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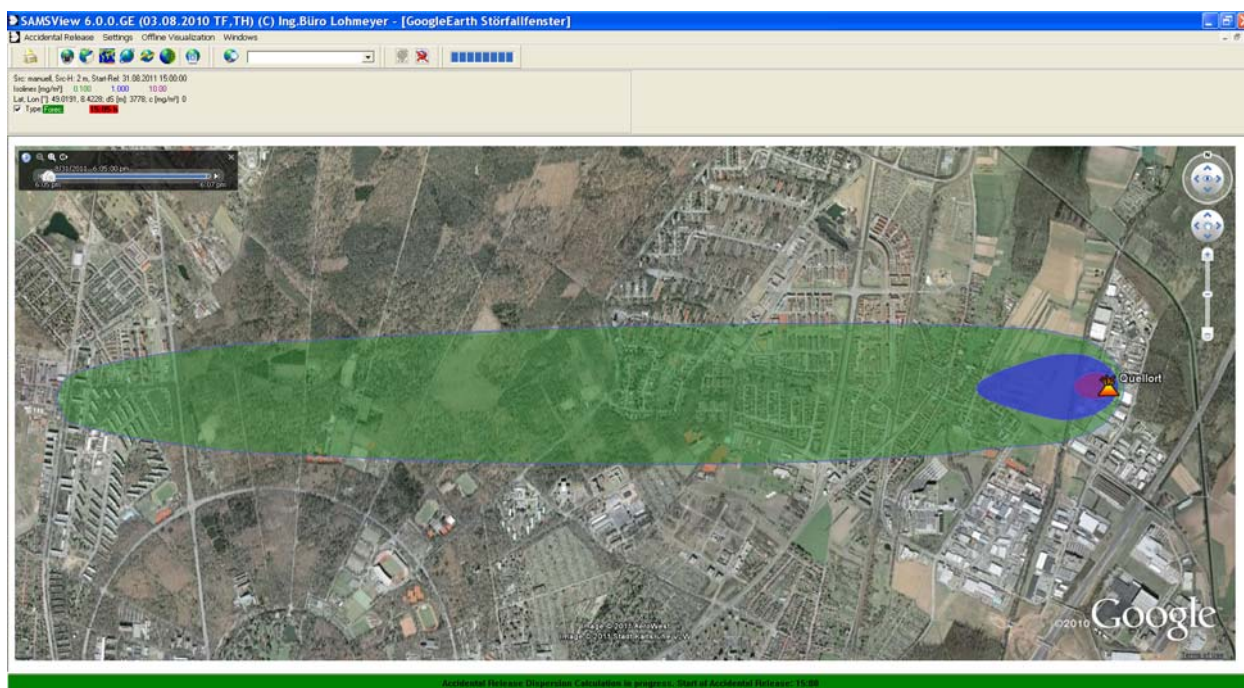
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SAMS-GLOBAL *DOCUMENTATION*



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1 WHAT IS SAMS-GLOBAL?

SAMS-GLOBAL is a PC-based system that simulates the dispersion of air pollutants. After an accidental release either in a stationary facility or during transport, it calculates the instantaneous and future concentrations of airborne pollutants in both the immediate and wider area around the release location (about 30 km x 30 km), taking into account meteorological conditions. This allows the user to identify at-risk areas and to take prompt action using targeted methods. The calculation results are shown as isolines of concentration on an area map.

During an accidental release calculation, SAMS-GLOBAL calculates a current **Diagnosis** (=concentration dispersion at the present time) and a **Forecast** (= expected concentration distribution in the future up to a maximum two hours ahead). The calculations for a selected day can be started up to five days in advance. The Diagnosis is updated every three minutes.

The SAMS-GLOBAL basic version includes the following modules:

- Gaussian Puff Model based on the guideline VDI 3945 sheet 1
 - Diagnostic mesoscale wind field model for complex terrain, used for processing meteorological data (10-minute average of wind speed, wind direction, turbulence, and atmospheric stability) from one or several meteorological stations
 - Release rate modelling for gases, liquids and liquid gases with pool vaporization or evaporation from a pool.
 - Database of substances and scenarios
-

2 STARTING ALL SYSTEM COMPONENTS

All components needed for accidental release calculation are started automatically when the computer is started up. These components include:

- The program SAMS.exe (control program including updating of meteorology; located in the folder "[InstallDir]\SAMS.exe"¹)
- The program SAMSView5.exe (interface for menu- and dialog-controlled input and for the graphical display of calculation results "[InstallDir]\elisin\SAMSView5.exe")
- GPMain.exe (Gaussian Puff dispersion model, started automatically by SAMS.exe).

The task bar shows that the three components have been started correctly:



After a system failure (e.g., power outage), all components will be restarted automatically. If one of the components is closed by mistake, it can easily be started from the SAMS-GLOBAL folder on the computer desktop.

IMPORTANT NOTES:

1. If the Gaussian Puff Model is accidentally closed but the SAMS.exe program is not, then SAMS.exe must be closed and started again so that the Gaussian Puff Model can also be restarted.
2. Please bear in mind that neither SAMS.exe nor SAMSView5.exe can be started a second time manually.
3. The SAMS.exe program must be running continuously (even if no accidental release calculation is in progress) so that meteorology time series can be recorded correctly.
4. After closing an accidental release calculation, neither SAMS.exe nor SAMSView5.exe needs to be closed and restarted. A new accidental release calculation can be started immediately.

¹ [InstallDir] is the SAMS-GLOBAL installation directory.

3 THE MAIN COMPONENTS OF SAMS-GLOBAL

3.1 The control components SAMS.exe

When "[InstallDir]\SAMS.exe" is started, a window appears with the following three status windows: "Messages", "GP Model" and "Diagnoses on Order" (see **Fig. 3.1**):

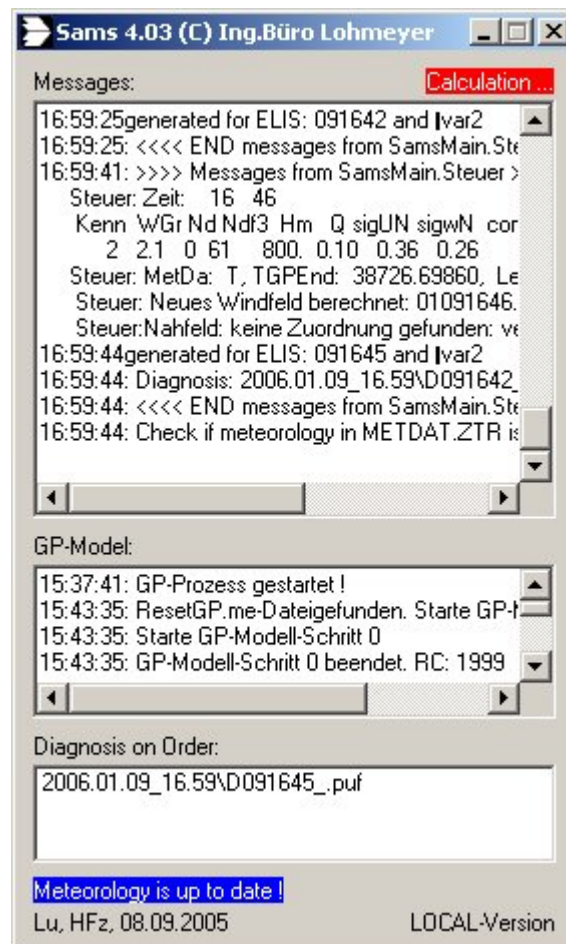


Fig. 3.1: Window **Sams 4.x** with three status windows for messages

IMPORTANT NOTE:

The messages shown by SAMS.exe in the three status windows serve the purpose of giving information on the current status of the system. The three status windows provide no accidental-release-relevant information. All accidental-release-relevant information is shown and supplied through the SAMSView5.exe program.

In the status window "Messages" appear the following:

- Work reports from the SAMS control program
- Information on the current meteorological file
- Information on the isoline file currently available for display
- Information on system status, and, if applicable, properties data for the accidental release calculation then in progress

The status window "GP Model" has the function of:

- Logging the calculation steps that are performed every three minutes during an accidental release calculation

The status window "Diagnoses on Order" has the function of:

- Logging all isoline files that are available for calculation

At the top right of the window is information on whether the system is currently carrying out a calculation



or whether it is waiting, i.e. is in stand-by mode.



IMPORTANT NOTE:

Accidental release calculations are started and closed using the program SAMSView5.exe, not SAMS.exe.

3.2 SamsView, the graphical user interface

Fig. 3.2 shows the Windows interface of the program SAMSView5.exe (referred to below as **SAMS-View**). The visualisation of the dispersion of air pollutant is shown in **Google Earth**². The **SAMS-View** program's menu bar includes the menu items "Accidental Release", "Settings", "Offline Visualization", and "Windows". In the "Accidental Release" menu, an accidental release calculation can be started or closed. The menu item "Settings" allows the user to change the scaling of isoline values during an accidental release calculation and to call up a graphic of the temporal course of release. Substance data and scenarios can be input in offline mode. The menu item "Offline Visualization" makes it possible to display isolines from previous accidental release calculations.

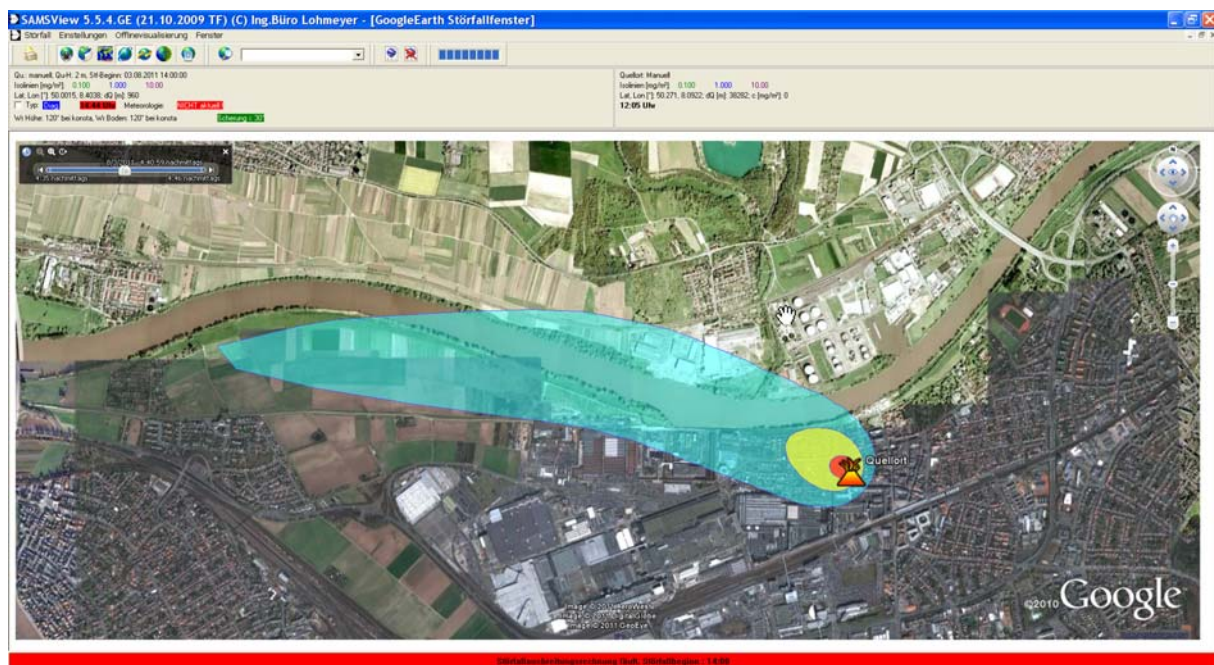


Fig. 3.2: The program SAMSView5.exe

² The visualisation with Google Earth works only if the PC is connected with the Internet.

4 PERFORMING AN ACCIDENTAL RELEASE CALCULATION

If all the system components described in Section 2 are active, an accidental release calculation can be started.

To start an accidental release calculation, go to the program **SAMView** and click the menu item "Accidental Release". This menu item offers the following submenu positions (see **Fig. 4.1**):

- Start Accidental Release Calculation ...
- Close Accidental Release Calculation ...
- Print ...
- Close

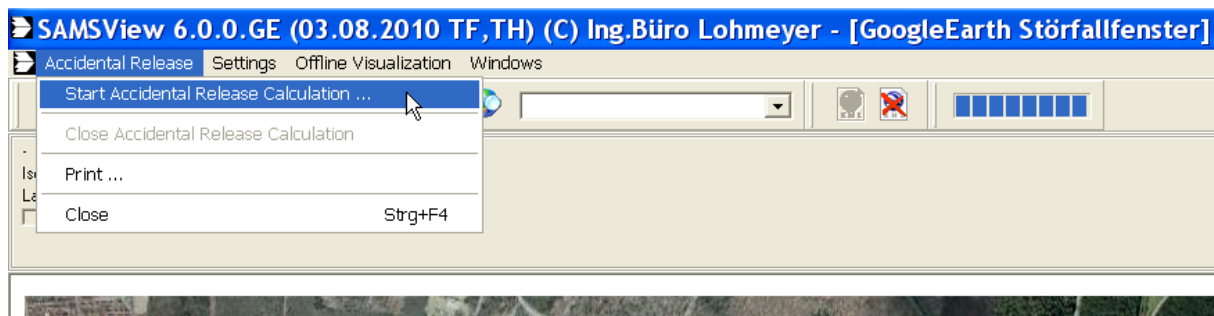


Fig. 4.1: The **SAMView** program with the "Accidental Release" menu

4.1 The "Accidental Release Calculation" window: the necessary parameters

Clicking on "Start accidental release calculation..." opens the "Accidental Release Calculation" window (see **Fig. 4.2**), which requests the parameters that are always necessary for an accidental release calculation.

Accidental Release Calculation

Start of Release

Current Time

Time Date

End of Release

Release continues

Release Location

Select from List

Geographical Coordinates

Lat N S

Lon W E

[GoogleEarth](#)

Wind Direction °

Wind Speed m/s

Anemometer H. m

Stability

Release ...

Isolines ...

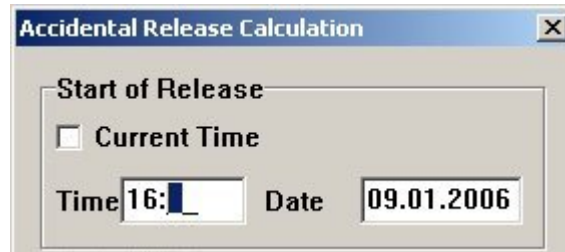
Additional Parameters ...

Cancel OK


Fig. 4.2: The "Accidental Release Calculation" window

The **necessary parameters** include release location and **Start of Release**, which must lie within the bounds set by the meteorology time series (see **Chapter 2.1**).

The start of release field is automatically filled with the current time. If this value differs from the start of release, then the correct time can be entered manually by deactivating the checkbox "Current Time".



If the **End of Release** time is known³, it should likewise be entered by disabling the checkbox "Release continues".

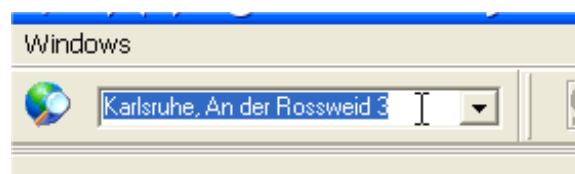


If no entry is made, it will be assumed that release is continuous up to the end of the accidental release.

The **Release Location** can be selected either by enabling the checkbox "Select from list" on the scroll box, by using the keyboard or by clicking the release location on the map⁴. If the release location wants to be entered by clicking on the map the button



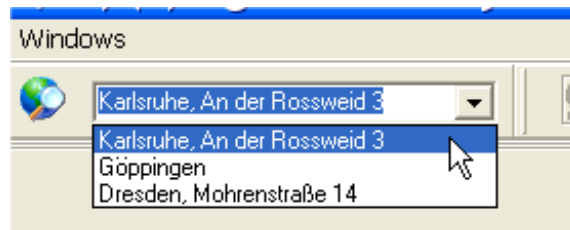
must be pressed. The map of the desired location can be shown when entering street and city name in the following edit field.



The entries from this edit field are stored in a list. Locations can be re-selected later from that list.

³ The end of release can also be entered at a later time.

⁴ Works only when the Google Earth Plugin is installed and the PC is connected with the Internet.



The meteorological data “wind direction”, “wind speed”, “anemometer height” and “stability“ have to be entered manually in the "Accidental Release Calculation" window.

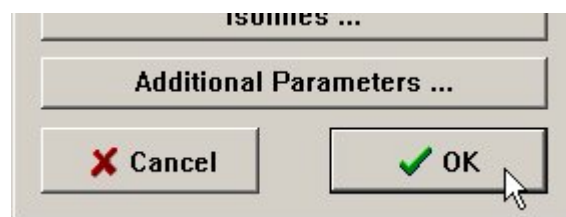
| | | |
|--------------|--------------------------------------|-----|
| Windrichtung | <input type="text"/> | ° |
| Windgeschw. | <input type="text"/> | m/s |
| Anemometerh. | <input type="text" value="10"/> | m |
| Stabilität | <input type="text" value="neutral"/> | |

IMPORTANT NOTE:

Optional parameters (the buttons "Release ...", "Isolines ..." and "Additional Parameters...") can be entered at this time or later.

If the button [**Release...**] is not pressed, then the standard setting will be used which assumes a chlorine gas release with a constant mass flow of 0.1 kg/s. The isoline values are pre-set at 0.1 mg/m³, 1 mg/m³ und 10 mg/m³.

Clicking "OK" to confirm the values in the **Accidental Release Calculation** window will start the accidental release calculation.



