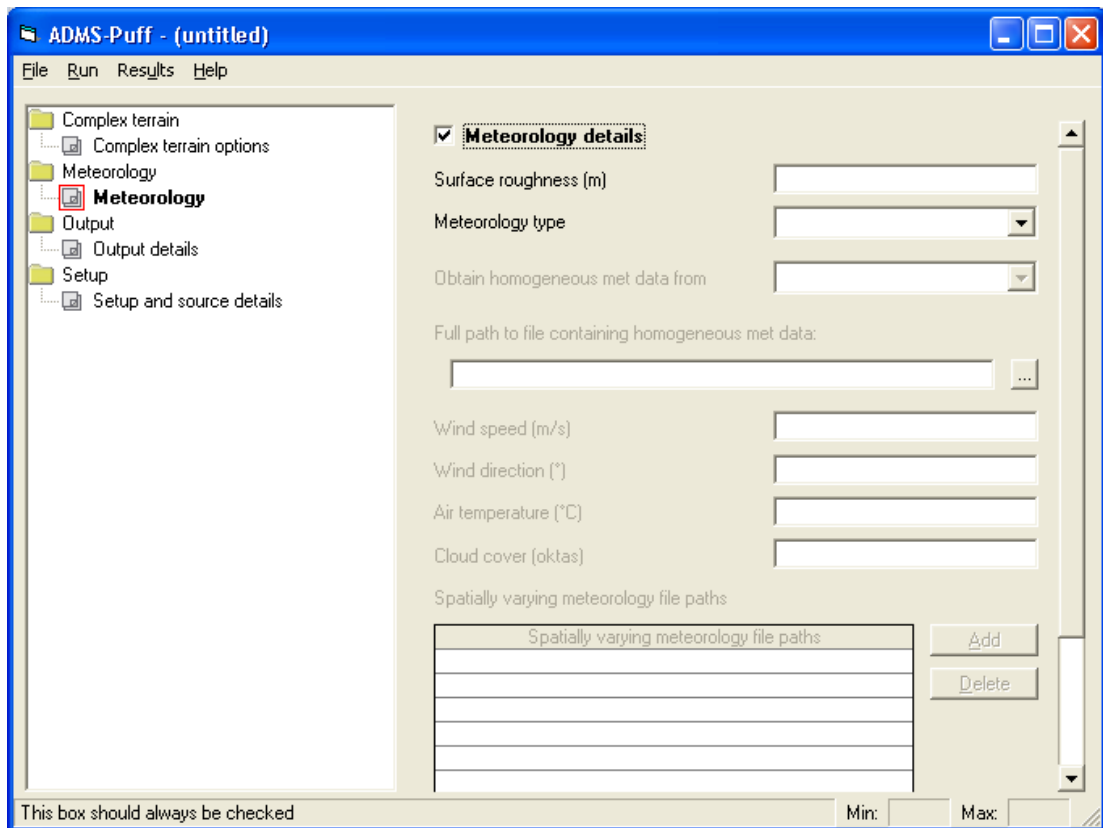
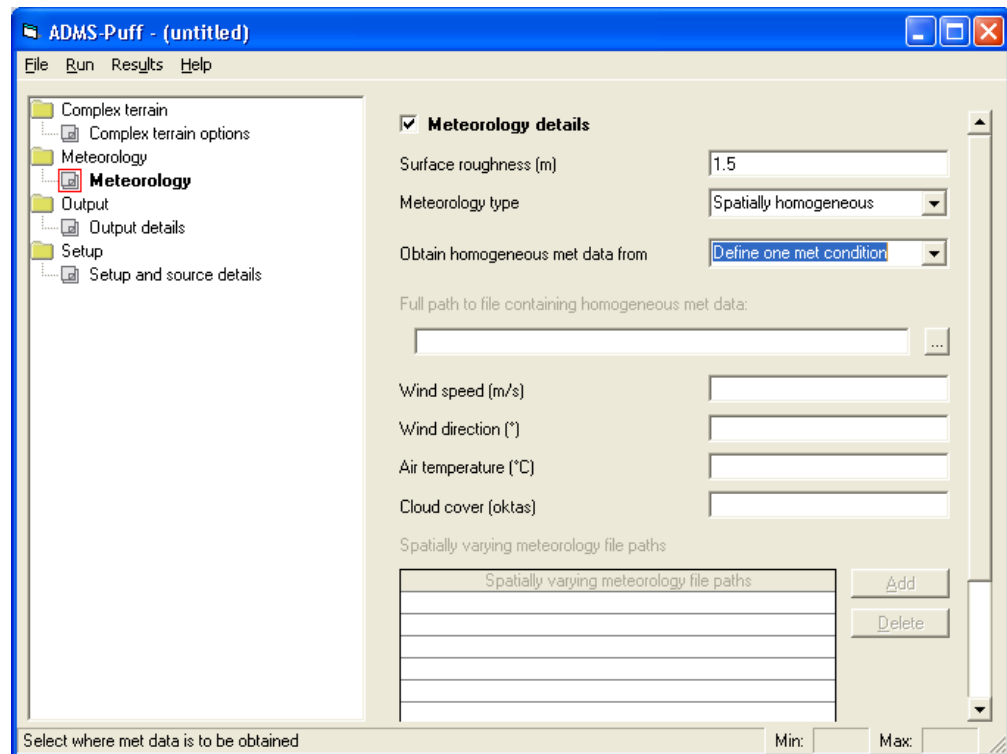


Figure 7: The meteorology screen.

- Enter a value of 1.5 in the cell for the **Surface roughness (m)**.
- Use the drop down menu next to **Meteorology type** to select **Spatially homogeneous** meteorological data.
- The cell for **Obtain homogeneous met data from** is no longer greyed out. The drop down menu here can be used to choose whether the meteorological data is to be entered by file or instead whether one meteorology condition is to be defined in the interface.
- Select **Define one met condition**. The cells for the meteorological data are no longer greyed out. See Figure 8.



**Figure 8: The meteorology screen when defining one condition for spatially homogeneous data.**

- e. In the cell next to **Wind speed (m/s)** enter 4.2. This is the wind speed at 10m in metres per second.

---

*Observe that in the bottom right hand corner of the interface the minimum and maximum allowed values are displayed in the cells labelled **Min:** and **Max:**. Also a description of each of the variables is given in the bottom left hand corner. This is the case for all of the cells.*

---

- f. In the cell next to **Wind direction (°)** enter 235. This is the wind direction at 10m in degrees from north.
- g. In the cell next to **Air temperature (°C)** enter 23. This is the air temperature in Celsius at screen height (1.2m).
- h. In the cell next to **Cloud cover (oktas)** enter 6. This is the cloud cover in oktas.

---

*A value of 8 oktas indicates a totally overcast sky, and a value of 0 oktas indicates a clear sky.*

---

- i. The meteorology screen is now complete; see Figure 9.

ADMS-Puff - (untitled)

File Run Results Help

Complex terrain  
Complex terrain options  
Meteorology  
Output  
Output details  
Setup  
Setup and source details

☒ **Meteorology details**

Surface roughness (m) 1.5

Meteorology type Spatially homogeneous

Obtain homogeneous met data from Define one met condition

Full path to file containing homogeneous met data:

Wind speed (m/s) 4.2

Wind direction (°) 235

Air temperature (°C) 23

Cloud cover (oktas) 6

Spatially varying meteorology file paths

Add Delete

Cloud cover (oktas) Min: 0 Max: 8

**Figure 9: The complete meteorology screen when defining one condition for spatially homogeneous data.**

- Now click on **Output details** in the menu screen to enter the data for the output grid, receptor points and output dates and times. The screen initially appears as shown in Figure 10.

**ADMS-Puff - (untitled)**

File Run Results Help

Complex terrain  
 Complex terrain options  
 Meteorology  
**Output**  
 Output details  
 Setup  
 Setup and source details

☐ **Output details**

Grid side length (km)

Number of grid lines

Receptor points

X, Y

Add Delete

☐ Receptor points file

Receptor points file path  ...

Output dates and times

DD MM YYYY, HH MM

Add Delete

☐ Instantaneous health limit contour output

Instantaneous health limits

Limit (g/m3)

Add Delete

☐ Time-integrated health limit contour output

Time-integrated health limits

Limit (gs/m3)

Add Delete

☐ Flammability limit contour output

Output details Min:  Max:

**Figure 10: The Output details screen.**

- Click in the box next to **Output details**. The mandatory options in the screen are no longer greyed out and the phrase **Output details** in the menu on the left now appears in bold.

- b. In the cell next to **Grid side length (km)** enter 25 for the length of the sides of each grid cell in kilometres.

---

*Notice again that a description of each cell appears in the bottom left hand corner and the minimum and maximum allowed values are displayed in the bottom right hand corner.*

---

- c. In the cell next to **Number of grid lines** enter 21 for the total number of grid lines.
- d. Click on the **Add** button to the right of the **Receptor points** table to enter the coordinates of a receptor point.
- Click in the cell where **<X,Y>** has appeared and delete the text.
  - Type **1000,800** in the cell. This is the distance of a receptor point from the source in metres in the E-W and N-S directions, respectively, with east and north being positive.
  - More receptor points can be added in the same way.
  - Receptor points can be deleted by use of the **Delete** button to the right of the table.
- e. Leave the **Receptor points file** unchecked, since we do not need to add additional receptor points.
- f. Click on the **Add** button to the right of the **Output dates and times** table to enter the dates and times when the output is required.
- Click in the cell where the date and time has appeared and delete the text.
  - Type **01 12 2011, 17 33** which is the 1<sup>st</sup> December 2011, 17:33 hours in local time.
  - More output dates and times can be added in the same way.
  - The **Delete** button to the right of the table can be used to remove data from the table.
- g. Leave the **Instantaneous health limit contour output** option box unchecked. Similarly, leave the **Time-integrated health limit contour output** and **Flammability limit contour output** boxes unchecked. We will not include these optional outputs.
- h. The **Output details** screen is now complete, see Figure 11.



**ADMS-Puff - (untitled)**

File Run Results Help

Complex terrain  
 Complex terrain options  
 Meteorology  
**Output**  
 Output  
**Output details**  
 Setup  
 Setup and source details

☒ **Output details**

Grid side length (km)

Number of grid lines

Receptor points

X, Y
1000, 800

☐ Receptor points file

Receptor points file path

Output dates and times

DD MM YYYY, HH MM
01 12 2011, 17 33

☐ Instantaneous health limit contour output

Instantaneous health limits

Limit (g/m3)