On the bottom frame of **SAMSVIEW** appears the message (blinking alternately red and green): "Accidental Release Dispersion Calculation in progress. Start of Accidental Release..."



Accidental Release Dispersion Calculation in progress. Start of Accidental Release: 09:00

After a short time (about 20 seconds) the isolines of pollutant concentration (cf. **Fig. 4.3**) for the first display date will appear on the map.



Fig. 4.3: Three isolines of pollutant concentration

Normally three isolines of pollutant concentration will be shown, coloured green, blue and purple. The concentration values corresponding to the colour are shown in the Information Bar described below.

An isoline of pollutant concentration forms a boundary around an area. The concentration is higher inside the area bounded by the isolines and lower outside. Unless the user enters different inputs in the **Isolines** window, the green isoline represents the lowest pollutant concentration while the purple isoline represents the highest.

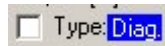
In the **Information Bar** (cf. **Fig. 4.4**) on the Accidental Release window, the following information is shown:

- Line 1: Name of the source location (Src), source height (Src-H), start of accidental release (Start-Rel)
- Line 2: Values of the isolines shown for concentration at 1.5 m above the ground
- Line 3: Current position of the cursor on the base map as northing/easting, distance from source in meters (dS), and concentration in [mg/m³]
- Line 4: Diagnosis/Forecast, date shown.

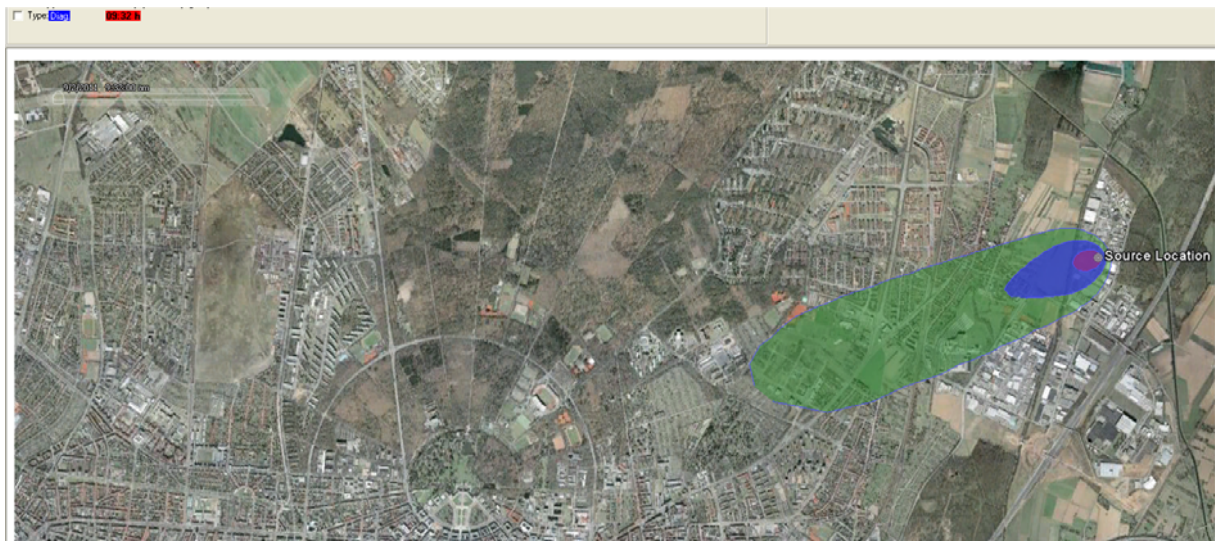


Fig. 4.4: Information Bar during an accidental release calculation

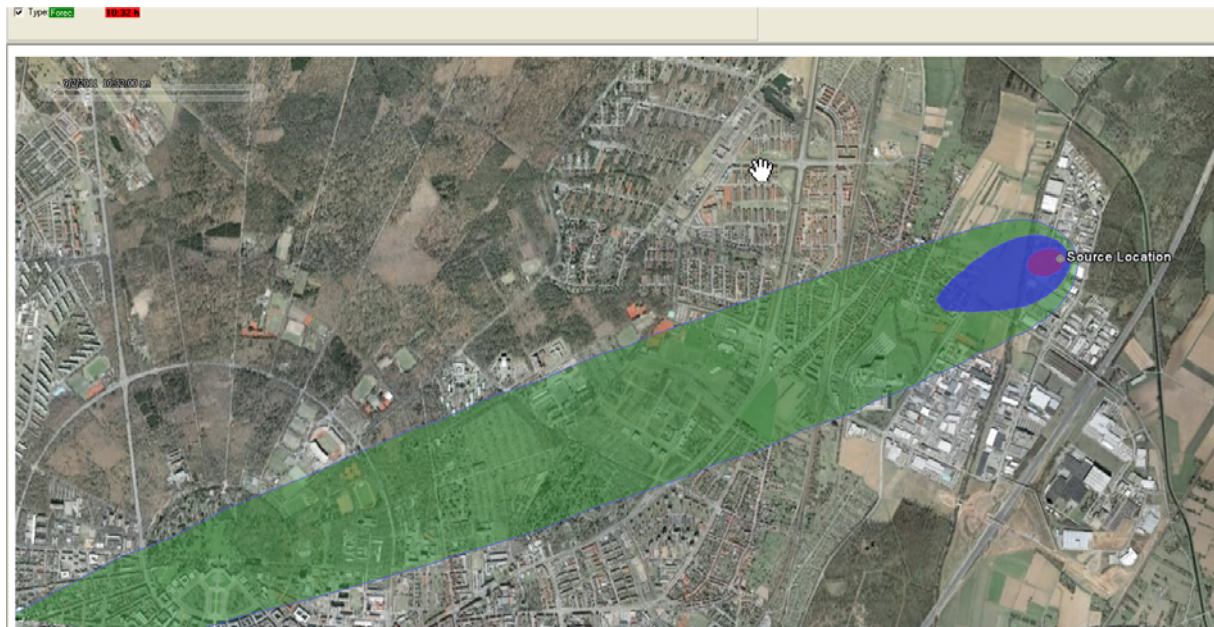
Diagnoses are displayed by default setting. In the Information Bar, the checkbox "Type" is not checked:



"Diag." appears on a blue background. By way of example, the concentration for 9:32h pm is shown:



If the "Type" checkbox on the Information Bar is checked, the Forecast will be displayed. "Forec." appears on a green background. In this case, the expected concentration for (e.g.) 10:32h pm is shown (the forecasting horizon is here set at 60 minutes; see the **Additional Parameters** window):



The displayed window can be printed by clicking the printer symbol (or by clicking the menu item "Accidental Release | Print..."):



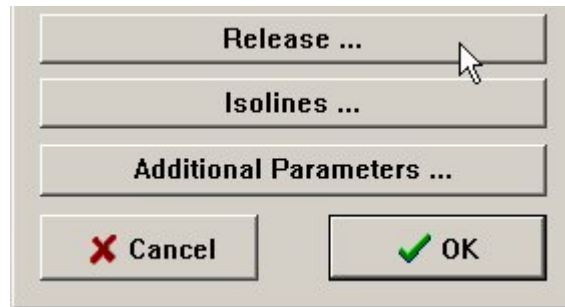
All additional functionalities of **SAMView** for use during an accidental release calculation are explained in **Chapter 5**.

4.2 Optional parameters for accidental release calculation

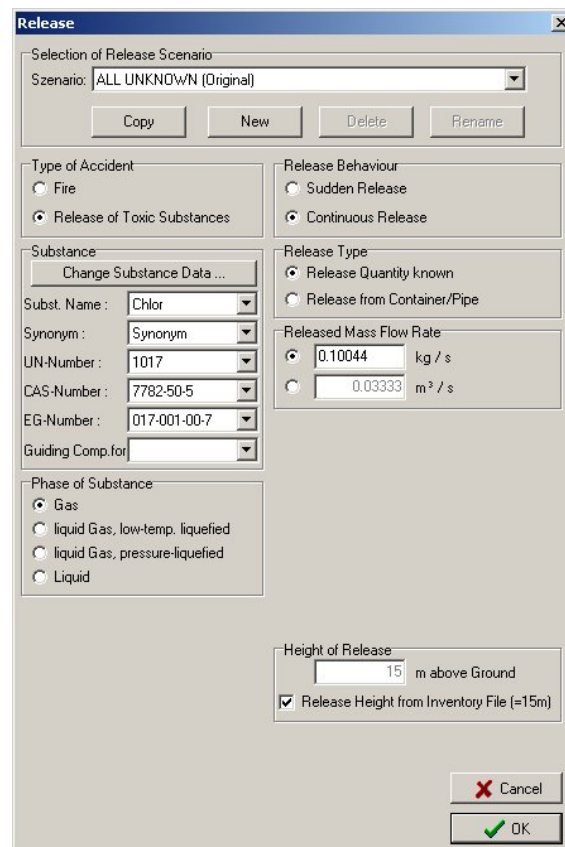
The optional parameters for accidental release calculation described below can be entered either at the beginning or during the course of an accidental release calculation or test calculation via the menu item "Accidental Release | Edit Accidental Release Parameters...". The **Accidental Release Calculation** window appears.

4.2.1 The Release window

The window in which the temporal course of release is input can be viewed by clicking on the **[Release...]** button of the **Accidental Release Calculation** window.⁵



If the **[Release...]** button is pressed, the **Release** window will appear:

A screenshot of the 'Release' dialog box. It has a title bar 'Release' and a close button. The dialog is divided into several sections:

- Selection of Release Scenario:** A dropdown menu showing 'ALL UNKNOWN (Original)'. Below it are buttons for 'Copy', 'New', 'Delete', and 'Rename'.
- Type of Accident:** Radio buttons for 'Fire' and 'Release of Toxic Substances' (selected).
- Release Behaviour:** Radio buttons for 'Sudden Release' and 'Continuous Release' (selected).
- Substance:** A 'Change Substance Data ...' button and dropdown menus for 'Subst. Name' (Chlor), 'Synonym' (Synonym), 'UN-Number' (1017), 'CAS-Number' (7782-50-5), 'EG-Number' (017-001-00-7), and 'Guiding Comp. for'.
- Release Type:** Radio buttons for 'Release Quantity known' (selected) and 'Release from Container/Pipe'.
- Released Mass Flow Rate:** Radio buttons for '0.10044 kg / s' (selected) and '0.03333 m³ / s'.
- Phase of Substance:** Radio buttons for 'Gas' (selected), 'liquid Gas, low-temp. liquefied', 'liquid Gas, pressure-liquefied', and 'Liquid'.
- Height of Release:** A text box with '15' and 'm above Ground'. A checked checkbox 'Release Height from Inventory File (=15m)'.
- Buttons for 'Cancel' and 'OK' at the bottom right.

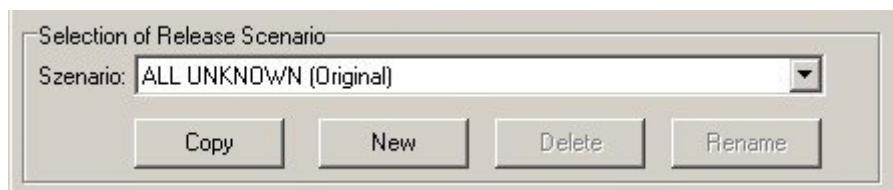
⁵ If the **[Release...]** button is not pressed, or if the **Release** window is exited using **[Cancel]**, then the standard setting of a chlorine gas release with a constant mass flow of 0.1 kg/s will be assumed.

Using this window, the temporal course of release – i.e., the quantity of the substance released in an accidental release – can be specified. A complete description of the **Release** window can be found in **Chapter 5.2**. This section of the manual only addresses the question of how to select a suitable pre-defined accidental release scenario. It should be noted that the temporal course of release can be changed during the course of an accidental release.

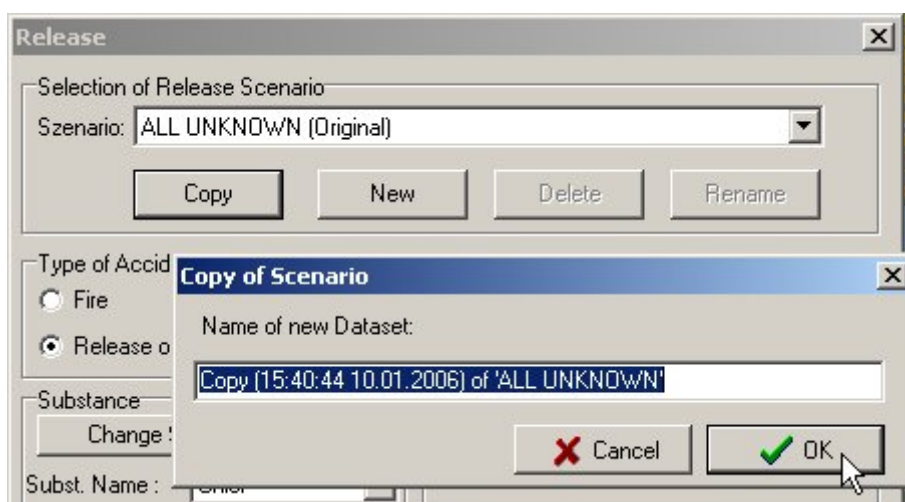
IMPORTANT NOTE:

A change in the temporal course of release has a retroactive effect back to the start of the accidental release, except in the case of release height. Changing the release height only impacts the calculation of concentration distribution beginning with the time of the change.

SAMS-GLOBAL files the possible paths of substance release using "release scenarios". Release scenarios that have been supplied in offline mode (cf. **Chapter 6.4**) can be called up in the **Release** window under "Selection of Release Scenario"



The scenario "ALL UNKNOWN (Original)" is always set when starting an accidental release calculation. This scenario represents a release of chlorine gas with a constant mass flow of 0.1 kg/s. A scenario with a name containing "(Original)" **cannot be modified** and is called a "**scenario template**". In order to modify a scenario template, it must first be copied by pressing the **[Copy]** button.



A scenario without the character string "(Original)" in the scenario name can be customized to fit the current accidental release (cf. **Chapter 5.2**).

SAMS-GLOBAL is delivered with the following three scenario templates:

- ALL UNKNOWN (Original)
- Fire major (Original)
- Fire medium (Original)

The scenario templates are defined in **Table 4.1**.

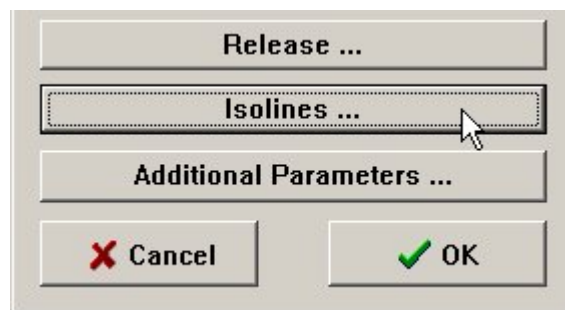
Table 4.1: Definition of the scenario templates

| Scenario name | Substance | Volume flow rate [m ³ /s] | Mass flow [kg/s] | Release height [m] |
|------------------------|--------------------|--------------------------------------|------------------|--------------------|
| ALL UNKNOWN (Original) | Chlorine (gaseous) | 0.03333 | 0.1 | 15 |
| Fire major (Original) | Carbon monoxide | 10 | ~ 12 | 50 |
| Fire medium (Original) | Carbon monoxide | 5 | ~ 6 | 25 |

A complete description of how to use the **Release** window can be found in **Chapter 5.2**.

4.2.2 The Isolines window

The window in which the three isoline values and the units are input can be viewed by clicking on the **[Isolines...]** button of the **Accidental Release Calculation** window.



The isoline values are pre-set at 0.1 mg/m³, 1 mg/m³ and 10 mg/m³. If the **[Isolines...]** button is pressed, the **Isolines** window will appear:

The screenshot shows the 'Isolines' dialog box with the following fields and controls:

- Isolines:**
 - Lower Isoline: 0.1 (with a 'Default' button)
 - Middle Isoline: 1
 - Upper Isoline: 10
- Unit:** Radio buttons for mg/m^3 (selected) and ppm.
- Conversion mg/m^3 into ppm and vice versa:**
 - Molar Mass: [] g/Mol
- Threshold Value:** []
- Unit:** Radio buttons for mg/m^3 (selected) and ppm.
- Buttons:** 'Get Molar Mass from DB', 'Get Threshold Value from DB', 'Cancel', and 'OK'.

The input fields for the three isolines contain the default setting mentioned above: The fields for Molar Mass and Threshold Value are initially empty. The option between the units " mg/m^3 " and "ppm" is disabled, and " mg/m^3 " is set as the unit.

The option is not activated until a valid value for molar mass is entered in the relevant field. The field Molar Mass can be filled either by pressing the button **[Get molar mass from DB]**⁶ or by inputting the value manually in g/Mol.

The field Threshold Value can be filled either by pressing the button **[Get threshold value from DB]** or by inputting the value manually in mg/m^3 or ppm.

IMPORTANT NOTE:

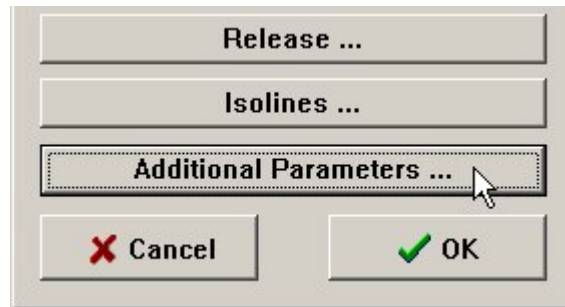
The molar mass entered in the **Isolines** window is used solely for converting mg/m^3 to ppm (and vice versa).

The threshold value entered in the Isolines window is used in displaying the concentration time series (see **Chapter 5.4**).

⁶ DB = database.

4.2.3 The Additional Parameters window

Optional parameters can be entered by clicking the **[Additional Parameters]** button of the **Accidental Release Calculation** window.



The **Additional Parameters** window will appear (see **Fig. 4.5**). This window allows the forecasting horizon to be set.

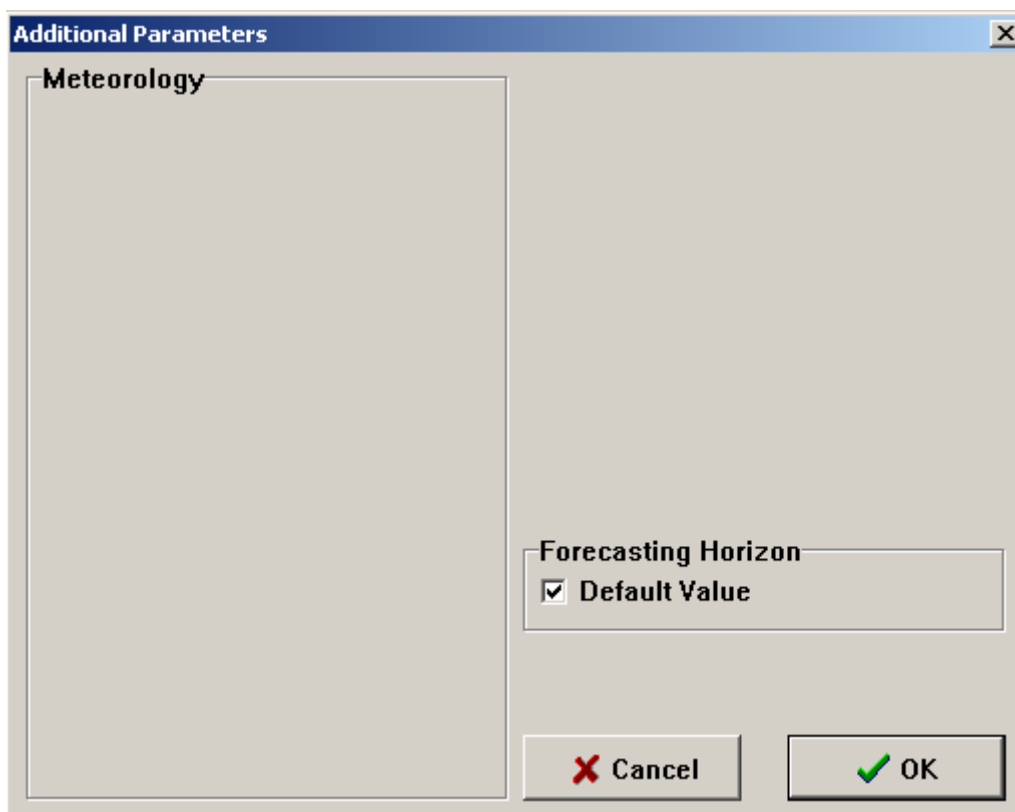
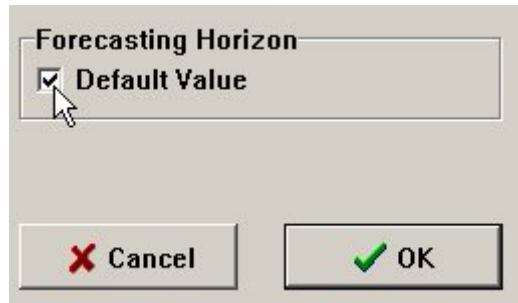


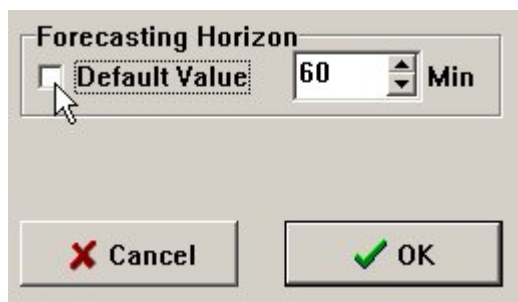
Fig. 4.5: The **Additional Parameters** window

Forecasting Horizon

In addition to Diagnoses, SAMS-GLOBAL is also able to calculate Forecasts. The forecasting horizon dialog allows the user to set how far into the future the calculation will go, starting at the current time. If "Default value" is selected, the forecasting horizon is 60 minutes:



If "Default value" is not selected, a forecasting horizon between 0 and 120 minutes can be input:



In calculating a forecast, it is assumed that meteorological conditions remain constant at current conditions.

SUMMARY:

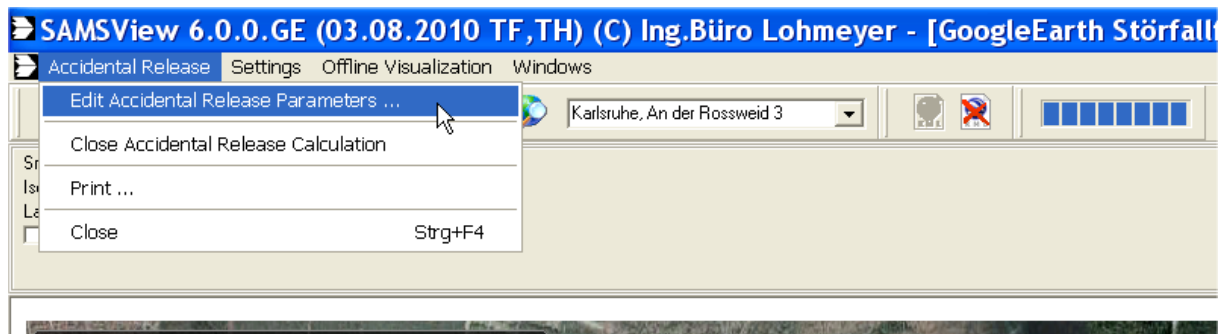
To start an accidental release calculation or a test calculation, the user must enter the answers for three questions into the system:

1. When? When is the start of accidental release? The start of accidental release should be entered, as well as the end of accidental release (if known).
2. Where? Where is the release location? The release location should be entered.
3. How much? How much of a substance was released? Either a release scenario should be selected, or a substance quantity should be entered. If no information on the released quantity is available, then the calculation can be made using a standard mass flow of 0.1 kg/s.

5 CONFIGURATION OPTIONS AND FUNCTIONS DURING AN ACCIDENTAL RELEASE CALCULATION

5.1 Menu item "Accidental Release | Edit Accidental Release Parameters..."

Under the menu item "Accidental Release", it is possible during an accidental release calculation to select the submenu position "Edit Accidental Release Parameters..."



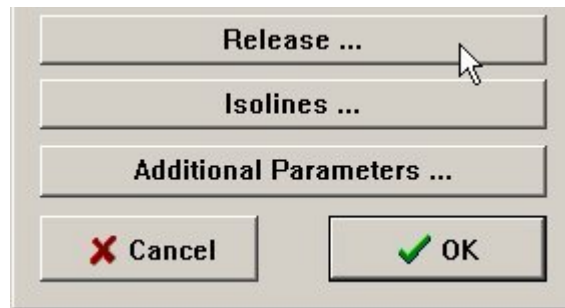
The **Accidental Release Calculation** window will appear (see **Chapter 4.1**). The following parameters can now be edited:

1. Input end of release.
2. Change the emission rate during an accidental release calculation. To do this, select the **[Release...]** button and edit the **Release** window⁷.
3. Changing the values of the isolines during an accidental release calculation: To do this, select the **[Isolines...]** button and edit the **Isolines** window. The new isoline levels will be retained until a new change is made.

5.2 The Release window

The window in which the temporal course of release is input can be viewed by clicking on the **[Release...]** button of the Accidental Release Calculation window.

⁷ A change in the temporal course of release has a retroactive effect back to the start of the accidental release, except in the case of release height. Changing the release height only affects the calculation of concentration distribution starting with the time of the change.



If the [Release...] button is pressed, the **Release** window will appear:

Using this window, the temporal course of release – i.e., the quantity of the substance released in an accidental release – can be specified.

The substance can be stored either

- as a gas,
- as a liquid, or
- liquefied by pressure or low temperature.

These storage conditions determine how it is released. Substances stored as gases enter the atmosphere directly after release. Substances that are stored as liquids or are liquefied by pressure or low

temperature normally form a pool upon being released and then vaporize or evaporate from the pool. Pressure-liquefied substances undergo what is called "flash evaporation". The droplets are atomized and sprayed into the atmosphere, partially vaporizing. The possible paths of substance release are shown in **Fig. 5.1**.

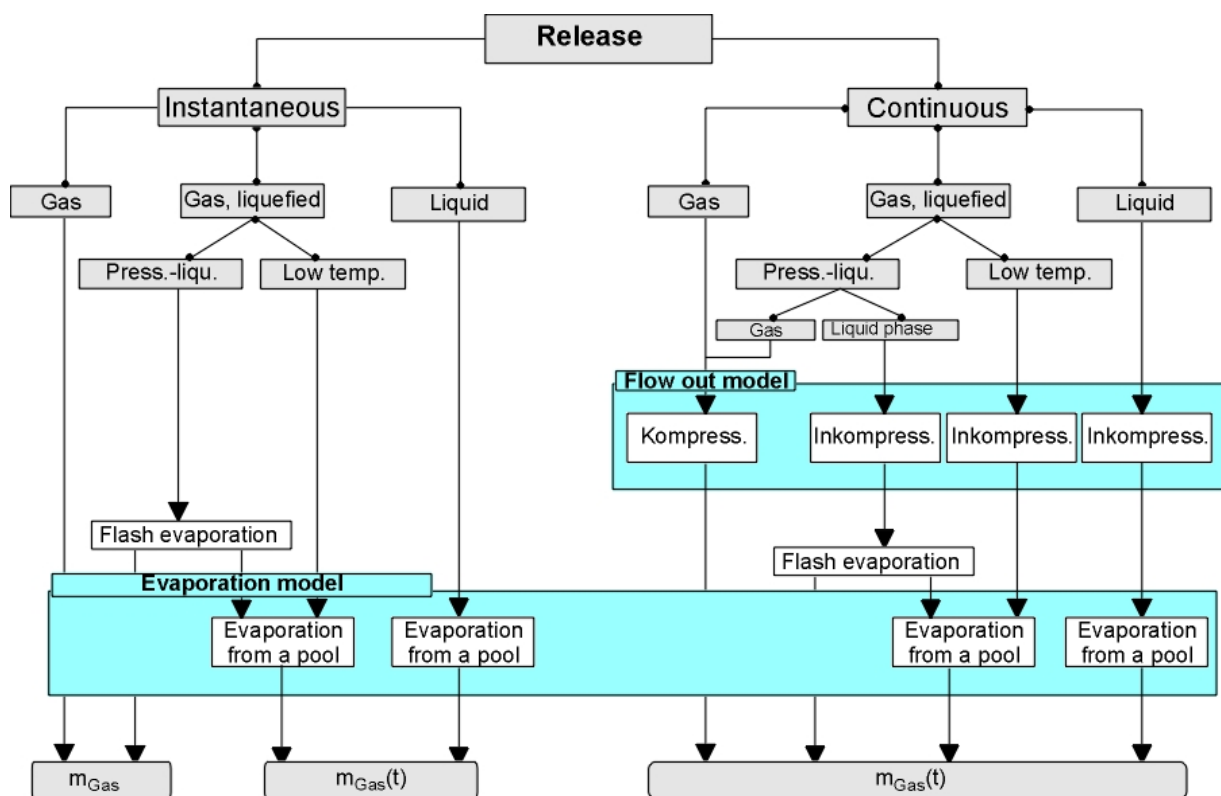
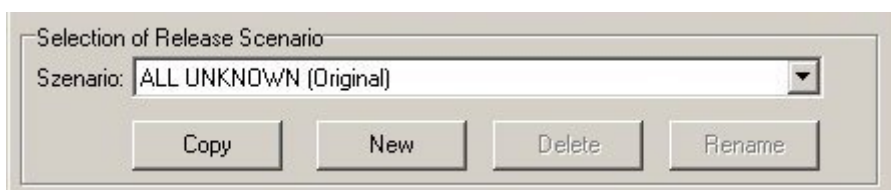


Fig. 5.1: Paths of substance release

5.3 Selecting the release scenario

SAMS-GLOBAL files the possible paths of substance release using "release scenarios". Release scenarios that have been supplied in offline mode (cf. **Chapter 6.4**) can be called up in the **Release** window under "Selection of Release Scenario"

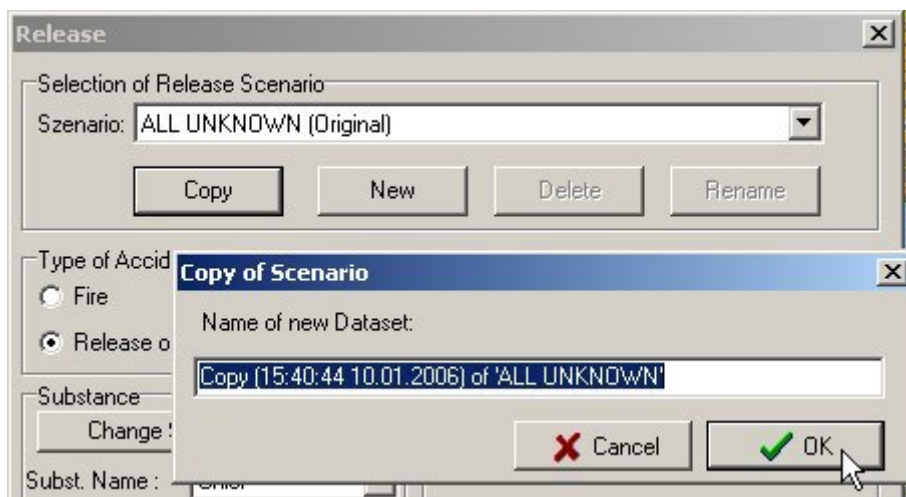


When starting an accidental release calculation, the scenario "ALL UNKNOWN (Original)" always appears as the default setting. This scenario represents a release of chlorine gas with a constant mass flow of 0.1 kg/s. A scenario with a name containing "(Original)" cannot be modified and is called a "scenario template". SAMS-GLOBAL is delivered with the following three scenario templates (cf. **Table 4.1**):

- ALL UNKNOWN (Original)
- Fire major (Original)
- Fire medium (Original)

Copy

In order to modify a scenario template, it must first be copied by pressing the **[Copy]** button. The name of the new scenario is requested:



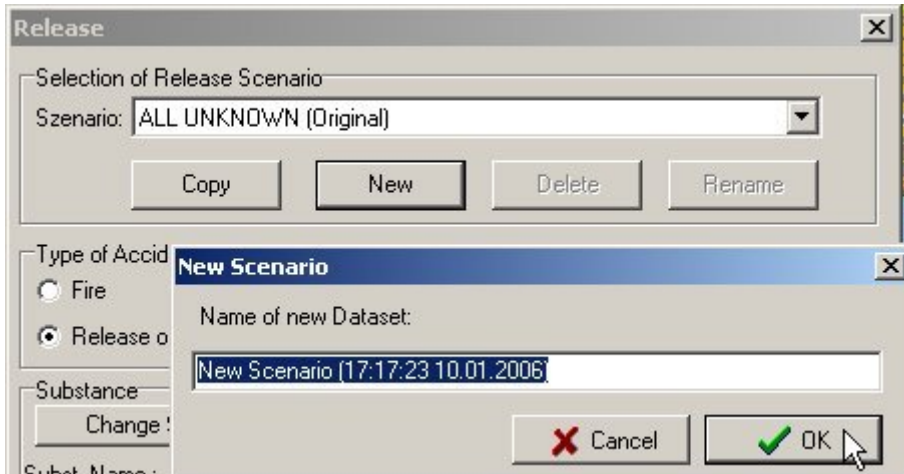
For the copy of a scenario, the name:

Copy (today's date) of "Name of the scenario to be copied, without the text string '(Original)'"

will be suggested. This suggestion can be changed. It should be noted that copies of templates containing the text string "(Original)" will become scenario templates that cannot be modified. The name of the copied scenario should be confirmed by clicking the **[OK]** button. After this, settings in the copied scenario can be made as desired.



To define a new scenario, press the **[New]** button. The name of the new scenario is requested:



For a new scenario, the name:

New scenario (today's date)

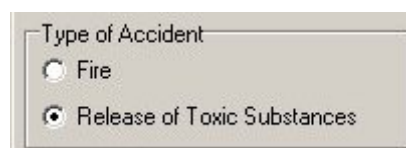
will be suggested. This suggestion can be changed. It should be noted that new scenarios containing the text string "(Original)" will become scenario templates that cannot be modified. The name of the new scenario should be confirmed by clicking the **[OK]** button. After this, settings can be made in the new scenario as desired.



Scenarios that do not contain the text string "(Original)" can be deleted or renamed. For scenarios containing the text string "(Original)", these buttons are disabled.

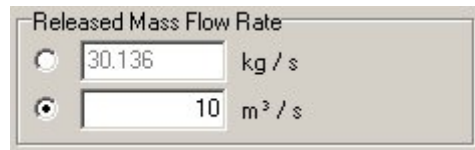
5.3.1 Type of Accident

The "Type of Accident" dialog makes it possible to inform the system as to whether the incident is a fire or (and) the release of a toxic substance.