☐ Time-integrated health limit contour output

Time-integrated health limits

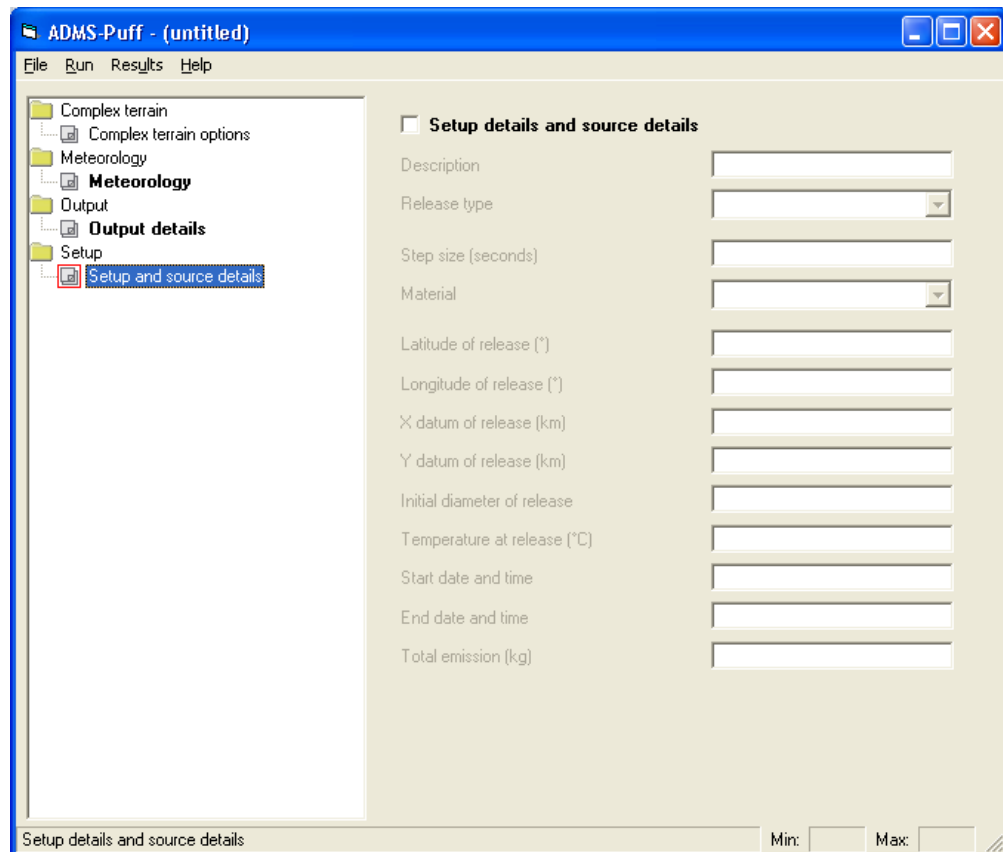
Limit (gs/m3)

☐ Flammability limit contour output

Enter output dates and time in DD MM YYYY, HH MM format Min:  Max:

**Figure 11: The completed screen for the output details**

4. Now click on **Setup and source details** in the menu on the left. The setup screen appears as shown in **Error! Reference source not found.**Figure 12.
  - a. Click in the box next to **Setup details and source details**. Most of the options are no longer greyed out and the phrase appears in bold in the menu on the left hand side of the screen.



**Figure 12: The setup and source details screen.**

- b. A description can be typed in the first cell. Type “Tank failure”.

---

*Note again that a description of what is to be entered in the cell is given in the bottom left hand corner of the interface and the minimum and maximum allowed values are displayed in the bottom right hand corner. The text here can be up to 80 characters in length.*

---

- c. From the drop-down menu next to **Release type** select **Instantaneous**.
- d. In the cell next to **Step size (seconds)** type 2. This means that every time step in the calculation is 2 seconds. Large time steps reduce computational time, but also reduce accuracy.
- e. From the drop down list next to **Material** select **Ammonia** as the pollutant.
- f. Enter 30 as the **Latitude of release (°)**.
- g. Enter 106 as the **Longitude of release (°)**.
- h. Enter 0 as the **X datum of release (km)**. This is the local datum in Cartesian coordinates.
- i. Enter 0 as the **Y datum of release (km)**. This is the local datum in Cartesian coordinates.
- j. Enter 20 as the **Initial diameter of release**. This is the initial diameter in metres.

- k. Enter -50 as the **Temperature at release (°C)**. This is the temperature of the material released.
- l. Enter 01 12 2011, 17 03 as the **Start date and time**. This is 1<sup>st</sup> December 2011, 17:03 local time. This should be before the output time and during or after the time covered in the meteorology file.
- m. Enter 20000 as the **Total emission (kg)**.
- n. The Setup and source details are now complete and the screen is as shown in Figure 13.

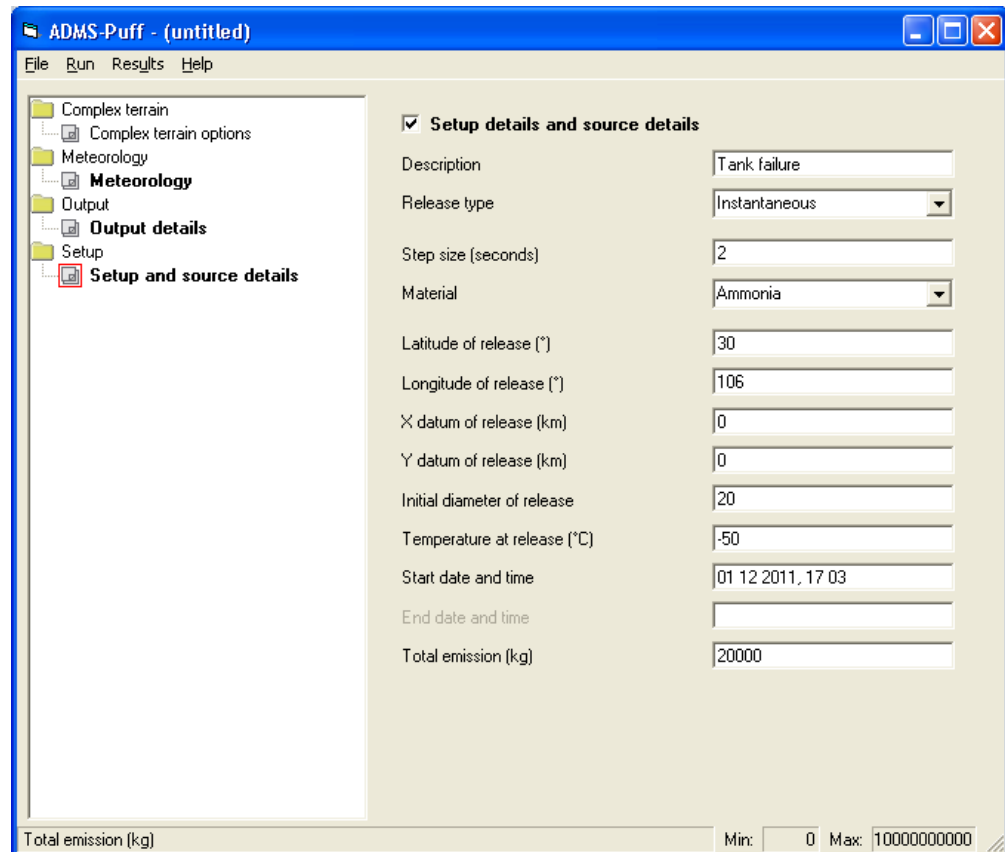


Figure 13: The setup and source details screen when completed.

- 5. We will not model the **Complex terrain** option in this example, so leave the **Complex terrain option** box unchecked. The phrase Complex terrain in the menu on the left should remain in normal font.
- 6. Click the **File** menu and **Save** the file as *Example.PPL*.
- 7. Click the **Run** menu and then click **Model**. The simulation will now run.
- 8. If you have Surfer installed, click the **Results** menu and then click **Contour plot in Surfer**. The ADMS Contour Plotter utility will appear, as shown in Figure 14.
  - a. Select *Example.glt* and click **Plot**

- b. **Save** the *.grd* file when prompted. This is a temporary file and can be deleted later.
  - c. A contour plot of the output will appear as shown in Figure 15. This can then be edited in Surfer as desired. See for example Figure 16.
  - d. Contour plots of the concentrations in the *Example.gst* file can also be plotted using this utility.
9. Navigate to the directory where you saved the *.PPL* file and open the *Example.plt* file in a spreadsheet package such as Microsoft Excel.
  10. The time integrated concentrations for all of the specified receptor points can be viewed.
  11. Similarly, open the *Example.pst* file. Instantaneous snapshots of concentration for all specified receptor points at each of the output times can be viewed.

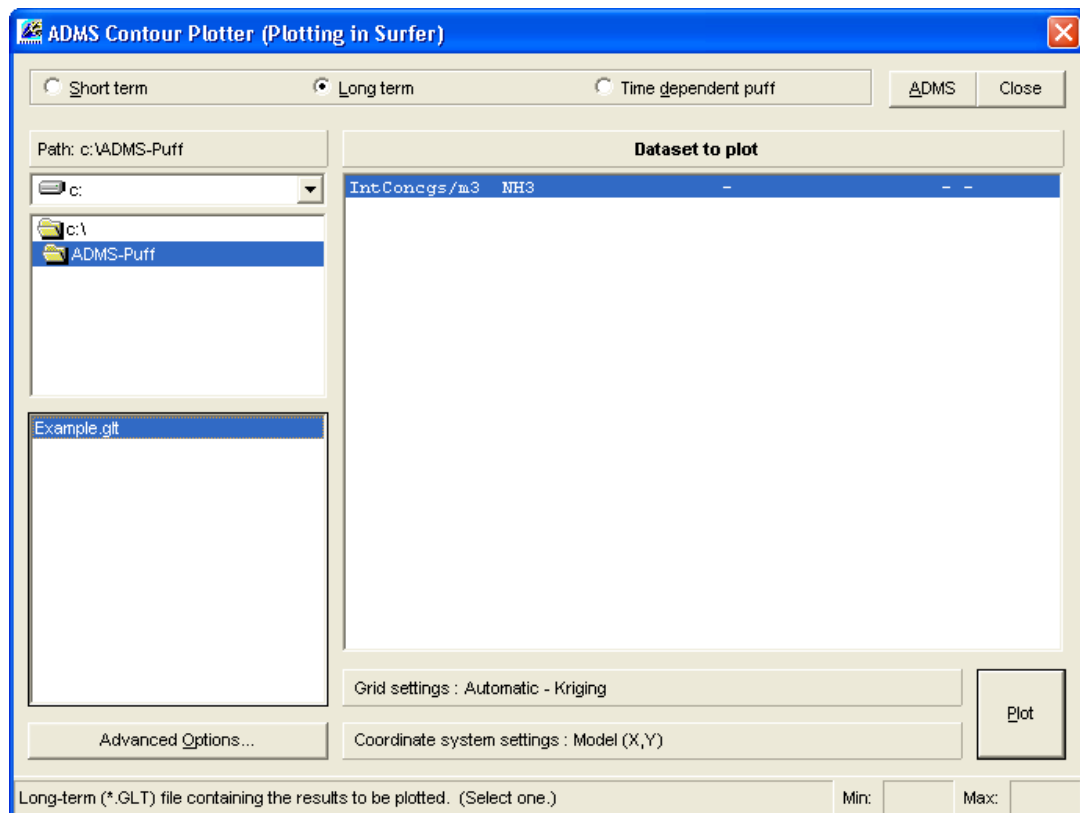


Figure 14: The ADMS Contour Plotter utility.

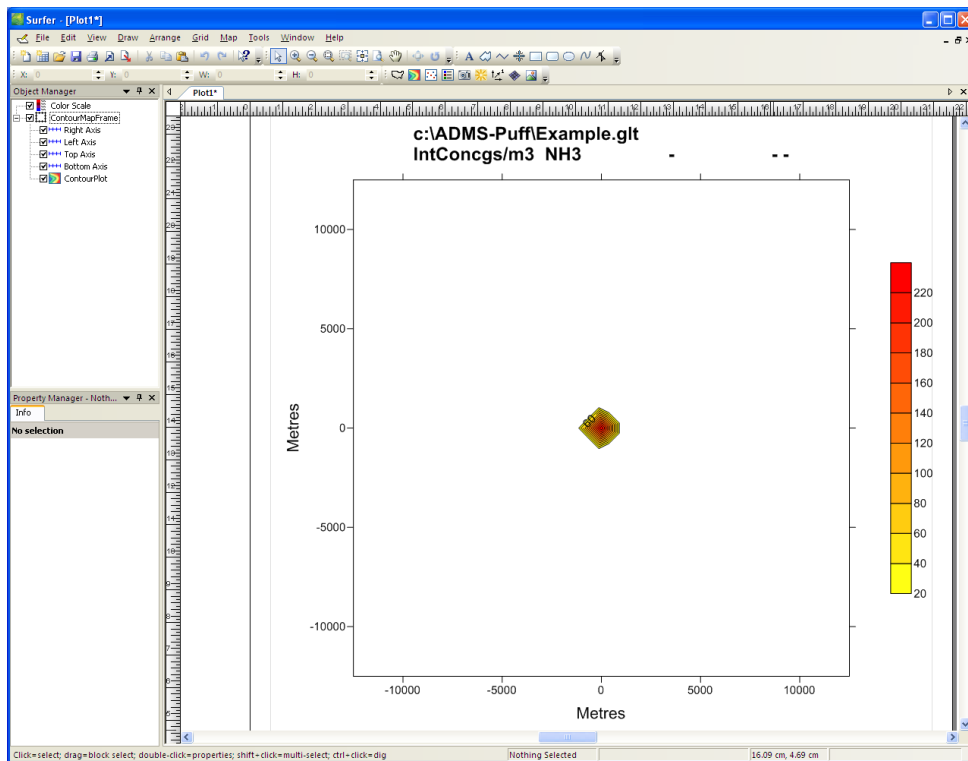


Figure 15: The contour plot produced by the utility.

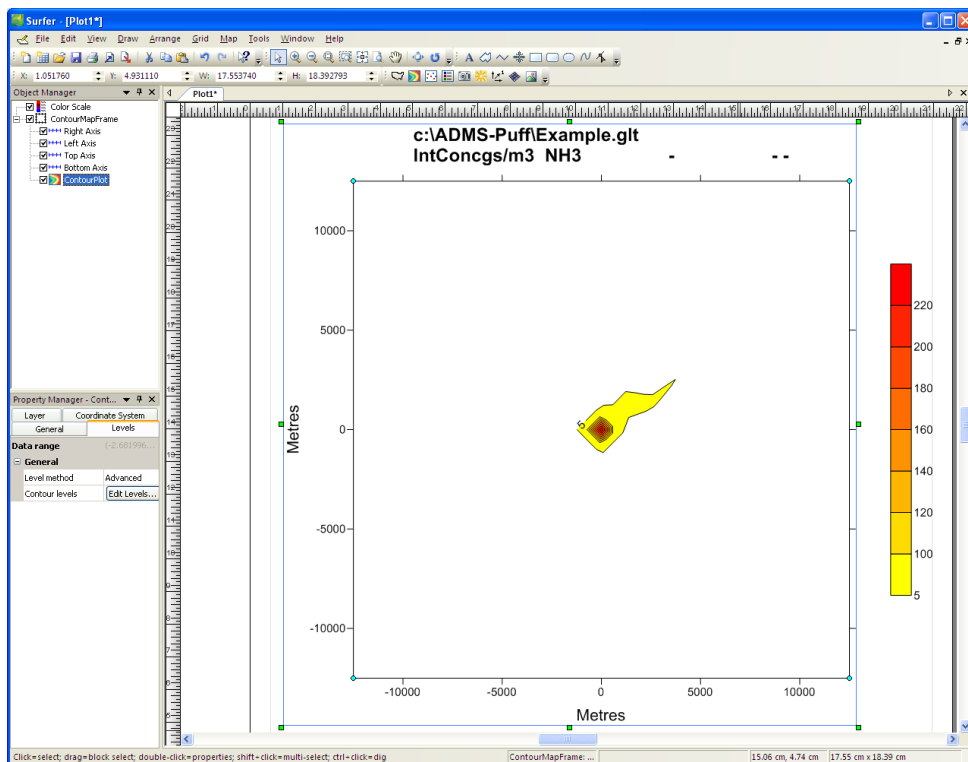


Figure 16: Editing the contour plot in Surfer.

## 4.2 Example 2

This example shows how to set up and run a model of a continuous release when using spatially-varying meteorological data.

1. To start ADMS-Puff, double click on the AdmsPuff.exe file in your install directory. The initial screen is as shown in Figure 17.
2. To enter the meteorological data first click on the phrase **Meteorology** in the menu on the left and click in the box next to **Meteorology details**. The **Surface roughness (m)** and **Meteorology type** are no longer greyed out and in the menu on the left **Meteorology** is now shown in bold.
  - a. Enter a value of 1.5 in the cell for the **Surface roughness (m)**.
  - b. Use the drop down menu next to **Meteorology type** to select **Spatially varying** meteorological data. The options in the lower part of the screen are no longer greyed out. You may have to scroll down to view all of the options available. See Figure 18.
  - c. Next to the table for **Spatially varying meteorology file paths** click on **Add**. The first cell in the table can now be edited.

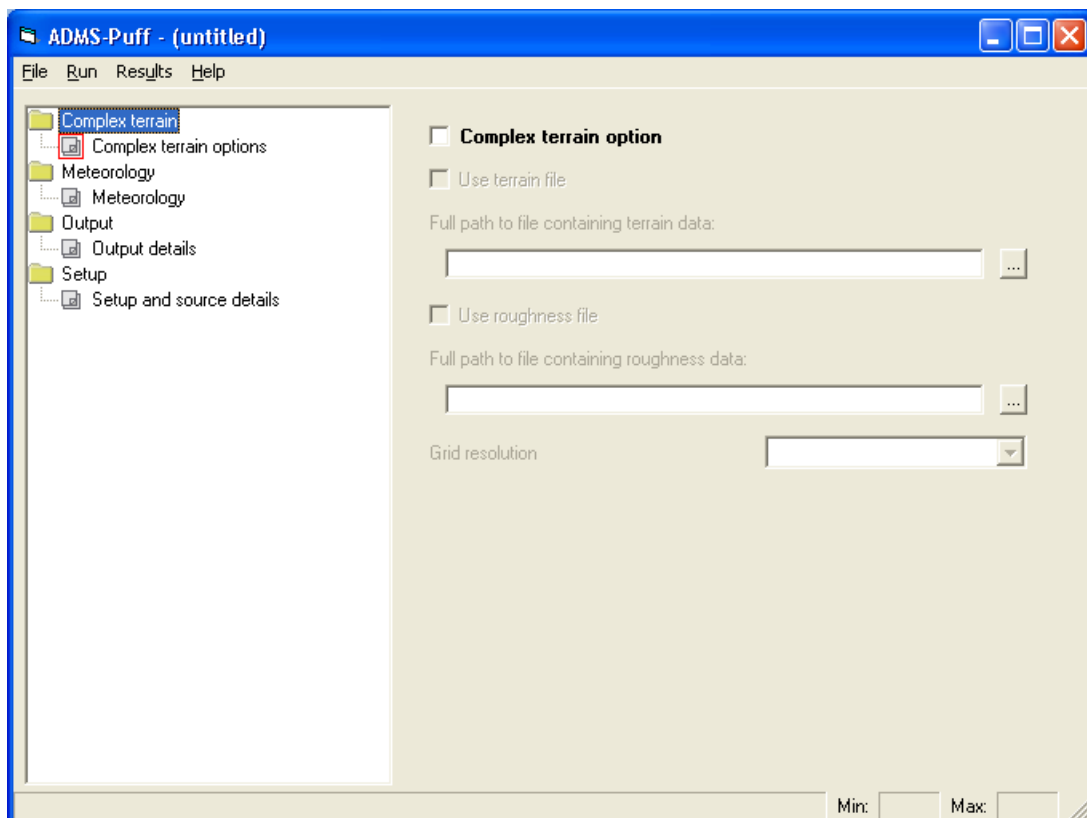


Figure 17: The initial screen after starting ADMS-Puff.

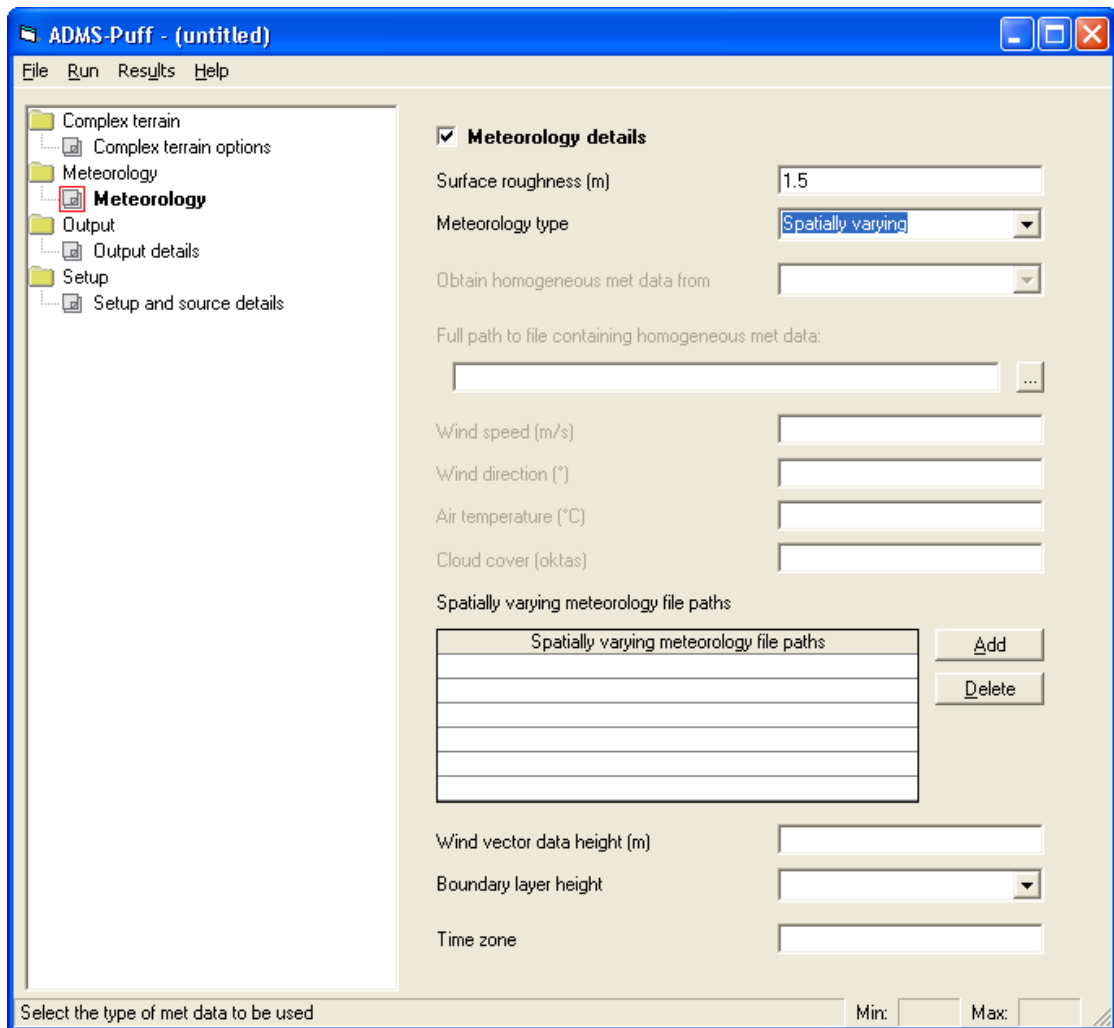


Figure 18: The meteorology screen.

- d. Click in the first cell and type or paste the full file path for a spatially varying meteorology file. This must be a file obtained from WRF.
- e. Up to 72 meteorology files can be added in this way. Files can be removed by clicking on the **Delete** button.
- f. In the cell next to **Wind vector data height (m)** enter 25. This is the height in metres at which the wind speed and direction data was measured.
- g. In the cell next to **Boundary layer height** choose **Calculated**. This means that the model will calculate the boundary layer height, rather than using the height specified in the WRF file.
- h. In the cell for **Time zone** enter 8. This is the time difference between local time and GMT. Longitudes east of the Greenwich meridian have positive time differences; those to the west have negative time differences. The times in a WRF file are in GMT but the times in the interface are in local time.

- i. The meteorology screen is now complete and will be similar to that shown in Figure 19.