"Fire" represents a subset of possibilities under "Release of toxic Substances". Accordingly, many input fields that appear in the case of "Release of toxic Substances" are invisible here. For a fire,

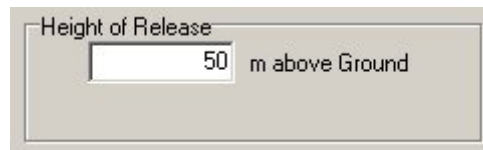
gaseous release is assumed. The substance is pre-set as carbon monoxide. If necessary, the substance can be modified. The released volume flow rate should be entered in m³/s in the field "Released Volume per Time"⁸:



IMPORTANT NOTE:

Normally it is very difficult to specify the released volume flow rate for carbon monoxide. It is therefore recommended to make concentration measurements. If the extension modules "Management of Measured Pollutant Concentrations" and "Source Term Back Calculation" have been licensed, then concentration measurements can be used in estimating the released volume flow rate on the basis of measured values.

The height of release must be estimated and entered into the "Height of Release" field in meters above the ground.



This value should be the effective height of release (actual height of release plus elevation from heat).

IMPORTANT NOTE:

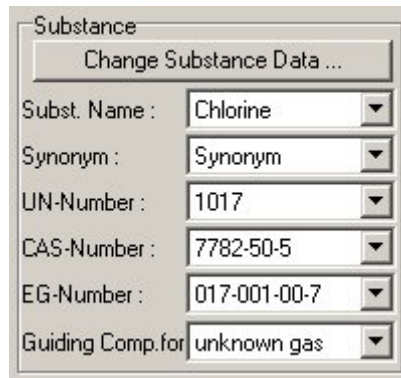
If the extension modules "Management of Measured Pollutant Concentrations" and "Source Term Back Calculation" have been licensed, and if concentration measurements are being used to estimate the released volume flow rate on the basis of measured values, then the height of release must be specified precisely. If not, the source term back calculation module will provide erroneous values for the released volume flow rate.

⁸ Conversion of a volume flow rate into a mass flow (and vice versa) is performed assuming an ambient temperature of 15° C.

If the incident is not a fire, then "Release of Toxic Substances" should be selected. Additional inputs are needed, e.g. "Phase of Substance", "Release Behaviour", and "Release Type".

5.3.2 Substance

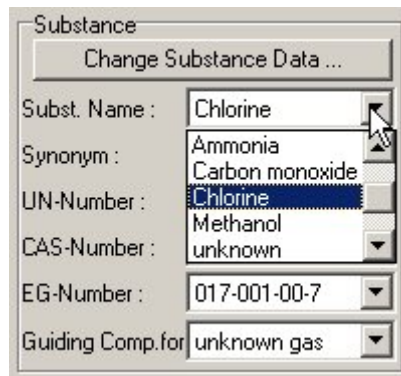
The released substance can be entered in the "Substance" dialog:



The screenshot shows a dialog box titled "Substance" with a "Change Substance Data ..." button at the top. Below the button are six fields, each with a drop-down arrow:

- Subst. Name : Chlorine
- Synonym : Synonym
- UN-Number : 1017
- CAS-Number : 7782-50-5
- EG-Number : 017-001-00-7
- Guiding Comp. for : unknown gas

The "Substance" dialog contains fields with drop-down lists for Substance Name, Synonym, UN Number, CAS Number, EU Number, and "Guiding component for..." Selections can be made by clicking on the selected substance name or identification number on the corresponding drop-down list:

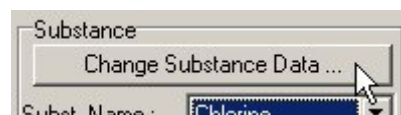


This screenshot shows the same "Substance" dialog box, but the "UN-Number" drop-down list is open. The list contains the following items:

- Chlorine (highlighted)
- Ammonia
- Carbon monoxide
- Methanol
- unknown

Alternatively, it is also possible to select a substance by typing in the first letter of its name or the first digit of (for example) its UN number. If several substances with the same initial letter are in the database, the user can scroll up or down the list using the cursor key.

If the desired substance is not in the database, or if the database contains only a similar substance, then the **[Change Substance Data...]** can be clicked.



This screenshot shows the "Substance" dialog box with the mouse cursor pointing at the "Change Substance Data ..." button. The "Subst. Name" field is visible below the button and contains "Chlorine".

The **Substance Database** window will appear:

The screenshot shows a software window titled "Substance Database" with a standard Windows-style title bar (minimize, maximize, close buttons). Below the title bar is a toolbar with navigation icons (back, forward, search, etc.). The main content area is divided into several sections:

- Identification:** Fields for Substance Name (Chlorine), Common Name (Synonym), Commercial Name (Trade name), Chemical Formula (Cl₂), UN Number (1017), CAS Number (7782-50-5), EG Number (017-001-00-7), and Guiding Component for (unknown gas).
- Chemical-physical Characteristics:** Fields for Molar Mass (70.91 g/mol), Fluid Density (1.239 kg/l), Heat of Vaporization (289000 J/kg), Boiling Temperature (-34.05 °C), Spec. Heat Capacity cp (479.48 J/(kg K)), and Isentropic Exponent (1.36).
- Vapor Pressure:** Fields for Vapor Pressure (6.731 bar) and at Temperature of (20 °C).
- Danger Threshold Values:** Fields for Threshold Value (0), Odor Threshold (0 mg/m³), Lower Ignition Limit (0 g/m³), and Upper Ignition Limit (0 g/m³). A "Unit" section has radio buttons for mg/m³ (selected) and ppm.
- Deposition:** Field for Deposition Speed (m/s).
- Notes:** A large empty text area for user notes.

At the bottom right, there are "Cancel" and "OK" buttons.

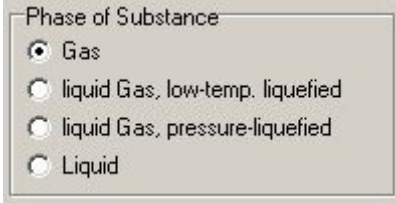
Chapter 6.3 explains how to use the Substance Database window.

IMPORTANT NOTE:

- Only properly trained staff should change substance data or enter new substances.
- If, on a one-time basis, an accidental release calculation is to be made with a different threshold value, it is sufficient to enter the threshold value desired in the **Isolines** window (cf. **Chapter 4.2.2**).

5.3.3 Phase of substance

The "Phase of Substance" area is only visible if the "Type of Accident" area shows "Release of Toxic Substances" as selected. In the "Phase of Substance" area, the substance's storage condition can be entered:



Phase of Substance

Gas

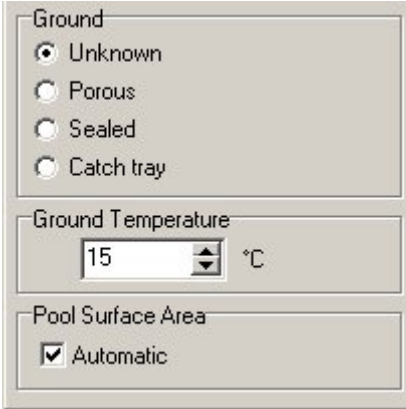
liquid Gas, low-temp. liquefied

liquid Gas, pressure-liquefied

Liquid

For the options "Liquid gas, low temperature", "Liquid gas, pressure-liquefied" and "Liquid", the following edit fields are displayed: "Ground", "Ground temperature" and "Pool surface area". However, the edit field "Height of release" will not be visible, since for the above-name phases of substance, release takes place close to the ground.

For the options "Liquid gas, low-temperature", "Liquid gas, pressure-liquefied" and "Liquid", it is assumed that a pool will form on the ground or in a catch tray and will then evaporate or vaporize. The edit fields "Ground", "Ground temperature" and "Pool surface area" should be filled out:



Ground

Unknown

Porous

Sealed

Catch tray

Ground Temperature

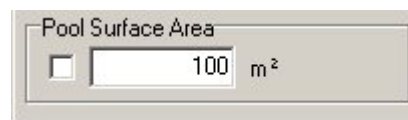
15 °C

Pool Surface Area

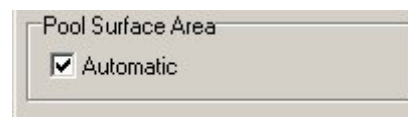
Automatic

Soil condition plays a big role in pool evaporation in relation to evaporation rates, i.e. to the quantity of a substance that enters the atmosphere. Accordingly, the selection for the "Ground" edit field should be made carefully. If the soil condition is unknown, select the setting "Unknown."⁹ Otherwise select "Porous", "Sealed" or "Catch tray".¹⁰

The "Pool Surface Area" edit field allows the pool size to be entered. Either the pool has a constant size, or the pool size changes with time. If the first case is true, uncheck the "Automatic" checkbox and enter the pool surface area:



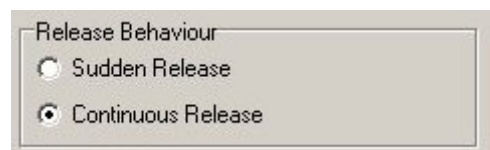
If the second case is true, the box should be checked. The word "Automatic" will appear after the checkbox.



The size of the pool, which is assumed to be a circle, will be calculated by the program.¹¹

5.3.4 Release behaviour

The substance, stored in the form entered in the "Phase of Substance" edit field, can be released either all at once or over a certain period of time.¹² In the "Release Behaviour" edit field, select either "Sudden Release" or "Continuous Release".



⁹ Internally, ground "unknown" is identical with ground "porous".

¹⁰ Internally, ground "sealed" is identical with "catch tray".

¹¹ A pool depth of 2 cm is assumed.

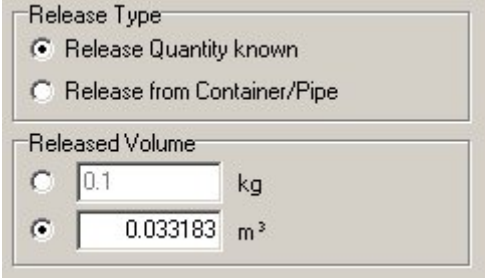
¹² If the total release of the stored substance lasts for shorter than five minutes, then "sudden release" can be selected.

5.3.5 Release type

In the "Release Type" edit field, the user states whether the released volume or volume flow rate is **known** (and thus can be entered in the "Released Volume" or "Released Volume Flow Rate" edit field), or whether the released volume or volume flow rate can be **calculated** based on the geometry of storage, the storage conditions (pressure and temperature), and the size of the leak.

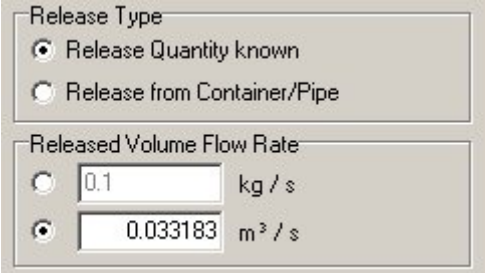
5.3.5.1 Release Quantity known

If the release quantity is known, and if "Sudden Release" has been selected, then the release volume should be entered in cubic meters:



The screenshot shows a dialog box titled "Release Type". It contains two radio buttons: "Release Quantity known" (selected) and "Release from Container/Pipe". Below this is a section titled "Released Volume" with two radio buttons and input fields: "0.1 kg" (unselected) and "0.033183 m³" (selected).

If "Continuous Release" has been selected, the released volume flow rate should be entered in [m³/s]:



The screenshot shows a dialog box titled "Release Type". It contains two radio buttons: "Release Quantity known" (selected) and "Release from Container/Pipe". Below this is a section titled "Released Volume Flow Rate" with two radio buttons and input fields: "0.1 kg / s" (unselected) and "0.033183 m³ / s" (selected).

It is also possible to enter the released quantity as a mass value or as mass flow. To do this, click on the respective buttons in front of the input field.¹³

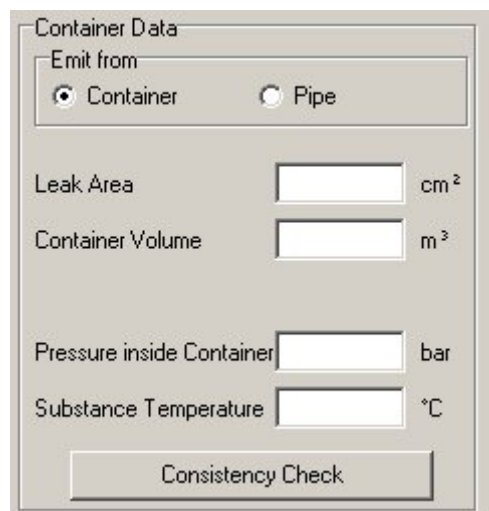
¹³ The conversion of a volume flow rate into a mass flow (and vice versa) is performed assuming an ambient temperature of 15° C.

IMPORTANT NOTE:

The released pollutant quantity value is heavily dependent on the "Phase of Substance" setting, as the density of liquids and liquid gas is greater than that of gas by several orders of magnitude. The released volume or volume flow rate is always linked to the aggregate status entered in the "Phase of Substance" edit field.¹⁴

5.3.5.2 Release from a container or pipe

If the release quantity is unknown, it is calculated based on the geometry of storage, the storage conditions (pressure and temperature) and the size of the leak. A range of data on the container is requested, based on the settings in the "Phase of Substance" and "Release Behaviour" edit fields. For example, the "Container Data" edit field appears as shown below in the case of a continuous gaseous release from a container:



The image shows a software dialog box titled "Container Data". At the top, under "Emit from", there are two radio buttons: "Container" (which is selected) and "Pipe". Below this, there are four input fields with labels and units: "Leak Area" (cm²), "Container Volume" (m³), "Pressure inside Container" (bar), and "Substance Temperature" (°C). At the bottom of the dialog is a button labeled "Consistency Check".

The leak area, container volume, internal container pressure, and substance temperature should be entered in the appropriate input fields.

Tab. 5.1 shows which container data must be entered as based on the "Phase of Substance" and "Release Behaviour" settings.

¹⁴ For liquids or liquid gas, the fluid densities stored in the Substance Database are used for conversion between volume and mass. For gases, the Ideal Gas Equation is used. Molar mass is taken from the Substance Database. If no temperature or pressure is requested, the calculation assumes 15° C and 1 bar.

Tab. 5.1: Parameters to be entered in the "Container Data" edit field

| Phase of Substance | Release Behaviour | Emission from | Parameter 1 | Parameter 2 | Parameter 3 | Parameter 4 | Parameter 5 |
|--------------------------------|-------------------|---------------|---------------|-----------------------------|-------------------------|---------------------------|-----------------------|
| Gas | Continuous | Container | Leak area | Container volume | | pressure Inside container | Substance temperature |
| | | Pipe | Pipe diameter | | | Pressure inside pipe | Substance temperature |
| | Sudden | Container | | Container volume | | pressure Inside container | Substance temperature |
| Liquid gas, low-temperature | Continuous | Container | Leak area | Filling volume in Container | Fill level of container | | |
| | | Pipe | Pipe diameter | | | Pressure inside pipe | |
| | Sudden | Container | | Filling volume in Container | | | |
| Liquid gas, pressure-liquefied | Continuous | Container | Leak area | Filling volume in Container | Fill level of container | | Substance temperature |
| | | Pipe | Pipe diameter | | | | Substance temperature |
| | Sudden | Container | | Filling volume in Container | | | Substance temperature |
| Liquid | Continuous | Container | Leak area | Filling volume in Container | Fill level of container | | |
| | | Pipe | Pipe diameter | | | Pressure inside pipe | |
| | Sudden | Container | | Filling volume in Container | | | |

5.3.6 Consistency check for release from a container or pipe

For releases from a container or pipe, the input data can be checked for consistency. To do this, click on the **[Consistency Check]** button:

Consistency Check

The following two examples demonstrate the consistency check function:

Example A

Continuous release of chlorine gas

The **Release** window has been filled out as follows:

Type of Accident

Fire

Release of Toxic Substances

Substance

Change Substance Data ...