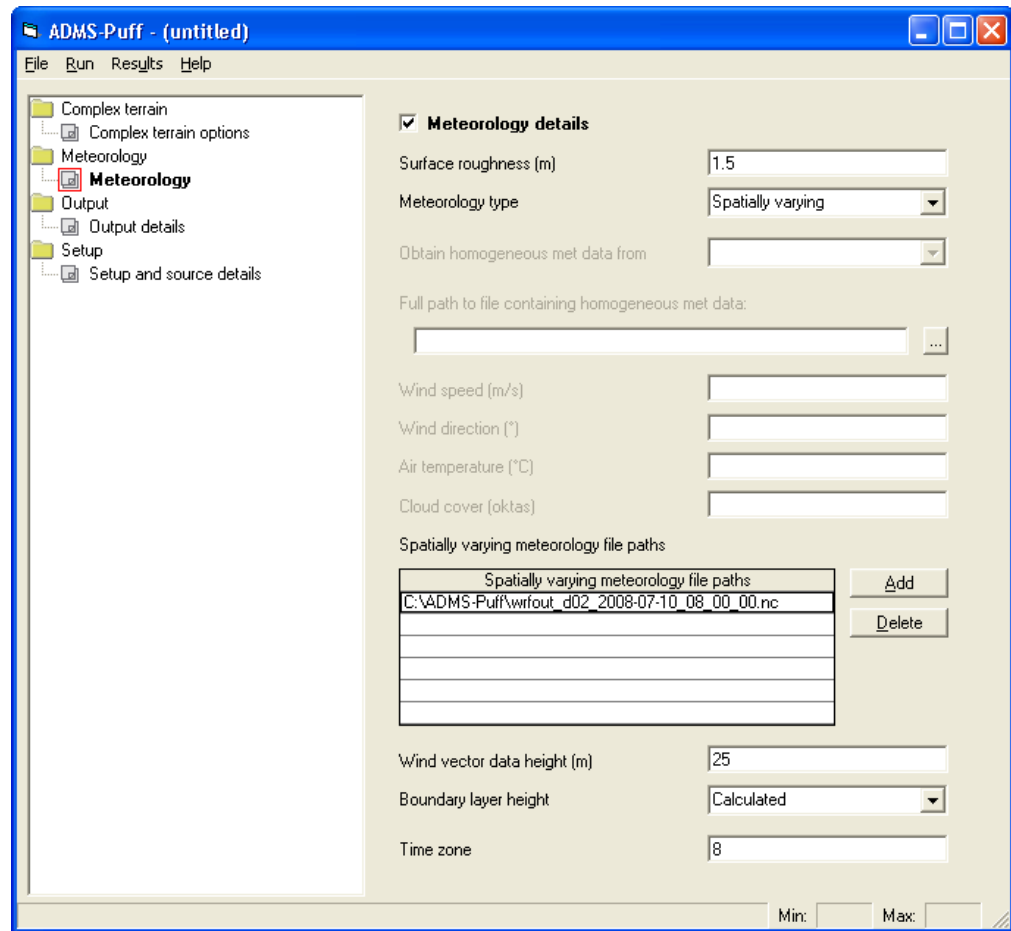


Figure 19: The meteorology screen for spatially-varying meteorological data.

3. Fill in the output screen as described in example 1, but make sure that the date and time entered is during or after the time period of the meteorological data. See Figure 20 for an example.



**ADMS-Puff - (untitled)**

File Run Results Help

Complex terrain  
 Complex terrain options  
 Meteorology  
**Meteorology**  
 Output  
**Output details**  
 Setup  
 Setup and source details

☒ **Output details**

Grid side length (km)

Number of grid lines

Receptor points

X, Y
1000,800

☐ Receptor points file

Receptor points file path

Output dates and times

DD MM YYYY, HH MM
10 07 2008, 16 00

☐ Instantaneous health limit contour output

Instantaneous health limits

Limit (g/m3)

☐ Time-integrated health limit contour output

Time-integrated health limits

Limit (gs/m3)

☐ Flammability limit contour output

Enter output dates and time in DD MM YYYY, HH MM format Min:  Max:

**Figure 20: The output details.**

- Click on **Setup and source details** to navigate to the screen where details of the source can be entered

- a. Click in the box next to **Setup details and source details**. Most of the options are no longer greyed out and the phrase appears in bold in the menu on the left hand side of the screen.
- b. Under **Description** type "Tank leak"
- c. Use the **Release type** drop-down menu to select **Continuous**.
- d. In the cell next to **Step size (seconds)** type 20.
- e. In the cell next to **Material** select **Propane**.
- f. Enter 40 as the **Latitude of release (°)**.
- g. Enter 110 as the **Longitude of release (°)**.
- h. Enter 0 as the **X datum of release (km)**. This is the local datum in Cartesian coordinates.
- i. Enter 0 as the **Y datum of release (km)**. This is the local datum in Cartesian coordinates.
- j. Enter 0.5 as the **Initial diameter of release**. This is in units of metres.
- k. Enter -40 as the **Temperature at release (°C)**.
- l. Enter a **Start date and time** that is during or after the meteorology period and before the output time
- m. Enter an **End date and time** that is during or after the meteorology period, after the start date and time, and before the output time. Thus this example models a continuous release of finite duration.
- n. Enter 5000 as the **Total emission (kg)**.
- o. The setup and source details are now complete and the screen will be similar to that shown in Figure 21.

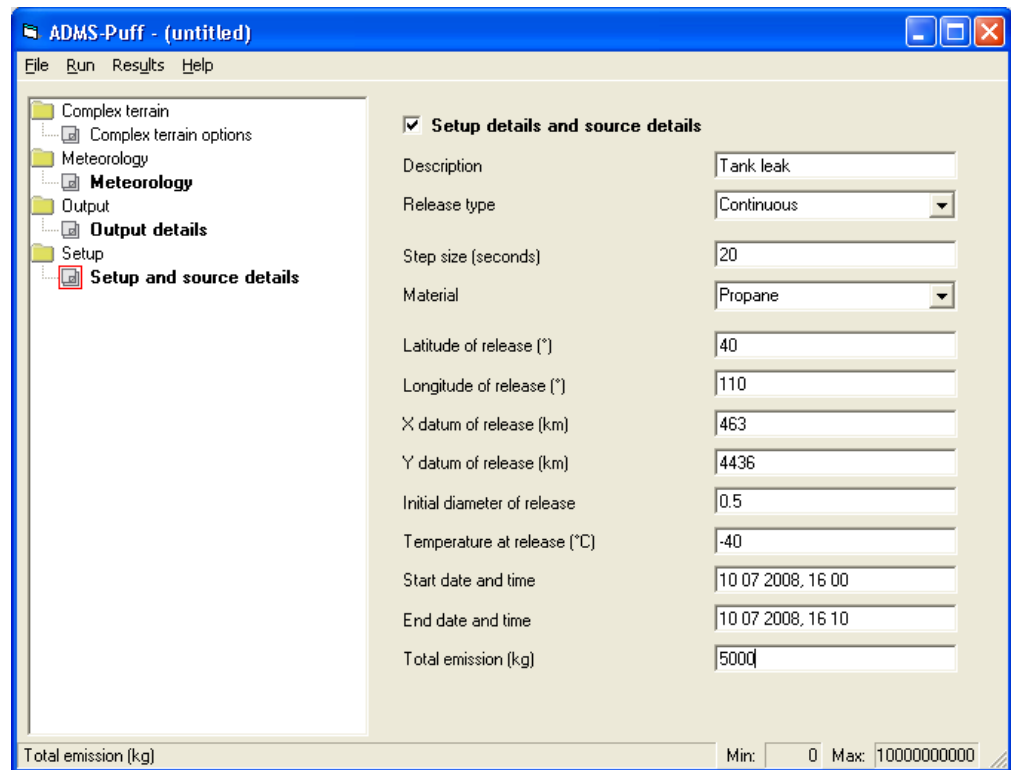
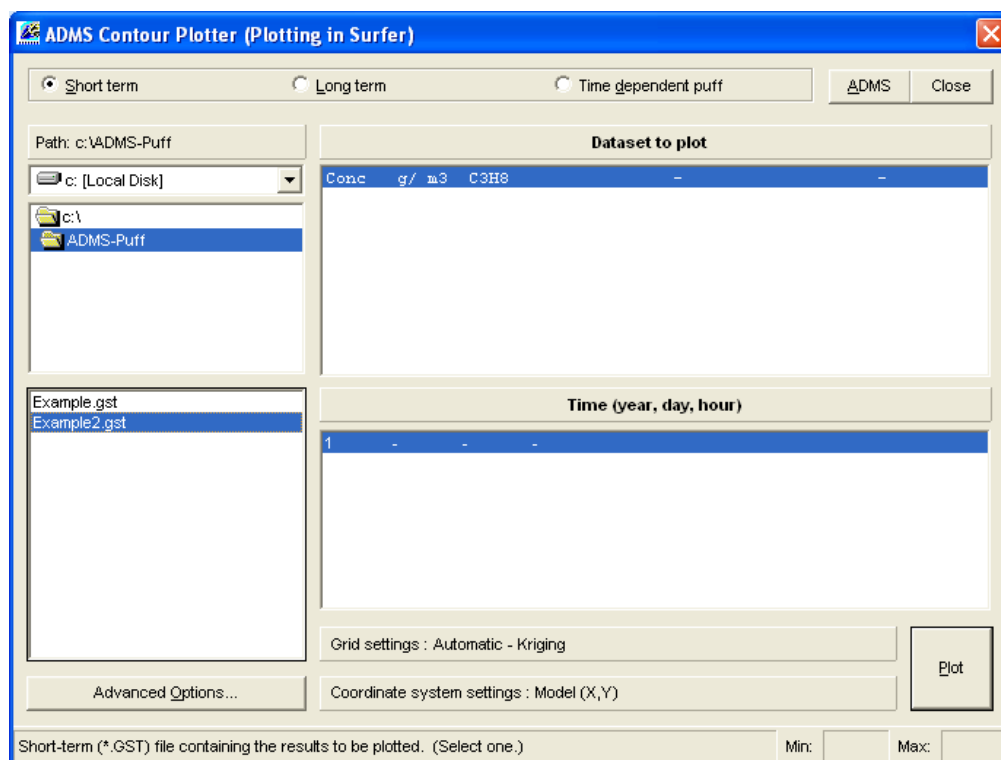


Figure 21: The Setup and source details.

5. Click the **File** menu and **Save** the file as *Example2.PPL*.
6. Click the **Run** menu and then click **Model**. The simulation will now run.
7. If you have Surfer installed, click the **Results** menu and then click **Contour plot in Surfer**. The ADMS Contour Plotter utility will appear, as shown in Figure 22.
  - a. Select the short term radio button to see a list of the \*.gst files. Select *Example2.gst* and click **Plot**
  - b. **Save** the .grd file when prompted. This is a temporary file and can be deleted later.
  - c. A contour plot of the output will appear. This can then be edited in Surfer as desired.
  - d. The *Example2.glt* file can also be plotted using the utility.



**Figure 22: The ADMS Contour Plotter utility.**

8. Navigate to the directory where you saved the *.PPL* file and open the *Example2.plt* file in a spreadsheet using a package such as Microsoft Excel.
9. The time integrated concentrations for all of the specified receptor points can be viewed.
10. Similarly, open the *Example2.pst* file. Instantaneous snapshots of concentration for all specified receptor points at each of the output times can be viewed.

## 5. Technical specification

### 5.1 Overview

This section describes the dispersion algorithms used within ADMS-Puff. ADMS-Puff models two types of release, a single instantaneous puff and a continuous plume. The continuous release is modelled as a series of puffs which are dispersed independently, but used collectively in the calculation of the concentration.

The general philosophy of the dispersion is that an individual puff is dispersed as a dense puff while its Richardson number is above a critical value. Then once the Richardson number goes below this critical value the puff is dispersed using passive algorithms. The concentration is also calculated in different ways depending on the Richardson number, with a weighted solution of the dense and passive calculations being used near the critical Richardson number to ensure a smooth transition in concentration values.

### 5.2 Input data and initial conditions

The following data are specified as input data by the user:

- The meteorological conditions.
- The material being released, this is selected from a list in the chemicals database, see Appendix B.
- The amount of material being release, either:
  - as total mass released,  $m_s$ , for an instantaneous puff,
  - as mass per second released,  $\dot{m}_s$ , for a continuous release.
- The width of the release,  $w_s$ .
- The temperature of the release,  $T_s$ .

The release is assumed to be initially unmixed with ambient air and the density of release,  $\rho_s$ , is calculated from the material being released as:

$$\rho_s = \frac{P_a M_{mol}}{RT_s}$$

where  $P_a$  is the ambient pressure,  $M_{mol}$  is the molecular mass of the material and  $R$  is the universal gas constant.

### 5.3 Dispersion of a dense puff

An instantaneous dense puff is treated as being a well mixed cylinder, i.e. the properties are constant across the puff. In the continuous case the puffs describe the flux properties at a

series of locations with the puff being well mixed in the crosswind direction at each of these locations and the puff properties varying continuously between these locations.

The dispersion algorithms used for the two release types are very similar, the main differences are in the entrainment rate and that in the instantaneous case the algorithms deal with absolute quantities whereas the continuous release use the fluxes of the quantities.

### 5.3.1 Integrated parameters

The main parameters describing each puff are calculated by integrating them up each time step. These parameters are:

- $x(t)$  the location of the puff
- $w(t)$  the width of the puff
- $\hat{m}(t)$  the mass,  $m(t)$ , of an instantaneous puff or mass flux,  $\dot{m}(t)$ , of a puff representing a continuous release
- $U_f(t)$  the front velocity, this is only an integrated parameter for an instantaneous release.

The initial values of these parameters are calculated from the input data. At each time step the derivatives of these properties are calculated and the value for that property advanced. In order to calculate the derivatives for these integrated parameters there are other properties of the puff which must be calculated. The algorithms used in the calculation of the derivatives are also given below.

### 5.3.2 Other puff parameters

The other parameters required in the dispersion or concentration calculations are calculated from the integrated parameters. The algorithms used to calculate these parameters are given in this section.

The puff radius,  $r$ , is calculated from:

$$r = \frac{w}{2}$$

The density difference,  $\Delta\rho$ , is given by

$$\Delta\rho = \frac{\rho - \rho_a}{\rho_a}$$

where  $\rho$  is the density of the puff and  $\rho_a$  is the ambient density.

The density of the puff is calculated from

$$\rho = \frac{\hat{m}}{\hat{v}}$$

where  $\hat{v}$  is the volume,  $v$ , or volume flux,  $\dot{v}$ , of the release. This relationship is used to calculate the initial volume (flux) of the release based on the initial mass (flux) and density.

The volume (flux) of the puff is calculated from

$$\hat{v} = \left(\frac{T}{T_a}\right) \left(\frac{\hat{m} - \hat{m}_s}{\rho_a}\right) + \left(\frac{T}{T_s}\right) \hat{v}_s$$

where  $T$  is the temperature of the puff and  $T_a$  is the ambient temperature.

The temperature of the puff is calculated from

$$T = \frac{T_a(\hat{m} - \hat{m}_s)C_{pair} + T_s\hat{m}_sC_{pv}}{(\hat{m} - \hat{m}_s)C_{pair} + \hat{m}_sC_{pv}}$$

where  $C_{pair}$  is the specific heat capacity of air and  $C_{pv}$  is the specific heat capacity of vapour for the material.

The height of the release,  $h$ , is calculated from

$$h = \begin{cases} \frac{v}{\pi r^2} & \text{instantaneous} \\ \frac{\dot{v}}{wU_a} & \text{continuous} \end{cases}$$

where  $U_a$  is the advection velocity of the puff.

The advection velocity of the puff is calculated from

$$U_a = F_{pert}F_{mix}U_w(h_{eff})$$

where  $U_w$  is the ambient wind speed at the specified height,  $h_{eff}$  is an effective height ( $=0.56h$ ) and  $F_{pert}$  and  $F_{mix}$  are factors relating the ambient wind speed to the advection velocity.

The Richardson number,  $Ri$ , is calculated as follows:

$$Ri = \frac{g\Delta\rho h}{U_r^2}$$

where  $U_r$  is a mixing velocity given by

$$U_r = u_*$$

where  $u_*$  is the friction velocity and  $w_*$  the convective velocity scale.

In the continuous case the front velocity is not an integrated parameter but is calculated from

$$U_f = C_e \left( \frac{gh\Delta\rho\rho_a}{\rho} \right)^{\frac{1}{2}}$$

where  $C_e$  is an edge coefficient which is dependent on the Richardson number.

For the calculation of the derivative of the mass (flux) we need the entrainment areas,  $A$ , and velocities,  $U$ , for the side,  $e$ , and top,  $t$ , of the puff. These are calculated as follows:

$$A_e = \begin{cases} \pi wh & \text{instantaneous} \\ 2hU_a & \text{continuous} \end{cases}$$

$$A_t = \begin{cases} \pi r^2 & \text{instantaneous} \\ wU_a & \text{continuous} \end{cases}$$

$$U_e = a_e U_f$$

$$U_t = \frac{\kappa U_r}{1 + \frac{Ri}{8}}$$

where  $a_e$  is a constant depending on the release type.

### 5.3.3 Derivatives of integrated parameters

The derivatives of the integrated parameters are calculated from the puff properties and these are then used to update the values of these properties. The derivatives are calculated as follows:



$$\frac{dx}{dt} = U_a$$

$$\frac{dw}{dt} = 2U_f$$

$$\frac{d\hat{m}}{dt} = \rho_a(U_e A_e + U_t A_t)$$

and in the instantaneous case

$$\frac{dU_f}{dt} = \frac{2g\Delta\rho\rho_a h}{\rho r} - \frac{U_f^2 \rho_a}{\rho} \left( \frac{C_3}{r} + \frac{C_4}{2h} \right) - \frac{2B_1 U_f^2}{r}$$

where  $B_1$  is dependent on the Richardson number and  $C_3$  and  $C_4$  are constants.

#### 5.4 Dispersion of a passive puff

The dispersion algorithms for a passive puff are much simpler than those of the dense puff. A passive puff is described by its location, height and its Gaussian spread parameters, see Figure 23. The location of the puff is updated based on the ambient wind velocity at the puffs location and the height of the puff remains constant.

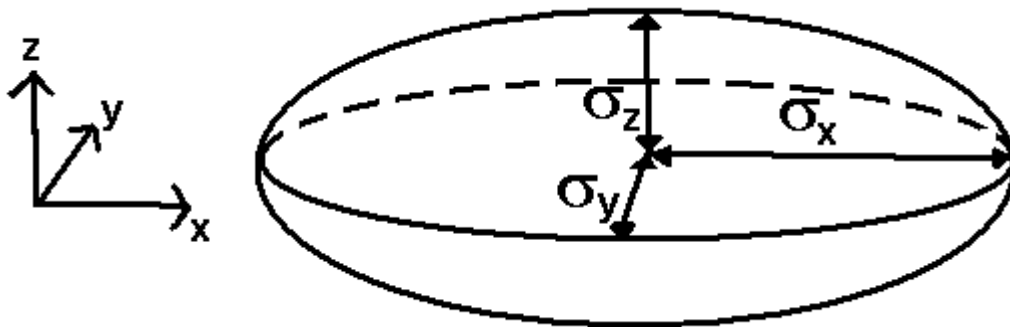


Figure 23: Diagrammatic representation of puff spread parameters

During the dense phase the puff spread parameters are set based on the width and height of the puff. The horizontal puff spread parameters ( $\sigma_x$ ,  $\sigma_y$ ) are set as

$$\sigma_x = (2\pi)^{-\frac{1}{6}} \frac{AWL}{2}$$

$$\sigma_y = (2\pi)^{-\frac{1}{6}} r$$

where  $AWL (= w)$  is the along wind length. The vertical puff spread parameter,  $\sigma_z$ , is based on an effective height of  $(2\pi)^{-\frac{1}{6}} h$ .

Once the puff has become passive the spread parameters are updated based on the following:

$$\sigma_x^2(t + \Delta t) = \sigma_x^2(t) + (\bar{\sigma}_x^2(t + \Delta t) - \bar{\sigma}_x^2(t))$$

and similarly for  $\sigma_y$  and  $\sigma_z$ , where the  $\bar{\sigma}$  represents the calculation assuming that the current meteorological conditions have persisted since the start of the release. These quantities are given by:

$$\bar{\sigma}_x = \sigma_u t \left\{ 1 + \frac{(15.6)^{\frac{1}{3}} u_* t}{H} \right\}^{-\frac{1}{2}}$$

$$\bar{\sigma}_y = \sigma_v t \left\{ 1 + \frac{(15.6)^{\frac{1}{3}} u_* t}{H} \right\}^{-\frac{1}{2}}$$

$$\bar{\sigma}_z = \sigma_w t \left\{ \frac{1}{b^2} + \frac{N^2 t^2}{1 + 2Nt} \right\}^{-\frac{1}{2}}$$

where  $H$  is the boundary layer height. See the ADMS 5 Technical Specification for full details<sup>2</sup>.

## 5.5 Concentration calculations

In order to calculate the concentration at any location two different concentration values are calculated; the concentration from the dense puffs and the concentration assuming the entire release is passive. In addition a value of concentration multiplied by Richardson number is calculated, again assuming the entire release is passive.

<sup>2</sup> [http://cerc.co.uk/environmental-software/assets/data/doc\\_techspec/CERC\\_ADMS5\\_P10\\_01\\_P12\\_01.pdf](http://cerc.co.uk/environmental-software/assets/data/doc_techspec/CERC_ADMS5_P10_01_P12_01.pdf)

The effective Richardson number,  $Ri$ , at the output location is then calculated by dividing the Richardson number multiplied by concentration value,  $RiC$ , by the passive concentration value,  $C_{pass}$ , i.e.

$$Ri(x, y, z) = \frac{RiC(x, y, z)}{C_{pass}(x, y, z)}$$

The final concentration  $C$  is then calculated by taking a weighted average of the dense and passive concentrations,  $C_{dense}$  and  $C_{pass}$ , with the weighting factor  $\lambda$  depending on the Richardson number of the output point as follows:

$$C(x, y, z) = (1 - \lambda)C_{dense}(x, y, z) + \lambda C_{pass}(x, y, z)$$

where

$$\lambda = \min\left(1, \left(\frac{Ri_{crit}}{Ri(x, y, z)}\right)^4\right).$$

Note that this means that for a dense release a weighted sum of the dense and passive concentrations is used, whereas once the release becomes passive it is purely the passive concentration which is used.

The time-integrated concentration is calculated by calculating the concentration at the output location for each advection time step and calculating the sum of these multiplied by the advection time step.

### 5.5.1 Dense concentration calculations

In the instantaneous case the puff is a well mixed cylinder, with the width and height given by the puff properties. The concentration,  $C$ , is taken to be constant within the puff and is given by:

$$C = \frac{m_s}{v}$$

i.e. the mass of released material divided by the current volume of the puff.

For a continuous release the concentration associated with each puff is calculated in a similar way, except that the flux values are now used, i.e.:

$$C = \frac{\hat{m}_s}{\hat{v}}$$

The concentration is calculated by first splitting the plume into polygonal sections defined based on the location and width of the puffs. Then for each output location it is determined which section of the plume the output location is in, if any, and a concentration is calculated based on the two puffs which define that section. In addition hemi-cylinders of constant concentration are placed at the front and back ends of the plume.