Subst. Name : Chlorine

Synonym : Synonym

UN-Number : 1017

CAS-Number : 7782-50-5

EG-Number : 017-001-00-7

Guiding Comp. for unknown gas

Phase of Substance

Gas

liquid Gas, low-temp. liquefied

liquid Gas, pressure-liquefied

Liquid

Release Behaviour

Sudden Release

Continuous Release

Release Type

Release Quantity known

Release from Container/Pipe

Container Data

Emit from

Container Pipe

Leak Area 1 cm²

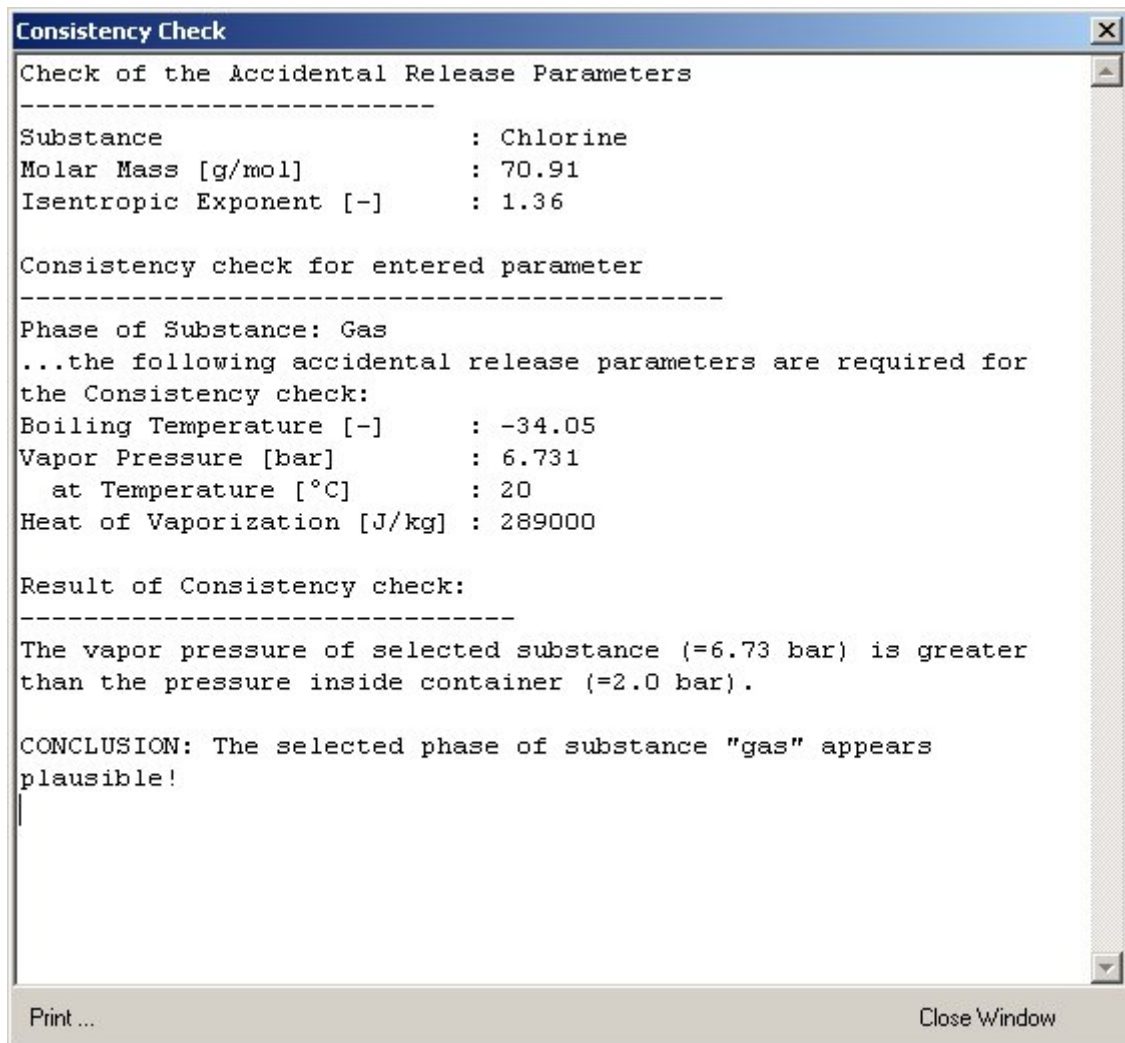
Container Volume 10 m³

Pressure inside Container 2 bar

Substance Temperature 20 °C

Consistency Check

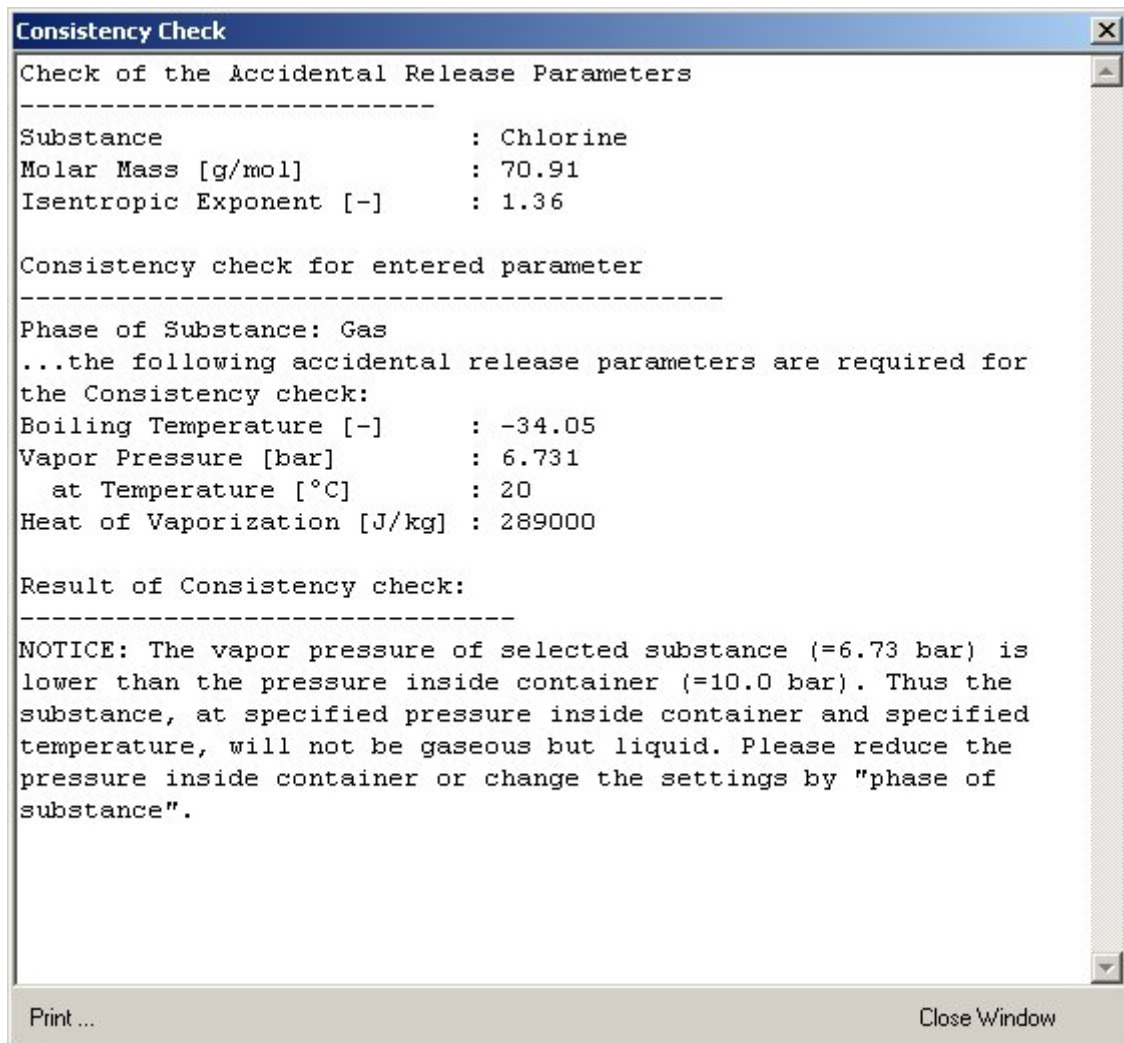
Upon pressing the **[Consistency Check]** button, this window will appear:



Thus, the entered inputs appear to be plausible.

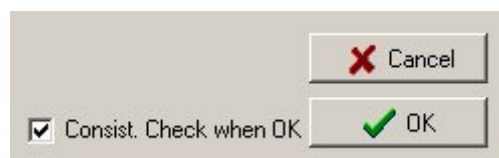
Example B

Like Example A (Continuous Release of Chlorine Gas), but with **10 bar** of pressure inside container instead of 2 bar as in Example A. Upon pressing the [**Consistency Check**] button, this window will appear:



The **Consistency Check** window serves notice that the entries are inconsistent, and proposes a possible remedy.

In the case of release from a container or pipe, the consistency check can also be performed automatically by clicking the **[OK]** button. To do this, the box next to "Consist. Check when OK" should be checked.



5.3.7 Checking substance data for consistency

When the **[OK]** button is clicked, a check will be performed as to whether the required substance data for the selected substance is in the substance database.¹⁵ If a value is missing or is zero, the Consistency Check window will appear and show the applicable message. In this case, no calculation can be carried out.

REMEDY:

- Add the missing parameters to the substance database.
- Select a different substance.
- Select a different setting in the "Phase of Substance" edit field.

Tab. 5.2 shows which parameters are required for which release path.

¹⁵ The system only checks whether relevant values are entered in the database and are greater than zero. The system does not check whether the numerical value is actually correct. In other words, the user has responsibility for the accuracy of all values he or she enters in the database. Special care should be given in ensuring that the values are input using the **required unit**.

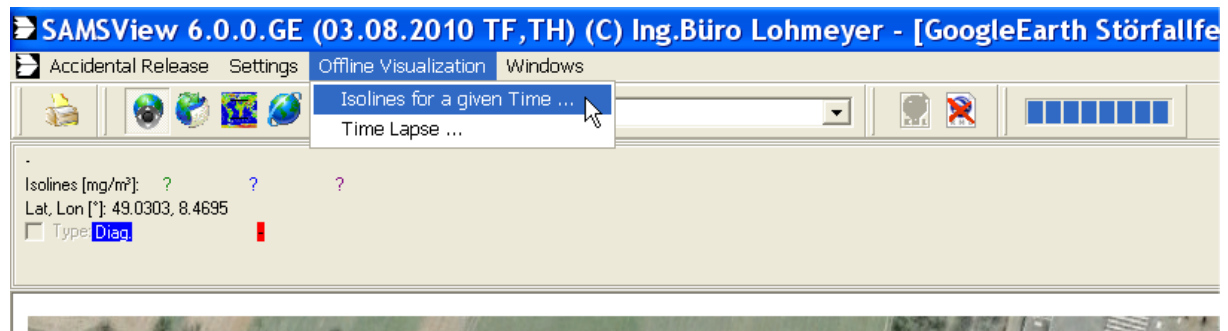
Tab. 5.2: Required physical parameters as dependent on the path of substance release

| Phase of Substance | Release quantity known | Molar mass | Fluid density | Heat of vaporization | Boiling temperature | Specific heat capacity C_p | Isentropic exponent | Vapour pressure and temperature |
|--------------------------------|------------------------|------------|---------------|----------------------|---------------------|------------------------------|---------------------|---------------------------------|
| Gas | Yes | X | | | | | | |
| | No | X | | | | | X | |
| Liquid gas, low-temperature | Yes | X | X | X^{16} | X | | | X |
| | No | X | X | X^{13} | X | | | X |
| Liquid gas, pressure-liquefied | Yes | X | X | X^{13} | X | X | | X |
| | No | X | X | X^{13} | X | X | | X |
| Liquid | Yes | X | X | X^{13} | X | | | X |
| | No | X | X | X^{13} | X | | | X |

5.4 Displaying previous concentration distributions when an accidental release calculation is in progress

When an accidental release calculation is in progress, concentration fields that have already been calculated can be displayed (see **Fig. 5.2**). To do this, go to the "Offline Visualization" menu item and click on "Isolines for a given Time..."

¹⁶ If the heat of vaporization is not known, it is estimated internally using the Clausius-Clapeyron Equation, taking into account the boiling temperature and vapor pressure at the specified temperature.



Proceed as described in **Chapter 6.1**. In order to show the concentration distribution, the window is split. Both halves can be maximized. However, as soon as a newly calculated concentration distribution is applied to the current accidental release calculation, this will be displayed. For this, the window will be split in half again. It is possible to print out the screen display by clicking on the printer symbol or by going to the menu item "Accidental Release | Print..."

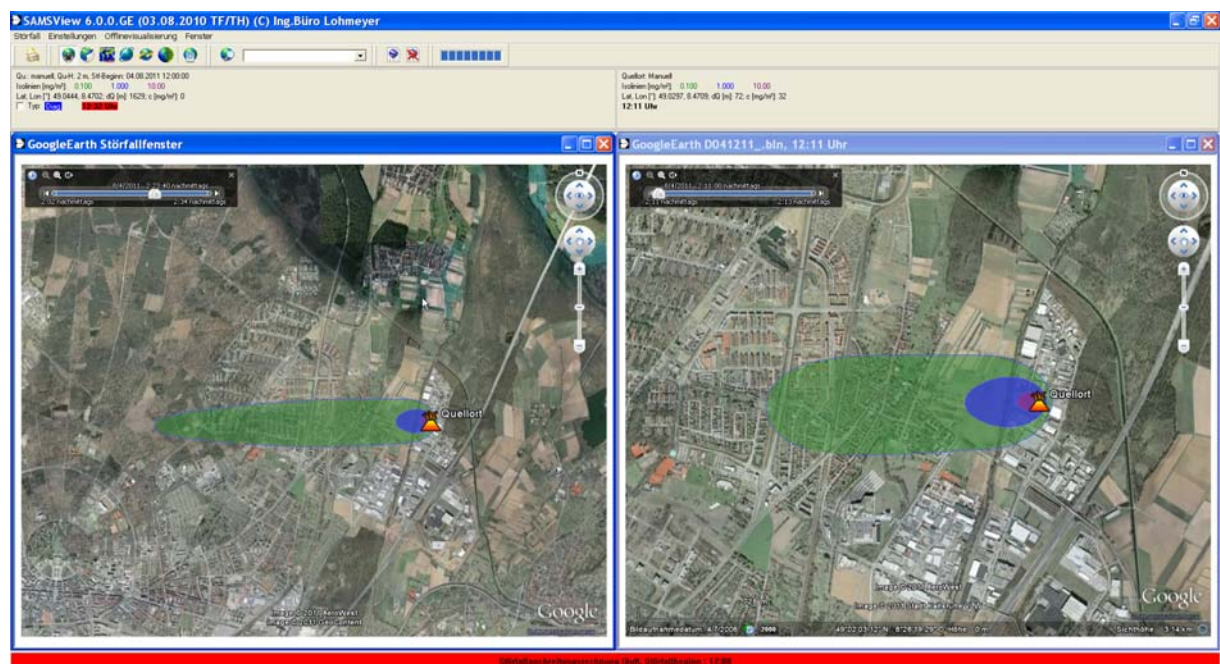
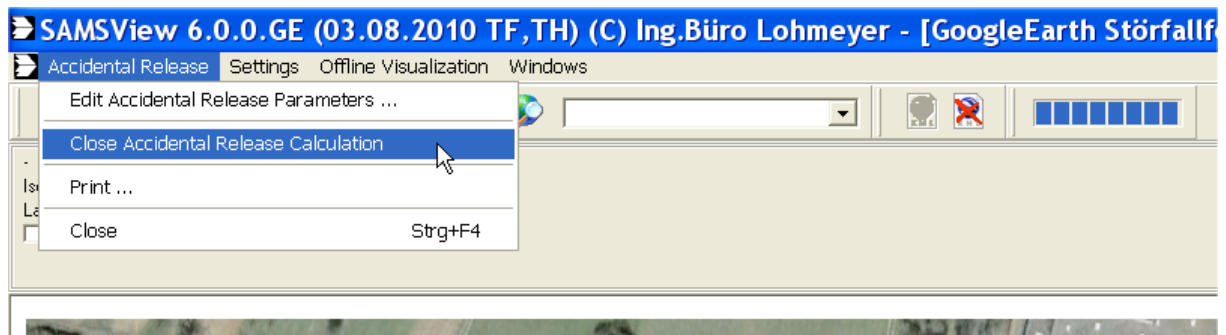


Fig. 5.2: **SAMSView** in accidental release mode with a split display showing the Accidental Release window (left) and the Offline window with isolines for a previous moment in time.

5.5 Closing a running accidental release calculation

An accidental release calculation can be closed in **SAMSView** by clicking on the menu item "Accidental Release | Close Accidental Release Calculation...":



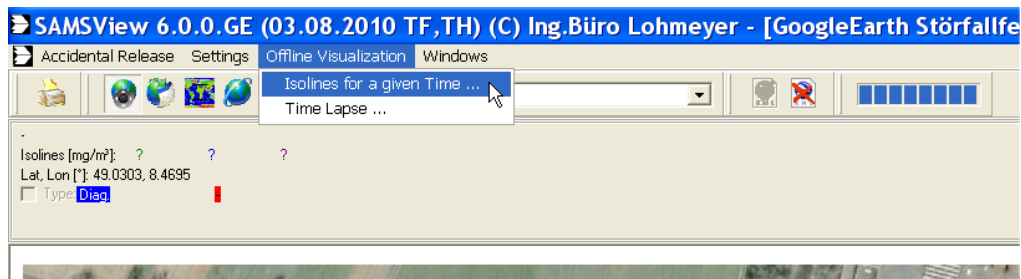
The "Close" command must be confirmed. The system will then require a short time (about 15 seconds) to "clean up" and save the calculation data in a security directory. During this time period, further inputs are blocked. After this, a new accidental release calculation can be started.

6 FUNCTIONS IN STAND-BY MODE

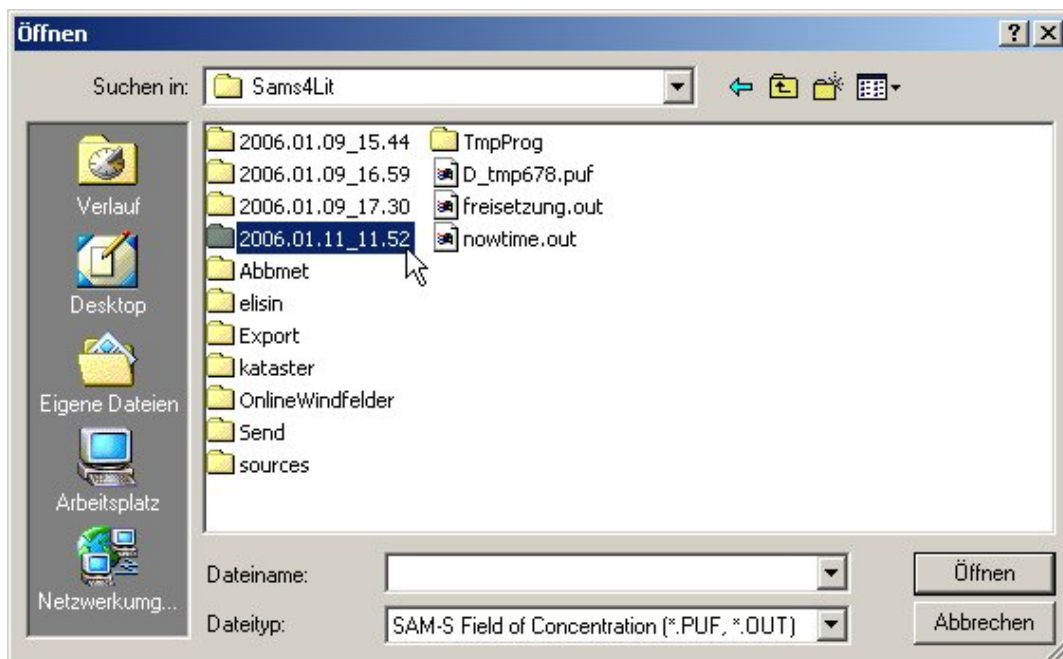
When in stand-by mode,¹⁷ it is possible to visualize isolines from closed accidental release calculations in a separate window (= offline window), as well as to update substance data and release scenarios.