An example of this can be seen in Figure 24, here there are 4 puffs making up the release (blue, red, green and purple). The plume has been split into three polygonal sections (blue/red, red/green and green/purple) along with two hemi-cylinders. The concentration within each hemi-cylinder is that of the puff it is associated with and the concentration within each section is calculated based on the weighted average of the values of the puffs at either end of the section.

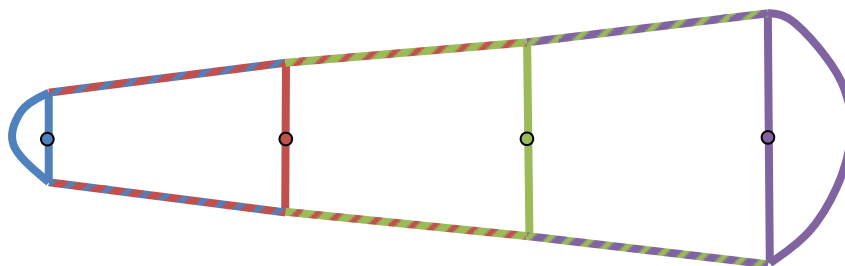


Figure 24: Schematic representation of the calculation of plume concentration with 4 puffs.

### 5.5.2 Passive concentration calculations

The concentrations assuming the entire release is passive are calculated in the same way for the instantaneous puff and continuous release cases (although there is only one puff in the instantaneous case). In each case the concentration at the output location is calculated by summing the contribution to the concentration at that location from each of the individual puffs.

The concentration at an output location due to a single puff is calculated from

$$C(x, y, z) = \frac{\dot{m}_s t_{puff}}{(2\pi)^{\frac{3}{2}} \sigma_x \sigma_y \sigma_z} \exp\left(-\frac{(x - x_c)^2}{2\sigma_x^2}\right) \exp\left(-\frac{(y - y_c)^2}{2\sigma_y^2}\right) \left\{ \exp\left(-\frac{(z - z_c)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z + z_c)^2}{2\sigma_z^2}\right) + reflection\ terms \right\}$$

where  $t_{puff}$  is the release time associated with that puff and  $(x_c, y_c, z_c)$  is the location of the centre of the puff.



## **Appendix A**

### **A.1 Permitted Materials**

A list of permitted materials that can be modelled in ADMS-Puff, together with their relevant physical parameters, is given below.

**Table I: Physical properties of permitted materials in ADMS-Puff, part 1.**

Name	Molecular Weight (g/mol)	Density of Liquid (kg/m <sup>3</sup> )	Boiling Point (K)	Latent Heat of Vaporization (kJ/kg)	Specific Heat Capacity of Vapour (kJ/Kkg)	Specific Heat Capacity of Liquid (kJ/Kkg)	Heat Transfer Group
1,2 Butadiene	54.091	676.00	284.00	448.63	1.4820	2.20800	0.0340
1,3 Butadiene	54.091	673.00	268.69	415.33	1.4740	2.27700	0.0351
1 Butene	56.107	645.00	266.90	390.61	1.5950	2.10200	0.0352
Acrylonitrile	53.064	806.00	350.50	615.00	1.2000	2.10000	0.0271
Ammonia	17.030	639.00	239.82	1374.00	2.1647	4.44790	0.0213
Boron Trichloride	117.169	1349.00	285.70	23.77	0.5353	0.91065	0.0216
Bromine	159.810	3119.00	331.90	188.90	0.2250	0.45200	0.0149
Carbon Monoxide	28.010	803.00	81.70	215.80	1.0370	2.38200	0.0202
Chlorine	70.910	1563.00	238.70	288.10	0.4796	0.89200	0.0154
Dimethyl Ether	46.070	735.00	248.30	467.12	1.4240	2.21900	0.0304
Ethylene	28.054	630.00	169.43	482.67	1.5530	2.43300	0.0248
Ethylene Oxide	44.053	897.00	283.50	581.19	1.0970	1.95100	0.0227
Hydrogen	2.016	70.78	20.268	445.59	14.8900	9.74000	0.0421
Hydrogen Chloride	36.461	1193.00	188.05	443.20	0.7950	1.61000	0.0160
Hydrogen Cyanide	27.026	688.00	298.90	933.70	1.3300	2.62700	0.0252
Hydrogen Fluoride	20.006	967.00	292.70	334.80	1.4550	2.58000	0.0204
Hydrogen Sulphide	34.080	993.00	212.80	547.90	0.9920	1.83000	0.0204
Iso-Butane	58.120	609.00	261.43	366.48	1.6660	2.17700	0.0393
Methane	16.043	422.36	111.66	509.73	2.2200	3.48110	0.0260
Methyl Bromide	94.940	1662.00	276.71	214.28	0.4460	0.83030	0.2320
Methyl Chloride	50.488	1050.00	248.90	424.60	0.8080	1.49900	0.0194
n-Butane	58.120	627.00	272.66	385.61	1.7000	2.19400	0.0533
Nitric Oxide	30.006	1280.00	121.40	460.50	0.9950	7.28200	0.0204
Nitrogen Dioxide	46.006	1450.00	294.30	402.00	0.8130	1.49200	0.1032



Table II: Physical properties of permitted materials in ADMS-Puff, part 1 continued.

Name	Molecular Weight (g/mol)	Density of Liquid (kg/m <sup>3</sup> )	Boiling Point (K)	Latent Heat of Vaporization (kJ/kg)	Specific Heat Capacity of Vapour (kJ/Kkg)	Specific Heat Capacity of Liquid (kJ/Kkg)	Heat Transfer Group
Oxides of Nitrogen <sup>3</sup>	46.006	1450.00	294.30	402.00	0.8130	1.49200	0.1032
Oxygen	32.000	1226.00	90.18	213.27	0.9130	1.67000	0.0211
Phosgene	98.920	1381.00	280.80	246.80	0.5847	1.02000	0.0265
Propane	44.100	590.00	231.11	425.74	1.6710	2.20200	0.0349
Propylene	42.080	612.00	225.45	437.82	1.5200	2.17700	0.0303
Propylene Oxide	58.080	829.00	307.50	464.90	1.5130	2.05100	0.0256
Sulphur Dioxide	64.060	1455.00	263.00	389.60	0.6230	1.38100	0.0158
Trimethyl Amine	59.110	658.00	276.10	407.98	1.5520	2.22300	0.0380
Vinyl Chloride	62.499	1031.00	259.80	355.92	0.8580	1.35800	0.0252

<sup>3</sup> In ADMS-Puff all NO<sub>x</sub> data in mass units are NO<sub>x</sub> as NO<sub>2</sub>, hence the properties of NO<sub>2</sub> are given here.

Table III: Physical properties of permitted materials in ADMS-Puff, part 2.

Name	Lower Flammability Limit (% v/v)	Upper Flammability Limit (% v/v)	Prandtl Number	Toxic Exponent	Antoine A	Antoine B (K)	Antoine C (K)
1,2 Butadiene	2.0	12.0	0.7649	1.0	9.11870	1041.1170	-30.8000
1,3 Butadiene	2.0	11.5	0.6948	1.0	8.97490	930.5450	-34.3000
1 Butene	1.6	9.3	0.8345	1.0	8.88960	926.1000	-33.1500
Acrylonitrile	3.0	17.0	0.7898	1.0	9.04120	1208.2985	-51.1500
Ammonia	16.0	25.0	0.9135	2.0	9.48540	926.1300	-32.9800
Boron Trichloride	0.0	0.0	0.8681	1.0	3.95145	973.9950	-38.9940
Bromine	0.0	0.0	0.7050	2.0	9.00600	1121.4900	-51.5600
Carbon Monoxide	10.9	74.0	0.7272	1.0	8.36500	230.2700	-13.1500
Chlorine	0.0	0.0	0.7467	2.0	9.05670	859.1700	-27.0100
Dimethyl Ether	3.4	18.0	0.7798	1.0	9.44130	1025.5600	-17.1000
Ethylene	2.7	36.0	0.7652	1.0	8.87240	585.0000	-18.1500
Ethylene Oxide	3.0	100.0	0.7872	1.0	4.38580	1114.9850	-29.0300
Hydrogen	4.0	75.0	0.6868	1.0	8.04571	71.6152	3.1900
Hydrogen Chloride	0.0	0.0	0.8011	1.0	9.29250	744.5000	-14.4500
Hydrogen Cyanide	5.6	40.0	0.2890	2.0	9.29670	1122.9900	-37.1500
Hydrogen Flouride	0.0	0.0	0.7049	1.0	9.81000	1478.5400	13.0600
Hydrogen Sulphide	4.3	45.5	0.6827	4.0	9.11878	768.1323	-26.0600
Iso-Butane	1.8	8.4	0.7654	1.0	8.94417	912.1410	-29.8080
Methane	5.0	15.0	0.7339	1.0	8.73670	389.9300	-7.1600
Methyl Bromide	10.0	16.0	0.7885	1.0	9.08460	986.5910	-34.8300
Methyl Chloride	10.7	12.4	0.7325	1.0	9.11930	902.4510	-29.5500
n-Butane	1.8	8.5	0.7801	1.0	8.85000	909.6500	-36.1456
Nitric Oxide	0.0	0.0	0.7525	1.0	10.86780	682.9300	-4.8800
Nitrogen Dioxide	0.0	0.0	0.0641	3.5	11.04190	1798.5200	3.6500

Table IV: Physical properties of permitted materials in ADMS-Puff, part 2 continued.

Name	Lower Flammability Limit (% v/v)	Upper Flammability Limit (% v/v)	Prandtl Number	Toxic Exponent	Antoine A	Antoine B (K)	Antoine C (K)
Oxides of Nitrogen <sup>4</sup>	0.0	0.0	0.0641	3.5	11.04190	1798.5200	3.6500
Oxygen	0.0	0.0	0.7128	1.0	8.81630	319.0100	-6.4500
Phosgene	0.0	0.0	0.5379	1.0	8.96790	941.2500	-43.1500
Propane	2.1	9.5	0.6924	1.0	8.98292	819.2960	-24.4170
Propylene	2.0	11.0	0.7556	1.0	8.94450	785.0000	-26.1500
Propylene Oxide	2.1	21.5	1.5268	1.0	8.77950	915.3100	-64.8700
Sulphur Dioxide	0.0	0.0	0.9385	2.0	9.40710	999.8980	-35.9700
Trimethyl Amine	2.0	11.6	0.7372	1.0	9.09530	968.7000	-39.1500
Vinyl Chloride	3.6	33.0	0.6524	1.0	8.62200	783.3980	-43.1500

<sup>4</sup>In ADMS-Puff all NO<sub>x</sub> data in mass units are NO<sub>x</sub> as NO<sub>2</sub>, hence the properties of NO<sub>2</sub> are given here.



## Appendix B

### B.1 Glossary of symbols

$a_e$	Constant, used in determining the edge velocity of the puff, whose value depends on release type.
$A_e$	Entrainment area on side of puff.
$A_t$	Entrainment area on top of puff.
$b$	Parameter pertaining to the structure of the boundary layer, which depends on ratio of source height to boundary layer height. It is a function of $z$ , $z_s$ , $u_{*}$ , and $t$ .
$C$	Concentration.
$C_e$	Edge coefficient, a function of the Richardson number.
$C_{p_{air}}$	Specific heat capacity of air.
$C_{p_v}$	Specific heat capacity of material as vapour.
$F_{pert}, F_{mix}$	Factors relating ambient wind speed to advection velocity.
$g$	Acceleration due to gravity.
$h$	Height of release.
$H$	Boundary layer height
$h_{eff}$	Effective height, $0.56h$ .
$M_{mol}$	Molecular mass of the material.
$m_s$	Total mass released in an instantaneous puff.
$\dot{m}_s$	Release rate (mass per second) for a continuous release.
$\hat{m}_s$	As defined above, but at the source location.
$\hat{m}_t$	Either mass of an instantaneous puff or mass flux $\dot{m}_t$ of a puff representing a continuous release.
$N$	The buoyancy frequency.
$P_a$	Ambient pressure.
$r$	Puff radius.