6.1 Displaying isoline data for a given moment in the Offline window

To display concentration fields that have been calculated, click on the menu item "Offline Visualization | Isolines for a given time...":



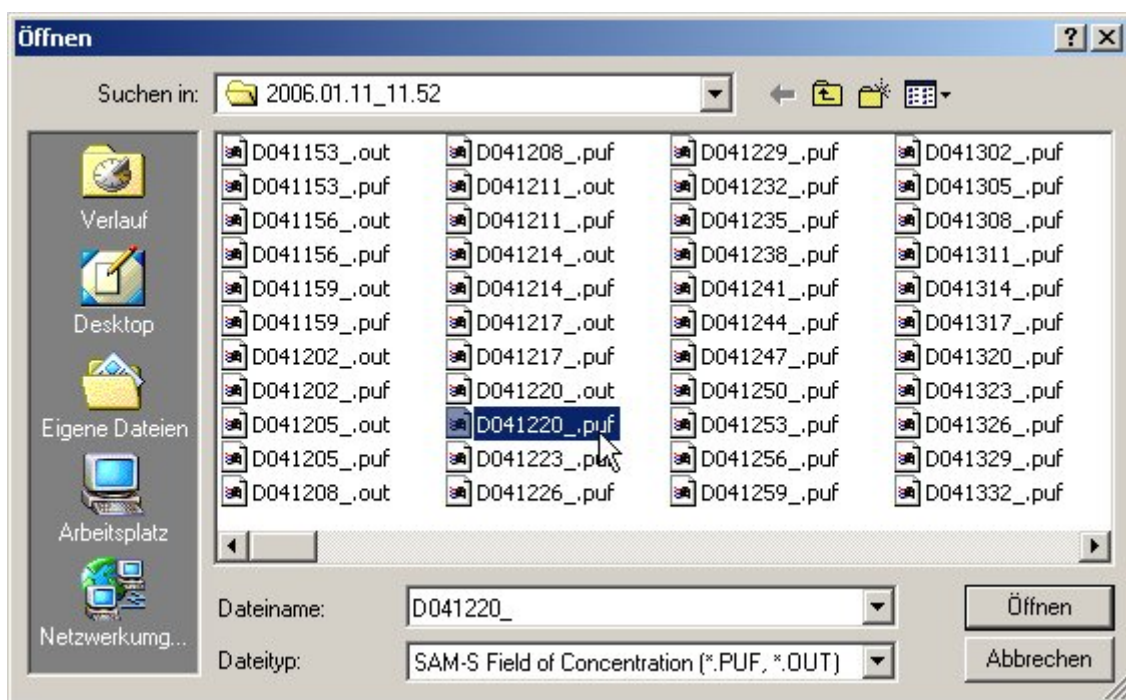
The "Open" window will appear:



¹⁷ "Stand-by mode" refers to when no accidental release calculation is running.

For each accidental release calculation, a security directory will be created in [InstallDir] (in the example: "Sams4Lu"), which will have the form yyyy.mm.dd_hh.nn (yyyy = year, mm = month, dd = day, hh = hour, nn = minute of the moment when the calculation was started; compare also the chapter in the appendix titled "Overview of the System's Directory Structure"). The calculated concentration distributions will be saved in this directory.

If a security directory is selected by clicking the [Open] button, the files will be displayed with the extension "puf" and "out". (In the example, for instance, the selected file is 2004.01.28_12.19, i.e. the accidental release calculation that was begun on 28 January 2004 at 12:19 p.m. Please note: This date is not the start of accidental release.) Normally, the files to select are those with the extension "puf". The file prefix indicates whether the file is for a Diagnosis (the first letter in the prefix is a D) or a Forecast (first letter in the prefix is a P). The digit sequence that follows the prefix gives the time of the Diagnosis or Forecast in ddhhnn_ format (dd = day, hh = hour, nn = minute):¹⁸



After selecting a file, use the **Set Isoline Levels...** window to enter values for the three isolines:

¹⁸ In the example, the file D221617_.puf is the diagnosed concentration distribution for the 22nd at 16:17h.

Set Isoline Levels: C:\Sams4Lit\2006.01.11_11.52\D041220_.puf

Isolines

Lower Isoline:

Middle Isoline:

Upper Isoline:

Unit mg/m³ ppm

Conversion mg/m³ into ppm and vice versa

Molar Mass g/Mol

Threshold Value

Unit mg/m³ ppm

IMPORTANT NOTE:

The molar mass entered in the "**Set isoline levels...**" window is used solely for converting mg/m³ to ppm (and vice versa).

The threshold value entered in the "**Set isoline levels...**" window is used in displaying the concentration time series.

If the window is exited by clicking **[OK]**, the three isolines will be shown on the map in the Offline window. The Accidental Release window and the Offline window are shown side by side. Both windows can be maximized. The **Offline** window can also be closed, while the **Accidental Release** window can only be minimized.

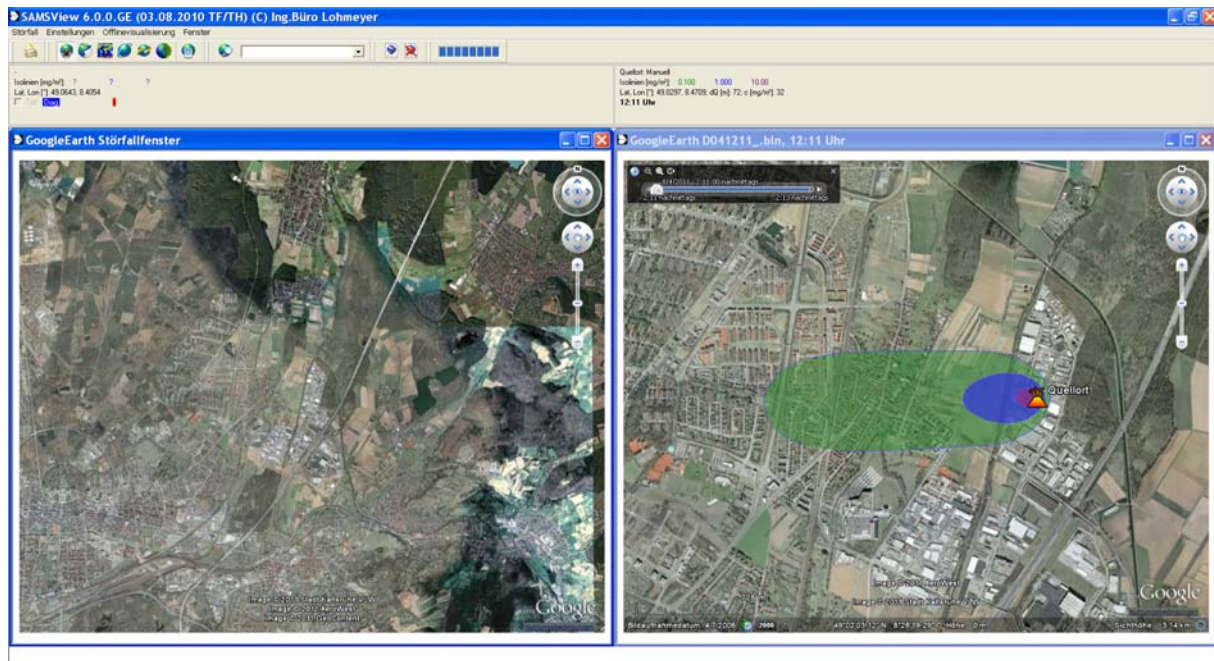


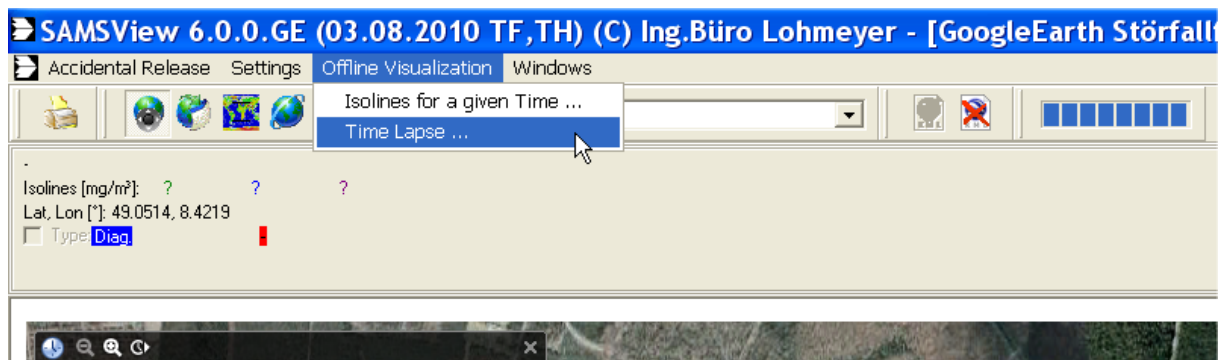
Fig. 6.1: **SAMSView** in offline mode with a split display showing the Accidental Release window (left) and the Offline window with isolines for a previous moment in time.

To print the displayed window, click on the printer symbol (or by clicking on the menu item "Accidental Release | Print..."):

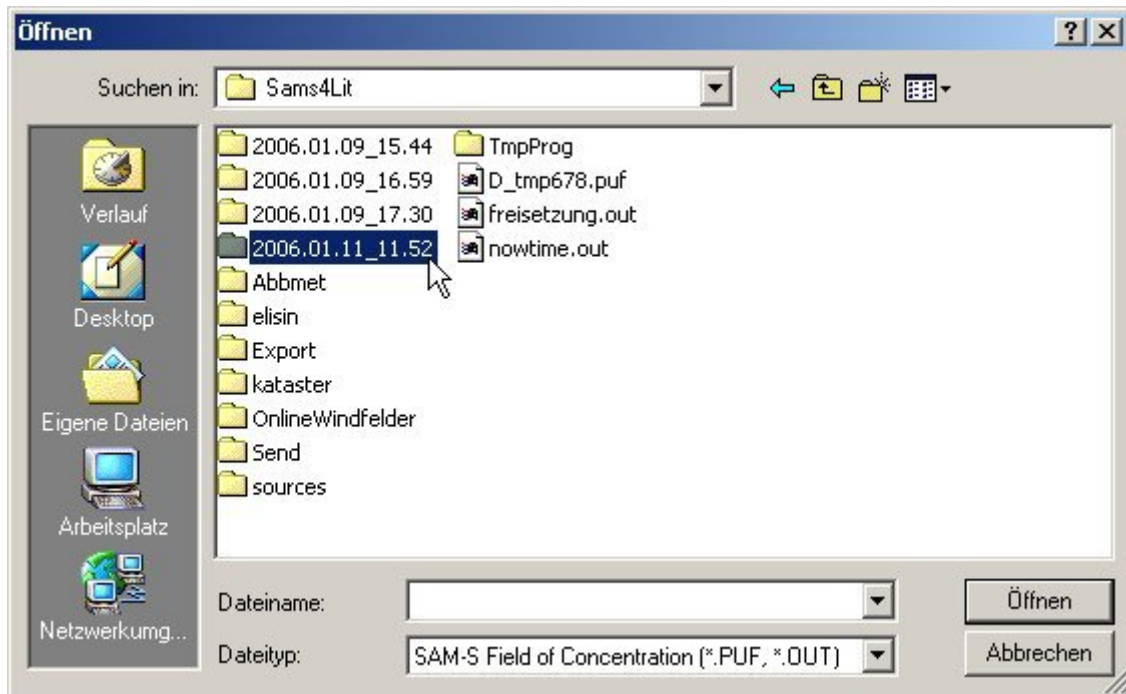


6.2 Displaying isolines with a time lapse in the Offline window

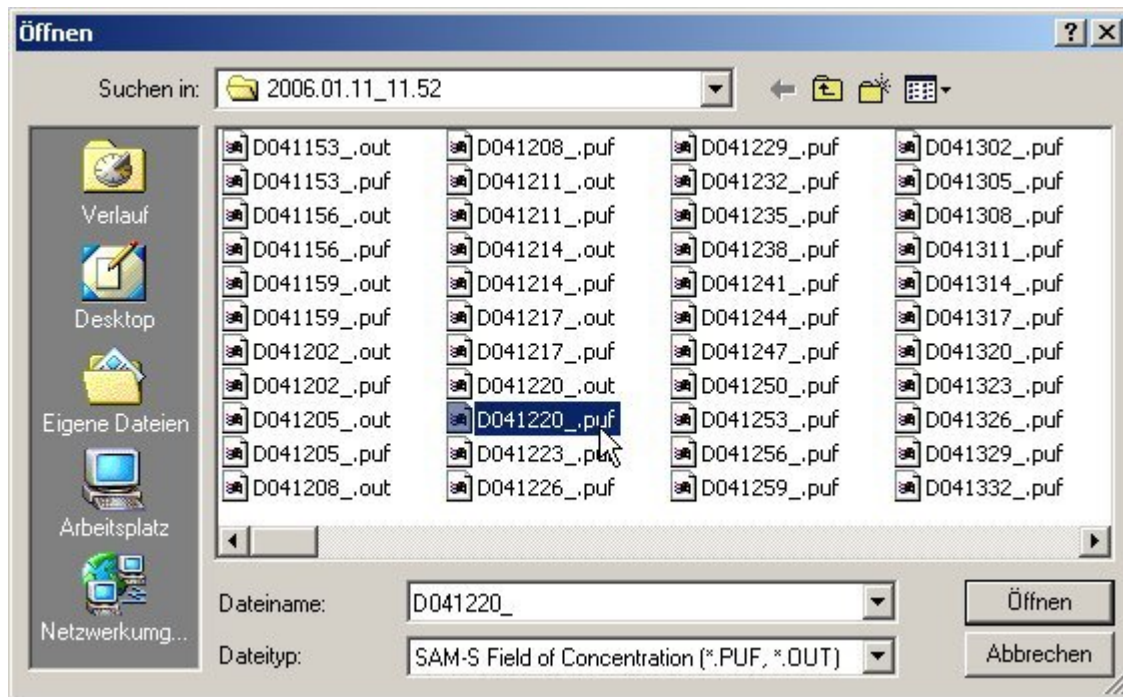
Concentration fields calculated for different times in an accidental release calculation can be displayed by the Offline window in a time lapse, one after the next. Click on the menu item "Offline Visualization | Time Lapse...":



The "Open" window will appear:



Select the desired security directory that has the form yyyy.mm.dd_hh.nn (yyyy = year, mm = month, dd = day, hh = hour, nn = minute of the moment when the calculation was started; see the chapter "Overview of the System's Directory Structure" and also the explanation in **Chapter 6.1**). Click the button **[Open]**. All files with the extension "puf" will be listed:



Select any file and click the button **[Open]**. The **Set Isoline Levels...** window will appear, just as with menu item "Offline Visualization | Isolines for a given Time..." (cf. **Chapter 6.1**). Enter values for the three isolines. If you exit this window by clicking **[OK]**, the calculated isolines will be displayed one after the other in the **Offline** window with a time lapse of about 60.¹⁹

¹⁹ That is about 60 times faster than in reality.

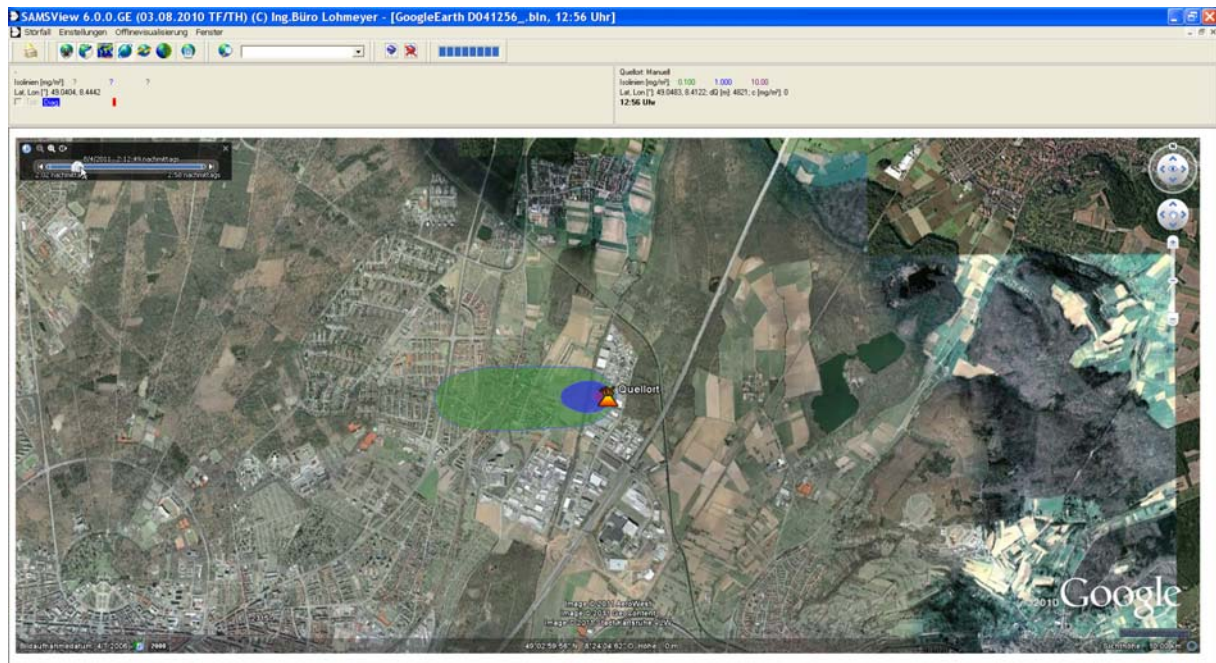
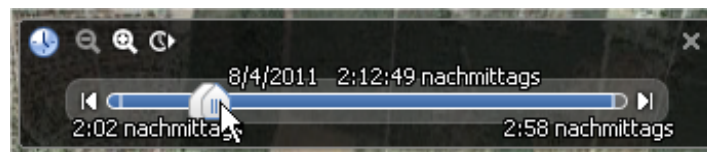
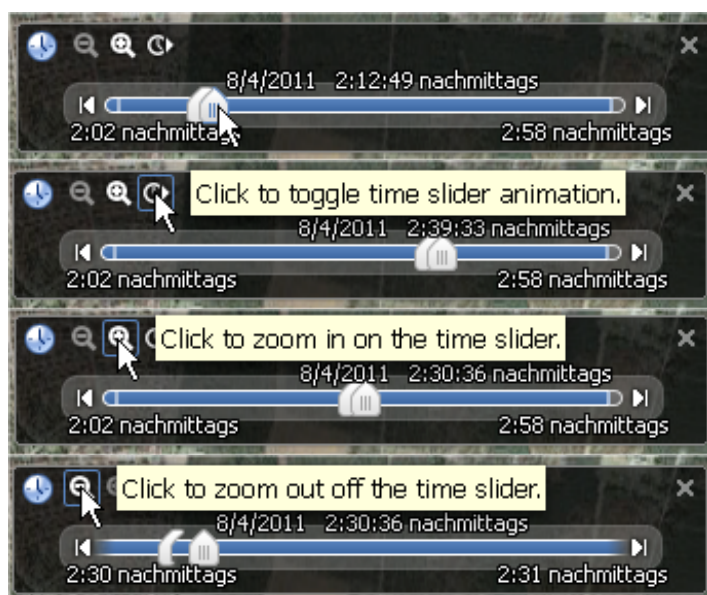


Fig. 6.2: **SAMSView** in offline mode with the Offline window with a time-lapse display.

During a time-lapse viewing, the Goggle Earth navigation tool is visible:



The Google Earth navigation tool has the following elements:



With the time slider the desired display time can be selected.

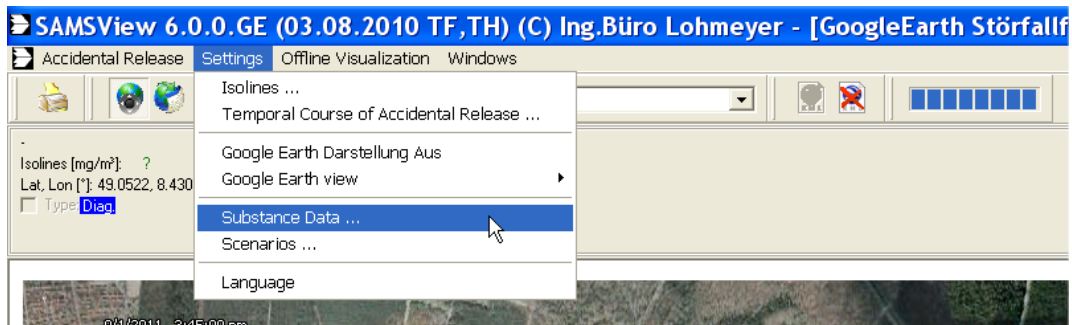
Start/Stop animation

Zoom in on the time slider

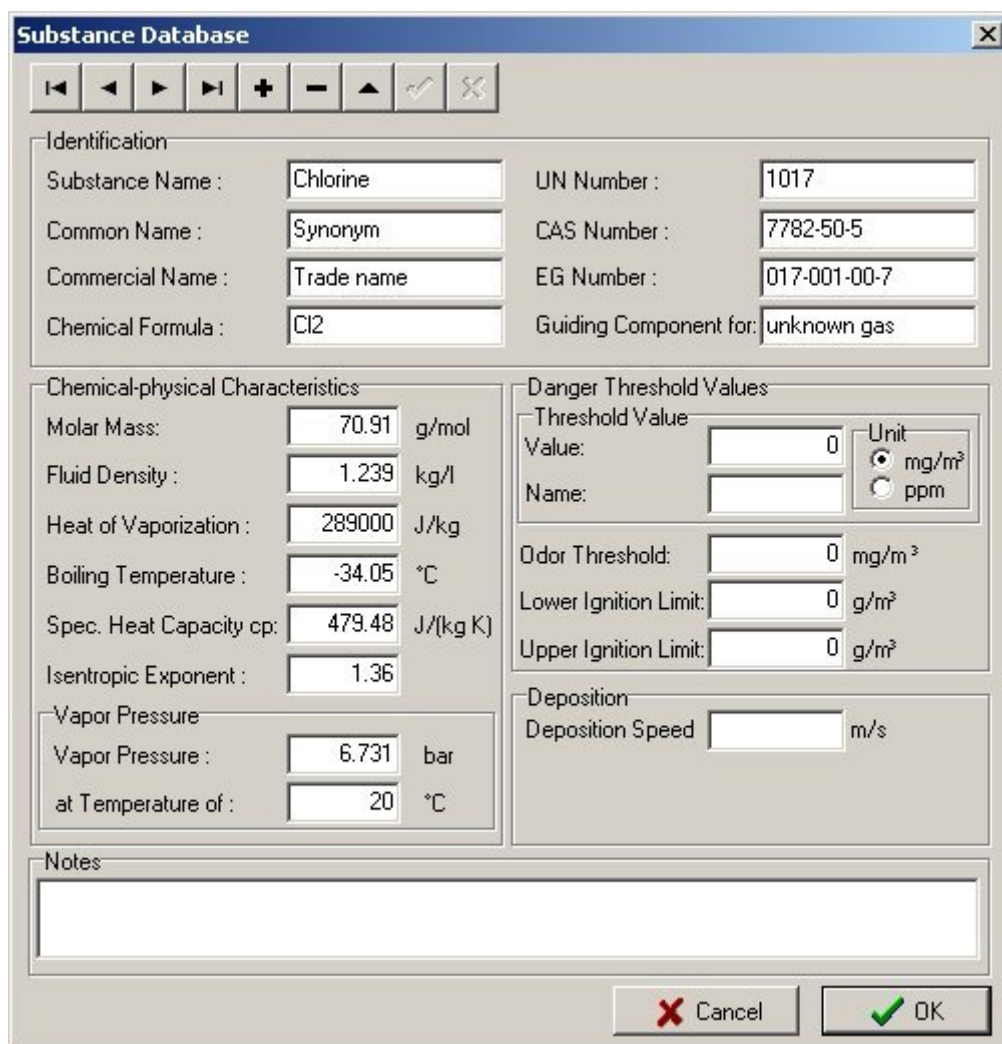
Zoom out off the time slider

6.3 Maintaining the Substance Database

In offline mode, go to menu item "Settings | Substance Data...":



Here you can edit existing substance data and input new substance data. The "Substance Database" window will appear.

The "Substance Database" dialog box is shown with the following fields:

| Identification | |
|------------------------|--------------|
| Substance Name : | Chlorine |
| UN Number : | 1017 |
| Common Name : | Synonym |
| CAS Number : | 7782-50-5 |
| Commercial Name : | Trade name |
| EG Number : | 017-001-00-7 |
| Chemical Formula : | Cl2 |
| Guiding Component for: | unknown gas |

| Chemical-physical Characteristics | |
|-----------------------------------|-----------------|
| Molar Mass: | 70.91 g/mol |
| Fluid Density : | 1.239 kg/l |
| Heat of Vaporization : | 289000 J/kg |
| Boiling Temperature : | -34.05 °C |
| Spec. Heat Capacity cp: | 479.48 J/(kg K) |
| Isentropic Exponent : | 1.36 |

| Danger Threshold Values | |
|-------------------------|---|
| Threshold Value Value: | 0 |
| Name: | |
| Unit: | <input checked="" type="radio"/> mg/m ³ <input type="radio"/> ppm |
| Odor Threshold: | 0 mg/m ³ |
| Lower Ignition Limit: | 0 g/m ³ |
| Upper Ignition Limit: | 0 g/m ³ |

| Deposition | |
|------------------|-----|
| Deposition Speed | m/s |





| Vapor Pressure | |
|---------------------|-----------|
| Vapor Pressure : | 6.731 bar |
| at Temperature of : | 20 °C |

Notes




Cancel OK

The navigation tool can be used to





- Display the first data record (press the button )
- Display the previous data record (press the button )
- Display the next data record (press the button )
- Display the last data record (press the button )

The navigation tool can also:

- Insert a data record (press the button )
- Delete a data record (press the button )
- Switch to editing mode (press the button )

When working in editing mode, the two buttons on the right of the navigation tool can also be used. In editing mode, you can:

- Accept changes (press the button ) , or
- Reject changes (press the button ) .

When the database is not in editing mode, **no changes** can be made. This is to prevent making changes by accident.

IMPORTANT NOTE:

The substances chlorine and carbon monoxide cannot be deleted from the Substance Database as they are used in the scenario templates (e.g. "ALL UNKNOWN (Original)"). In addition, the chemical and physical properties of these two substances cannot be changed in editing mode.

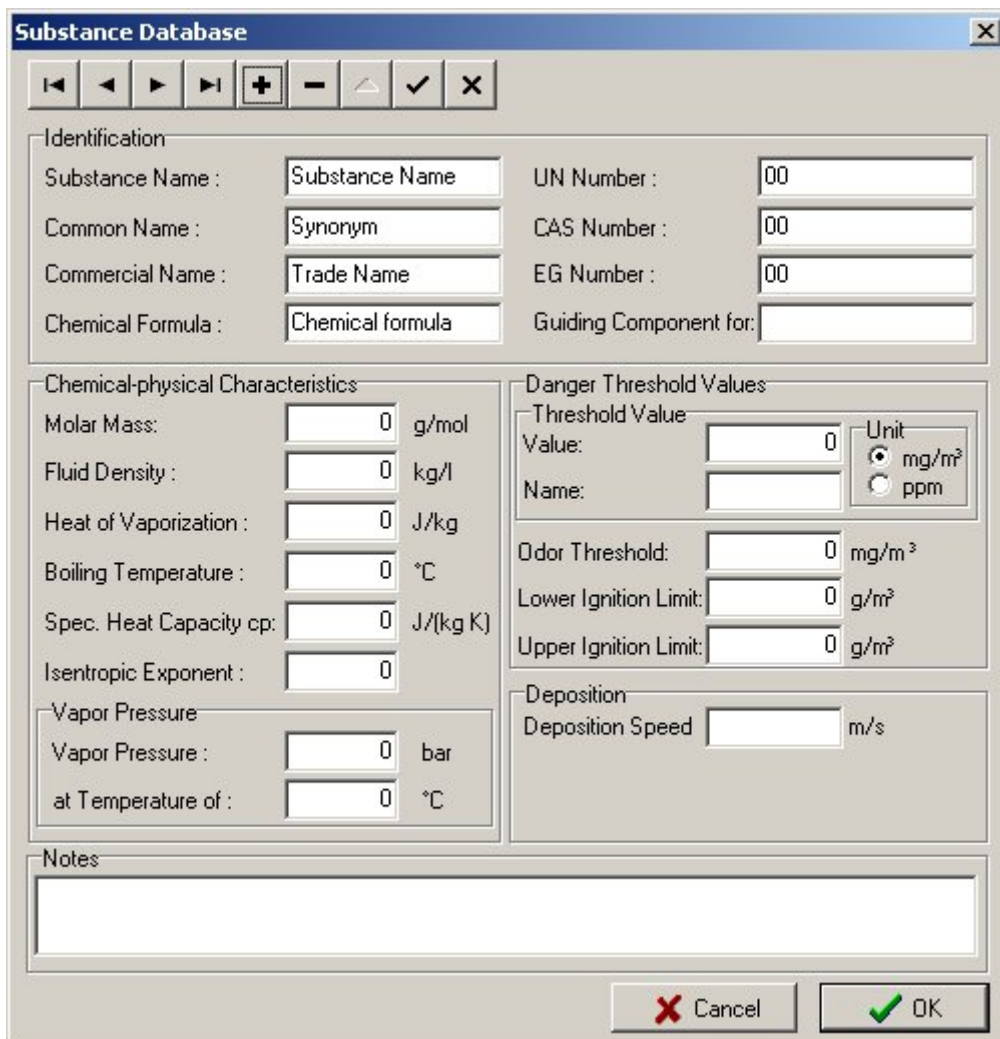
To delete a substance, the final deletion must be confirmed:



In order to enter a new substance in the Substance Database, click the button



on the navigation bar of the Substances Database window. The window will then look like this:

The "Substance Database" window is shown with a navigation bar at the top containing several icons, including a plus sign. The main area is divided into several sections:

- Identification:** Fields for Substance Name (placeholder: Substance Name), UN Number (00), Common Name (placeholder: Synonym), CAS Number (00), Commercial Name (placeholder: Trade Name), EG Number (00), Chemical Formula (placeholder: Chemical formula), and Guiding Component for.
- Chemical-physical Characteristics:** Fields for Molar Mass (0 g/mol), Fluid Density (0 kg/l), Heat of Vaporization (0 J/kg), Boiling Temperature (0 °C), Spec. Heat Capacity cp (0 J/(kg K)), Isentropic Exponent (0), and Vapor Pressure (0 bar at Temperature of 0 °C).
- Danger Threshold Values:** Fields for Threshold Value (0), Name, Odor Threshold (0 mg/m³), Lower Ignition Limit (0 g/m³), and Upper Ignition Limit (0 g/m³). A unit selector is set to mg/m³.
- Deposition:** Field for Deposition Speed (m/s).
- Notes:** A large empty text area at the bottom.

At the bottom right, there are "Cancel" and "OK" buttons.

The database is now in editing mode. Under "Substance Name", enter the relevant name. If the name entered is already in the database, the error message "Index error" will appear upon clicking the **[Accept changes]** button.



If this error message appears, a different name must be selected for the "Substance Name" input field.

The input fields for the following:

- Common Name
- Commercial Name
- Chemical Formula
- UN Number
- CAS Number
- EU Number
- Guiding Component for...

can be filled out, but need not be. It is recommended to fill them out so as to be able in an accidental release to select the released substance using these fields.

For chemical and physical properties, the input fields for the following:

- Molar Mass
- Fluid Density
- Heat of Vaporization
- Boiling Temperature
- Specific Heat Capacity c_p
- Isentropic Exponent
- Vapour Pressure at a given...

- Temperature

can be filled out.²⁰ When inputting values, particular notice should be paid to the measurement units used (cf. **Tab. 6.1**)

²⁰ Please note that only trained staff should input substance data.

Tab. 6.1: Chemical and physical properties saved in the Substance Database, with their respective measurement units

| Measurement | Unit |
|------------------------------|----------|
| Molar mass | g/mol |
| Fluid density | kg/l |
| Heat of vaporization | J/kg |
| Boiling temperature | °C |
| Specific heat capacity c_p | J/(kg K) |
| Isentropic exponent | - |
| Vapour pressure | bar |
| Temperature | °C |

As already explained in **Chapter 5.2.8 "Checking the Substance Data for Consistency"**, not all substance properties are required for each of the different paths of substance release. Substance properties are not always available. **Table 6.2** shows which parameters are required for which release path.

Tab. 6.2: Physical parameters required depending on the path of substance release

| Phase of Substance | Release quantity known | Molar mass | Fluid density | Heat of vaporization | Boiling temperature | Specific heat capacity C_p | Isentropic exponent | Vapour pressure and temperature |
|--------------------------------|------------------------|------------|---------------|----------------------|---------------------|------------------------------|---------------------|---------------------------------|
| Gas | Yes | X | | | | | | |
| | No ²¹ | X | | | | | X | |
| Liquid gas, low-temperature | Yes | X | X | X | X | | | X |
| | No ²² | X | X | X | X | | | X |
| Liquid gas, pressure-liquefied | Yes | X | X | X | X | X | | X |
| | No ²² | X | X | X | X | X | | X |
| Liquid | Yes | X | X | X | X | | | X |
| | No ²² | X | X | X | X | | | X |

IMPORTANT NOTE:

The Substance Database is set up in such a way that for each substance, four parameters must be entered: **Molar Mass**, **Boiling Temperature**, and **Vapour Pressure** with its associated **Temperature**. If one of these parameters is missing, the attempt to save the substance in the database will not be accepted.

If the heat of vaporization of a substance is not known, it can be estimated internally and drawn on for the calculation. The estimate is made using the Clausius-Clapeyron Equation, taking into account the boiling temperature and vapour pressure at the specified temperature. For an estimate of the heat of

²¹ In this case, the release quantity is calculated based on the geometry of storage, the storage conditions (pressure and temperature) and, in the case of continuous release, the size of the leak.

vaporization to be possible, the **boiling temperature and the temperature entered for the specified vapour pressure** must **differ by at least 10° K**.