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$R$	Universal gas constant.
$Ri$	The Richardson number.
$RiC$	At each output location, the sum over all puffs of the Richardson number multiplied by concentration, i.e. $\sum_{n=1}^{n_{puff}} Ri_n \cdot C_{pass_n}(x, y, z)$ .
$t$	Time since start of release.
$T_a$	Ambient temperature.
$t_{puff}$	The release time of an individual puff.
$T_s$	Temperature of release.
$u_*$	The friction velocity.
$U_a$	Advection velocity of puff.
$U_e$	Velocity at the side of the puff.
$U_f(t)$	Front velocity, only an integrated parameter for an instantaneous release.
$U_t$	Velocity at the top of the puff.
$U_w$	Ambient wind speed.
$\hat{v}$	Volume $v$ or volume flux $\dot{v}$ of the release.
$\hat{v}_s$	As defined above, but at the source location.
$w_s$	Width of release.
$x(t)$	Location of the puff at time, $t$ .
$x_c, y_c, z_c$	The location of the puff centre.
$\Delta\rho$	Density difference.
$\kappa$	Von Kármán constant.
$\lambda$	Weighting factor between passive and dense concentrations used in calculating the final concentration at an output location, a function of the Richardson number.
$\rho_a$	Ambient density.
$\rho_s$	Density of release.

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$\sigma_x, \sigma_y, \sigma_z$  Spread parameters.

$\bar{\sigma}_x, \bar{\sigma}_y, \bar{\sigma}_z$  The values the spread parameters would take were the met conditions to remain constant since the start of the release.

$\sigma_u, \sigma_v, \sigma_w$  Components of turbulent velocity.





## Appendix C

### C.1 Comparison to GASTAR

In order to establish the accuracy of ADMS-Puff, comparisons have been made to GASTAR. GASTAR is a well validated dense gas release model<sup>5</sup> suitable for modeling many types of dense gas release with spatially and temporally homogeneous meteorological data. Comparisons are made for both instantaneous and continuous releases for a period when the release remains dense. Comparisons cover all three atmospheric stability types.

The scenarios investigated are

1. A 100kg instantaneous release of chlorine from a 3m wide source. Output is given at 2 minutes after the release start time for stable, neutral and convective conditions. Output after 10 minutes is also given for the stable condition. At this time, the puff has become passive for the neutral and convective conditions and so a comparison to GASTAR is not appropriate.
2. A continuous release of 360000kg of chlorine from a 3m wide source lasting 1 hour. Output is given 15 minutes after the release start time for stable, neutral and convective conditions.

The various atmospheric conditions were defined as shown in the table below.

**Table V: Meteorological conditions for representative atmospheric stability types.**

Condition	Date	Time	Wind speed (m/s)	Temperature (°C)	Cloud cover (oktas)	Monin-Obukhov length (m) (GASTAR only)
Stable	Jan 29	1300	2	0	8	34.48
Neutral	May 06	0700	2	12	0	833.33
Convective	Jun 29	1300	1	20	0	-3.52

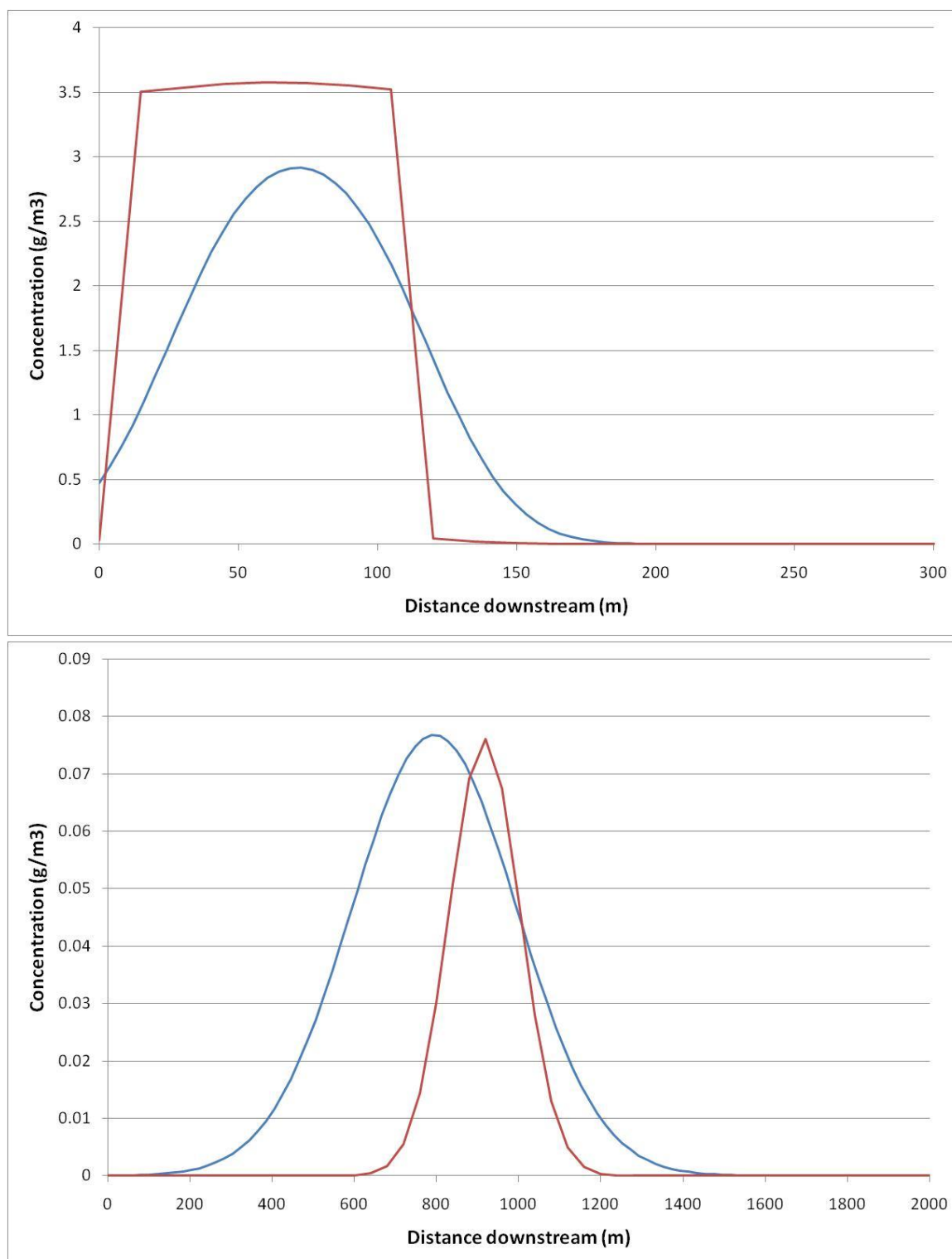
The figures below show the output from GASTAR and ADMS-Puff for each of these scenarios. The curves show the ground level concentrations at the plume centre line.

First Figure 25 - Figure 27 show that for scenario 1 the results match well. The magnitude of the maximum concentrations, the width of the distribution and the location of the maximum match well in all cases. In ADMS-Puff the distribution shows the puff to be better mixed than the distribution seen in GASTAR. Note that the lower plot in Figure 25 shows the results for scenario 1 after 10 minutes for the stable atmosphere. Here the peak concentrations again match very well, but the location in ADMS-Puff is shifted slightly

<sup>5</sup> See for example "Hazardous Gas Model Evaluation With Field Observations", SR Hanna, JC Chang, DG Strimaitis, Atmos. Env., Vol 27A, Issue 15, pp 2265-2285 (1993), Pergamon Press; or "Evaluation of 14 hazardous gas models with ammonia and hydrogen fluoride data", SR Hanna, DG Strimaitis, JC Chang, J. Haz. Mat., Vol 28, pp 127 – 158, (1991), Elsevier Science Publishers.

downstream and the width of the distribution is narrower. In this case both distributions are Gaussian in shape. At this time the puff is just reaching ambient density and as GASTAR and ADMS-Puff have different algorithms once the puff has become passive some differences in the solution may be expected at this stage.

Finally Figure 28 – Figure 30 show that the results agree excellently for the continuous case for stable, neutral and convective conditions. The shape of the distributions match very closely and the curves virtually coincide.



**Figure 25: Scenario 1 – results from ADMS-Puff (red) and GASTAR (blue) for an instantaneous chlorine release after (a) 2 minutes in stable conditions (top) and (b) 10 minutes in stable conditions (bottom) .**

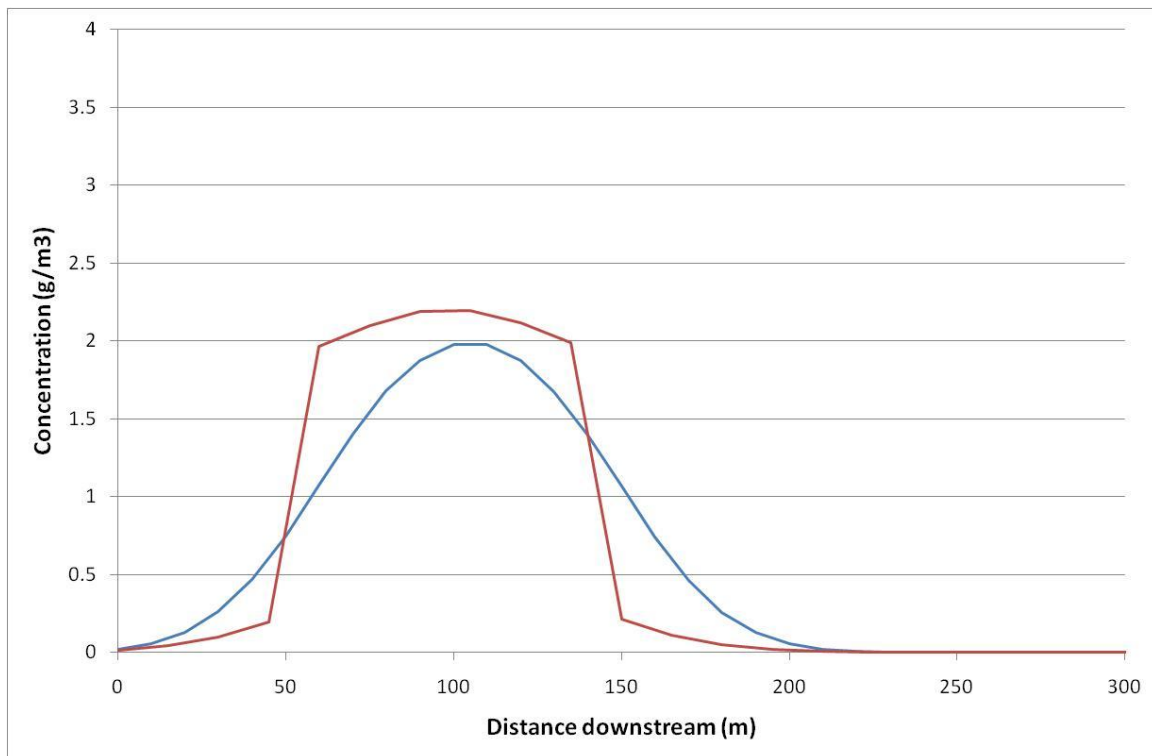


Figure 26: Scenario 1– results from ADMS-Puff (red) and GASTAR (blue) for an instantaneous chlorine release after 2 minutes in neutral conditions.

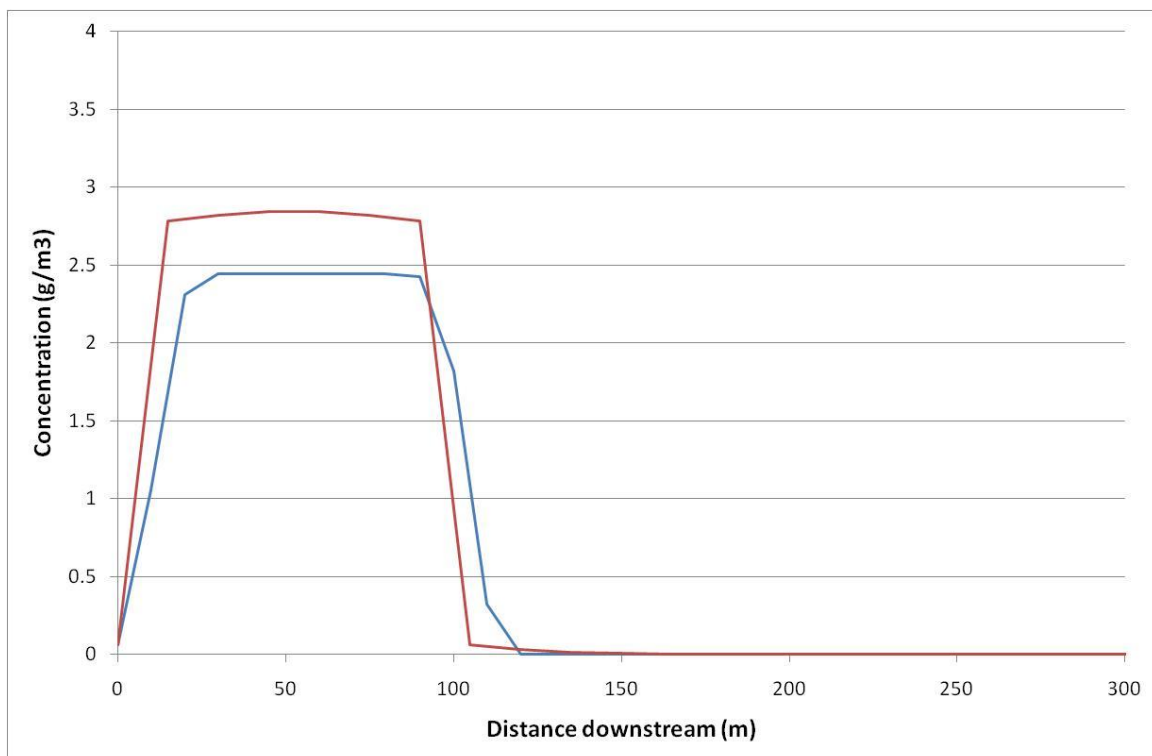
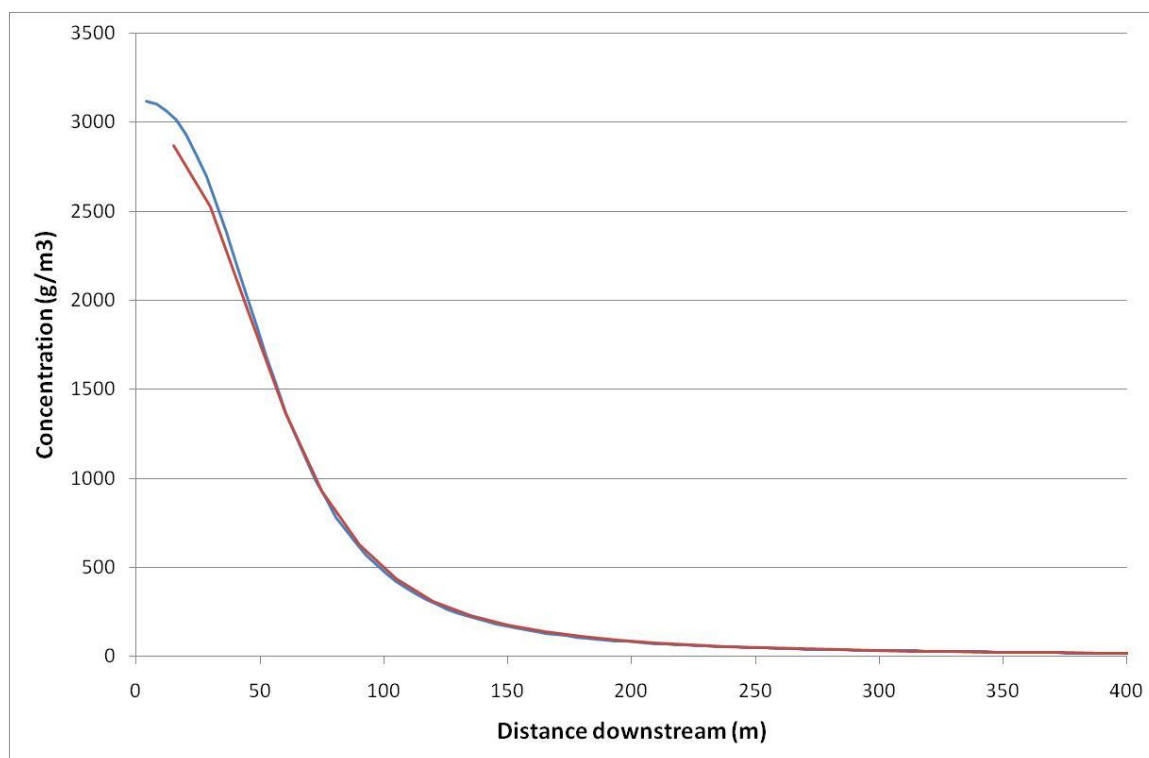
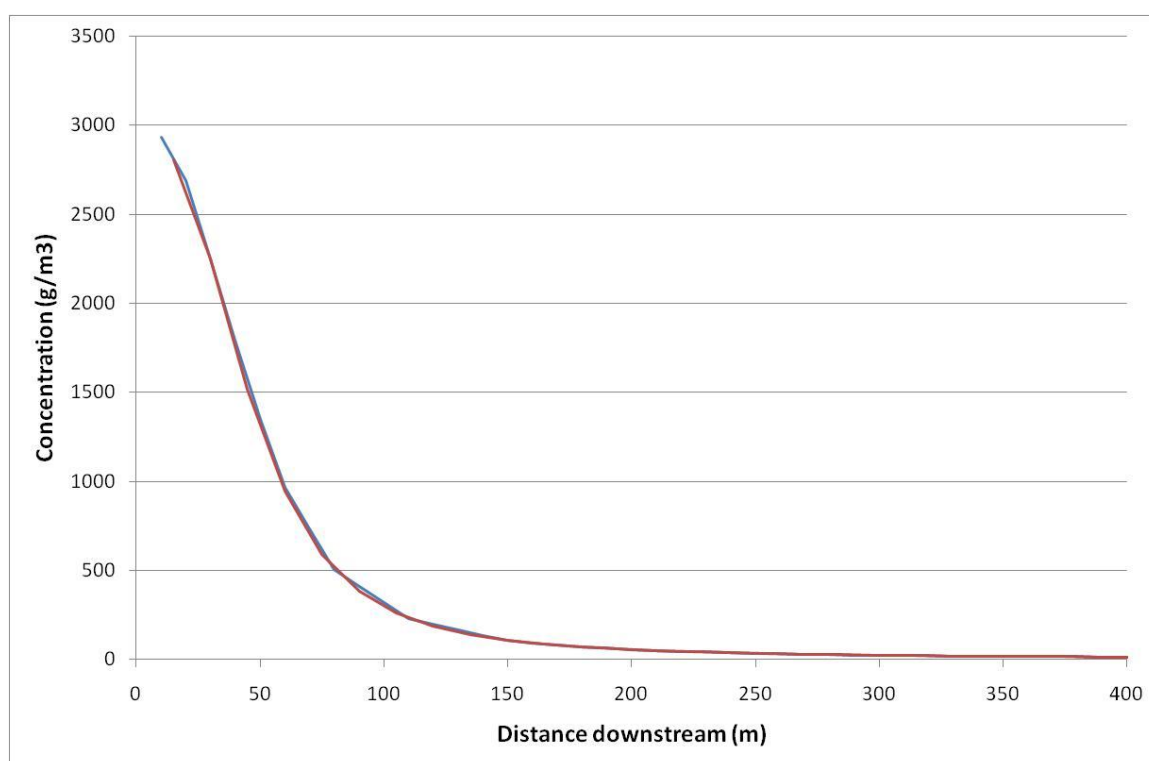


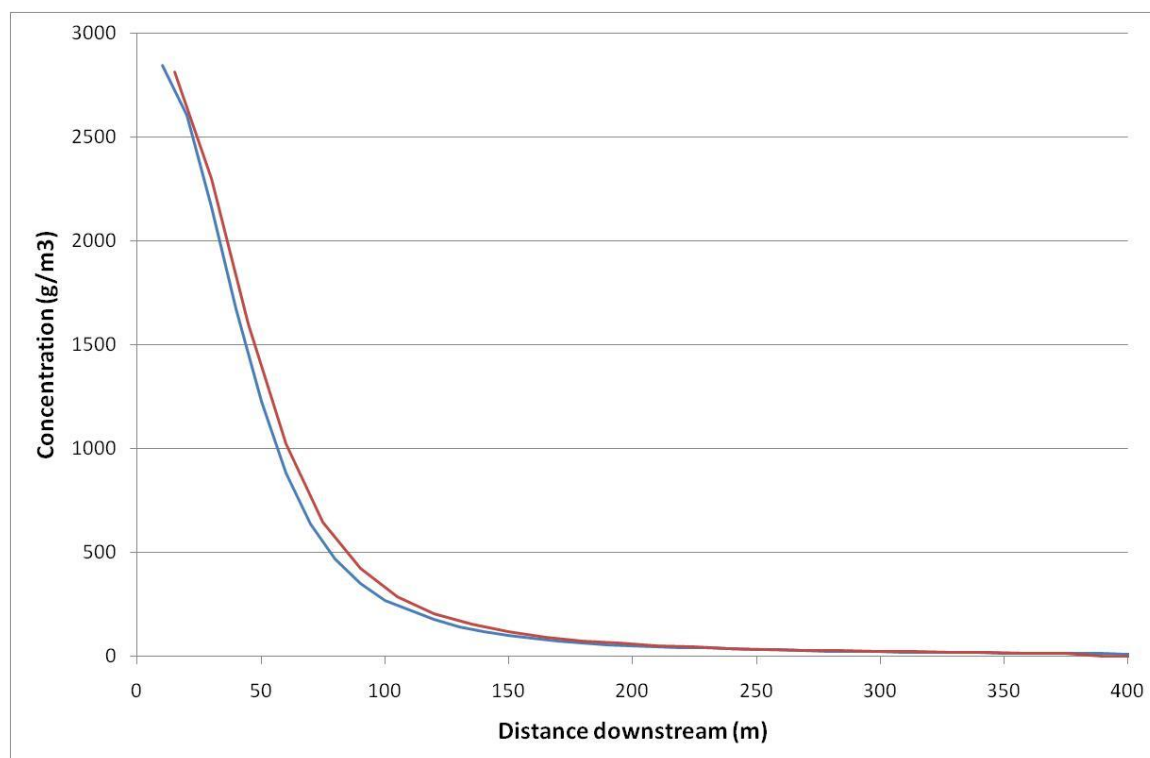
Figure 27: Scenario 1 – results from ADMS-Puff (red) and GASTAR (blue) for an instantaneous chlorine release after 2 minutes in convective conditions.



**Figure 28: Scenario 3 – results from ADMS-Puff (red) and GASTAR (blue) for a continuous chlorine release after 15 minutes in stable conditions.**



**Figure 29: Scenario 3 – results from ADMS-Puff (red) and GASTAR (blue) for a continuous chlorine release after 15 minutes in neutral conditions.**



**Figure 30: Scenario 3 – results from ADMS-Puff (red) and GASTAR (blue) for a continuous chlorine release after 15 minutes in convective conditions.**



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