The isentropic exponent is only required for substances that are stored as gases. This storage condition is only possible if the substance's boiling temperature is lower than the ambient temperature.²² Put the other around, this means that the isentropic exponent need only be given for substances whose boiling temperature is higher than the ambient temperature.

Appropriate values must be entered for danger threshold values. In the "Danger Threshold Values" edit area, the following input fields can be filled out, though they need not be:

- Threshold value, with a
- Name and
- Unit
- Odour Threshold
- Lower Ignition Limit
- Upper Ignition Limit

It is recommended to fill out the fields for threshold value, name (e.g. MAK or ERPG) and unit (mg/m³ or ppm) so as to be able to access these in case of an accidental release.

The Gaussian Puff Model can take dry deposition into account. In the "Deposition" edit field, a value can be entered for speed of deposition in [m/s].

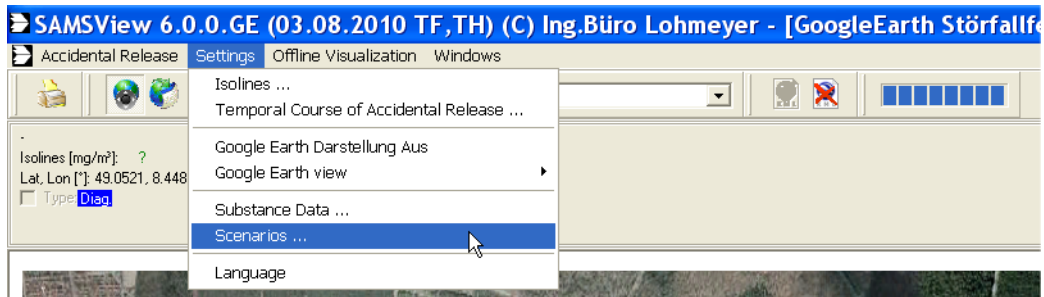
The "Notes" edit field can be used for entering optional text.

To transfer the data into the Substance Database, click either the **[OK]** button or the **[Accept changes]** button in the navigation area.

6.4 Maintaining the Release Scenarios

In offline mode, the menu item "Settings | Scenarios..."

²² The assumption here: The substance is stored at a pressure that is greater or equal to ambient pressure.



can be used for updating existing accidental release scenarios and for entering new accidental release scenarios or scenario templates. The "Release" window will appear.

Release

Selection of Release Scenario
Scenario: ALL UNKNOW'N (Original)

Copy New Delete Rename

Type of Accident
 Fire
 Release of Toxic Substances

Release Behaviour
 Sudden Release
 Continuous Release

Substance
Change Substance Data ...

Subst. Name : Chlorine
Synonym : Synonym
UN-Number : 1017
CAS-Number : 7782-50-5
EG-Number : 017-001-00-7
Guiding Comp. for unknown gas

Release Type
 Release Quantity known
 Release from Container/Pipe

Released Mass Flow Rate
 0.10044 kg / s
 0.03333 m³ / s

Phase of Substance
 Gas
 liquid Gas, low-temp. liquefied
 liquid Gas, pressure-liquefied
 Liquid

Height of Release
15 m above Ground

Cancel OK

SAMS-GLOBAL files the possible paths of substance release in what are called "release scenarios". The release scenarios can be input in offline mode. In the case of an accidental release, the release scenarios can be called up in the **Release** window under "Selection of Release Scenario".

A complete description of how to use the **Release** window can be found in **Chapter 5.1**.

7 SHUTTING DOWN THE SYSTEM

The components described in **Chapter 2** should not be closed during operational use if they are running. The system components may only be shut down for maintenance or after failures.

To shut down the system, take the following steps:

- Close any accidental release calculation that may be running
- Close the SAMS program
- Close **SAMView**

This disables the accidental release system. The computer can now be shut down.

APPENDICES

A OVERVIEW OF THE SYSTEM'S DIRECTORY STRUCTURE

Below is an overview of the structure and contents of the installed system directories. The main installation directory is called [InstallDir]. The following subdirectories are filed beneath it:

| | |
|---|--|
| lelisin | Contains the SAMSVIEW program, with user interface and graphics |
| Security directories with names in yyyy.mm.dd_hh.nn format (yyyy = year, mm = month, dd = day, hh = hour, nn = minute of the time when the calculation was started ²³): | <p>These directories contain:</p> <p>a.) Input data:</p> <ul style="list-style-type: none"> The input data common.nnn (nnn=000 to a maximum 999) of the Gaussian Puff Model for dispersion calculations (these make it possible to reconstruct the calculations). Input data for calculating the temporal course of release (Freisetzung.inp). <p>b.) Result data</p> <ul style="list-style-type: none"> Gaussian Puff Model results for Diagnoses (file prefix is Dddhhnn_) and for Forecasts (file prefix is Pddhhnn_). <ul style="list-style-type: none"> Status of the Gauss Puff (*.puf). In some cases: The concentration distribution (*.out) as calculated on the basis of Freisetzung.out, and the isoline files (*.bln). These do not necessarily exist. They can be calculated based on Freisetzung.out and puf file. Calculated temporal course of release (Freisetzung.out). |

The directory structure may not be changed. Likewise, no data (apart from those explicitly specified below) may be deleted or changed.

²³ The time at which the calculation was started may differ from the start of accidental release.

B RELEASE MODELLING

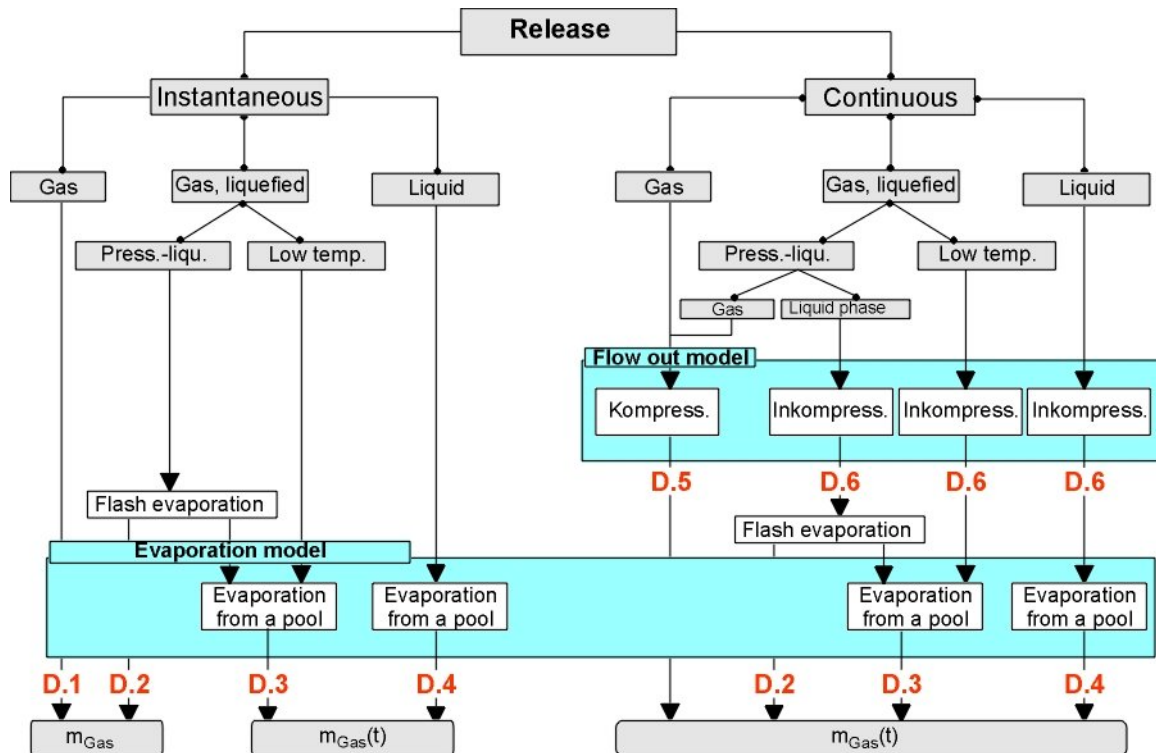


Fig. D.1: Paths of substance release

Fig. D.1 shows the relevant chapters for the respective paths in red type.

B.1 Sudden release of a gas

$$m_g = M \cdot \frac{p_{con} \cdot V_{con}}{\mathfrak{R} \cdot T_{con}}$$

m_g Released mass of gas in [kg]

M Molar mass of the substance in [kg/mol]

p_{con} Pressure inside container in [Pa]

V_{con} Container volume in [m³]

T_{con} Gas temperature in the container in [K]

\mathfrak{R} Universal gas constant (=8.314 J/(mol K))

If "Release Quantity Known" is selected in the "Release Type" edit field of the **Release** window, then the value entered in the edit field "Release Volume" will be used for V_{con} with temperature at 15° C and pressure at 1 bar.

B.2 Flash evaporation of pressure-liquefied gas

Part of the pressure-stored substance (the flash portion) evaporates spontaneously upon release. The flash portion can be calculated with the expression:

$$\Phi = 1 - \exp\left(-\frac{c_p}{h_v}(T_{con} - T_s(p_u))\right)$$

with

$$\begin{aligned} \Phi \leq 0.05 : \quad & m_{g,flash} = 4 \cdot \Phi \cdot m_{fl} \\ 0.05 < \Phi \leq 0.5 : \quad & m_{g,flash} = 2 \cdot \Phi \cdot m_{fl} \\ 0.5 < \Phi : \quad & m_{g,flash} = m_{fl} \end{aligned}$$

| | |
|------------|---|
| Φ | Flash portion in [-] |
| c_p | Specific heat capacity at constant pressure in [J/kg/K] |
| T_{con} | Storage temperature in the container in [K] |
| $T_s(p_u)$ | Boiling temperature at ambient pressure in [K] |

The portion that vaporizes into the atmosphere but does not do so through flash evaporation forms a pool and is calculated in accordance with D.3 or D.4.²⁴

B.3 Mass flow of a liquid gas vaporizing from a pool

$$\dot{m}_g = \frac{\lambda_{bb}(T_B - T_s(p_u))}{h_v \sqrt{\pi \cdot k_B t}} \cdot F(t)$$

To calculate the mass of gas vaporized from a pool for the interval from time t to time t + Δt, the following equation must be integrated:

²⁴ The greater of the two values is used.

$$\dot{m}_g(t \div t + \Delta t) = \frac{\lambda_B (T_B - T_S(p_u))}{h_v \sqrt{\pi \cdot k_B}} \cdot F(t) \cdot 2 \cdot (\sqrt{t} - \sqrt{t + \Delta t})$$

| | |
|-------------|---|
| \dot{m}_g | Vaporized mass flow in [kg/s] |
| λ_B | Heat conduction coefficient of the ground in [W/(mK)] |
| k_B | Thermal conductivity of the ground in [m ² /s] |
| h_v | Heat of vaporization in [J/kg] |
| T_B | Ground temperature in [K] |
| $T_S(p_u)$ | Boiling temperature at ambient pressure in [K] |
| t | Time since start of accidental release in [s] |
| F | Surface area of the pool of liquid or of the catch tray, in [m ²] |

For $\lambda_B / \sqrt{\pi \cdot k_B}$ the value 774 W s^{0.5}/(m² K) is used for sealed ground (i.e. non-porous ground); the value used for permeable ground is eight times that. If the surface area of the pool is not specified, then a pool depth of 2 cm is assumed.

B.4 Mass flow of a liquid gas evaporating from a pool

$$\dot{m}_g(t) = 0.002 \cdot u_o \frac{(u/u_o)^{0.78} \cdot (r/r_o)^{-0.11} \cdot M \cdot F \cdot p_u}{\mathfrak{R} \cdot T} \cdot \ln\left(\frac{p_u}{p_u - p_d}\right)$$

| | |
|----------------|---|
| $\dot{m}_g(t)$ | Evaporated mass flow in [kg/s] |
| u | Wind speed at 10 m above the surface in [m/s] |
| r | Radius of the pool of liquid or of the catch tray, or the longer side in the case of rectangular pools or catch trays |
| T | Temperature of the liquid in [K] |
| p_d | Vapor pressure on the surface of the liquid in [Pa] |
| p_u | Ambient pressure in [Pa] |
| F | Surface area of the pool of liquid or of the catch tray, in [m ²] |
| \mathfrak{R} | Universal gas constant (8.314 J/(mol K)) |

u_0 Reference velocity (= 1 m/s)

r_0 Reference radius (= 1 m)

If the surface area of the pool is not specified, then a pool depth of 2 cm is assumed.

B.5 Continuous emission of a gas

B.5.1 Continuous emission of a gas from a container

Critical emission takes place if the container pressure exceeds the critical pressure:

$$p_{con} \geq p_k = p_u \left(\frac{\kappa + 1}{2} \right)^{\frac{\kappa}{\kappa - 1}}$$

For CRITICAL emission, the following applies:

$$\dot{m}_g(t) = C_F F \sqrt{\kappa \left(\frac{2}{\kappa + 1} \right)^{\frac{\kappa + 1}{\kappa - 1}}} \cdot \frac{p_{con}(t)}{\sqrt{\frac{\mathfrak{R}}{M} \cdot T_{con}(t)}}$$

If the pressure in the container has decreased to the point that the critical pressure condition is no longer reached, or if the container pressure is in any case lower than critical pressure, then the following applies for mass flow for NON-CRITICAL emission:

$$\dot{m}_g(t) = C_F A \sqrt{\frac{2\kappa}{\kappa - 1} \left[1 - \left(\frac{p_u}{p_{con}(t)} \right)^{\frac{\kappa - 1}{\kappa}} \right]} \cdot \left(\frac{p_u}{p_{con}(t)} \right)^{\frac{1}{\kappa}} \cdot \frac{p_{con}(t)}{\sqrt{\frac{\mathfrak{R}}{M} \cdot T_{con}(t)}}$$

$\dot{m}_g(t)$ Time-dependent released mass flow in [kg/s]

C_F Discharge coefficient (= 0.61 for a round opening with sharp edges)

A Area of the leakage position or of the broken pipe in [m²]

p_u Ambient pressure in [Pa]

$p_{con}(t)$ Time-dependent pressure inside the container in [Pa] (in the case of pressure-liquefied gases and release in the gas phase: vapour pressure at ambient temperature)

| | |
|----------------|--|
| $T_{con}(t)$ | Time-dependent gas temperature in the container in [K] |
| κ | Isentropic exponent in [-] |
| M | Molar mass of the substance in [kg/mol] |
| \mathfrak{R} | Universal gas constant (8.314 J/(mol K)) |

B.5.2 Continuous emission of a gas when volume flow rate is known

If "Release Quantity Known" is selected in the "Release Type" edit field of the **Release** window, then the mass flow can be calculated with the Ideal Gas Law, assuming a temperature of 15° C and pressure of 1 bar:

$$\dot{m} = M \cdot \frac{p}{\mathfrak{R} \cdot T} \cdot \dot{V}$$

| | |
|-------------|--|
| \dot{m}_g | Released mass flow in [kg/s] |
| p | Pressure (calculation assumes 1 bar) |
| T | Temperature (calculation assumes 15°C) |
| \dot{V} | Volume flow rate [m³/s] |

(compare: The input field in the **Release** window)

B.6 Emission of a liquid or of a liquid gas (pressure-liquefied or low-temperature) from a container

The following equation is used to calculate the continuous emission of a liquid or of a liquid gas (pressure-liquefied or low-temperature) from a container:

$$\dot{m}_{fl}(t) = c_F A \rho \sqrt{2 \left(\frac{p_{con}(t) - p_u}{\rho} + g \cdot (h_0(t) - h_u) \right)}$$

| | |
|-------------------|---|
| $\dot{m}_{fl}(t)$ | Emission rate of liquid gas in [kg/s] |
| p_u | Ambient pressure in [Pa] |
| p_{con} | Pressure inside container in [Pa] |
| C_F | Discharge coefficient in [-] |
| A | Area of the leakage position or of the broken pipe in [m ²] |
| ρ | Density in [kg/m ³] |
| g | Acceleration of gravity (= 9.81 m/s ²) |
| h_0 | Height of the liquid surface in the container in [m] |
| h_u | Height of the point of emission in [m] |

For pressure-liquefied gases, the pressure in the container falls upon emission down to vapour pressure, which is dependent on the temperature of the liquid gas. For the calculation, the internal container pressure is deemed equal to the vapour pressure at the specified storage temperature. For low-temperature liquid gas, the pressure inside the container is deemed equal to the ambient pressure.

B.7 Size of pool (if this is not pre-given)

If the pool surface area is not specified, then the size of the pool is determined from the mass balance:

$$F(t) = \frac{\int_0^t \dot{m}_{fl} dt - \int_0^t \dot{m}_g dt}{\rho \cdot h_l}$$

| | |
|-------------------|---|
| $\dot{m}_{fl}(t)$ | Liquid mass flow emitted according to D.6 |
| $\dot{m}_g(t)$ | Gaseous mass low from evaporation or vaporization according to D.3 or D.4 |
| ρ | Density of the liquid in [kg/m ³] |
| h_l | Depth of pool in [m] |

Here, a pool depth of 2 cm is assumed. The above equation expresses the fact that the mass situated in the pool at time t is the difference between the liquid mass emitted up to time t and the gaseous mass that has entered the atmosphere.

For pressure-liquefied gas, the calculation of pool surface area is modified on account of flash evaporation. Flash evaporation is calculated as in D.2. For pressure-liquefied gas, pool surface area is calculated as follows:

$$F(t) = \frac{\int_0^t (\dot{m}_{fl} - \dot{m}_{g,flash}) dt - \int_0^t \dot{m}_g dt}{\rho h_t}$$