GasSimLite User Manual

Release 1

CHAPTER 1: INTRODUCTION TO GASSIMLITE

1.0 INTRODUCTION TO GASSIMLITE

This chapter aims to describe the background to GasSimLite, outline the program, detail how the manual is organised and inform you what you will need to run GasSimLite and where to obtain technical support.

About GasSimLite

The principal driver behind the development of GasSimLite is the requirement for a tool to estimate annual mass emissions to air of Pollution Inventory (PI) substances from landfills.

Since 1998, the Environment Agency has required the reporting of certain emissions from industrial processes regulated under Integrated Pollution and Control. The reporting of annual emissions from most landfills will become necessary under The Pollution Prevention and Control (England & Wales) Regulations, 2000 in early 2003 for emissions during 2002. Additionally, newly permitted facilities will be required to report PI emissions annually. Reported data may derive from measurement, calculation or estimation techniques and GasSimLite provides the capability to calculate the annual releases and report them in a format suitable to meet PI requirements.

The Environment Agency provides a standard list of substances to be reported based on operation during the previous year to reporting. GasSimLite reports the gases and volatile compounds on the PI list, which are known to occur at reasonably measurable concentrations in landfill gas, as detailed in (Gillett and Gregory, 2002). This list includes forty-five species, which are reported at the 25, 50 and 75 percentiles in the units required for PI purposes. The 50th percentiles can then be used to complete the non-notifiable air emission section of the PI reporting form.

It is under this framework of mainly new Regulations and technical guidance that GasSimLite was developed from GasSim (Environment Agency, 2002), which itself was developed using the HELGA framework (Gregory *et al.*, 1999), for the Environment Agency under the contract "Development of the Health and Environmental Risks from Landfill Gas".

The Conceptual Model

GasSimLite considers the landfill as one unit as, unlike leachate, cells are rarely isolated with respect to Landfill Gas (LFG). The model is divided into two modules the:

- ☐ source term;
- ☐ emissions module;

The source term determines the generation of LFG based on the mass of waste deposited and its composition for an individual site for the year following that for which data has been entered. The emission model takes this output and uses it to calculate the LFG emission, of bulk and trace gases, to the environment after allowing for LFG collection, flaring, utilisation (energy recovery), and biological methane oxidation. This is undertaken by using information on the site gas collection system, flare, engine, and engineered barriers (cap and liner) if present. It is assumed that LFG generated and not collected is in equilibrium and will be emitted from the landfill cap or liner at a steady state. Additionally the model calculates the concentrations of other major and trace gases emitted from flares and engines.

GasSimLite General Assumptions

GasSimLite has been developed from GasSim which itself has been developed to provide a standard risk assessment methodology that will aid a nationally consistent approach to the Agency's statutory duty in respect of gaseous emissions from landfill sites. GasSimLite has the following general assumptions:

- ☐ GasSimLite can only be used determine gas emissions from landfills and cannot be used for emissions from soils or groundwaters;
- ☐ the model operates at steady state with a minimum time period of 1 year;
- ☐ the model does not determine the pressure generated by the landfill and to simplify the model, pressure has been excluded from all modules;
- ☐ LFG is only abstracted from the capped area of the landfill and gas generated from the operational area is emitted directly to the atmosphere.
- ☐ GasSimLite determines the emissions for the landfill surface, and emissions for engines and flares. Lateral emissions are not determined, as these are relatively small and are therefore not considered to be significant.

Uses of GasSimLite

GasSimLite is designed to provide those concerned (waste regulators, operators, local authority planners and others) with the management of landfill gas with a means of calculating emissions necessary to meet the PI reporting requirements.

Program Outline

GasSimLite has been designed to be similar in design and layout to its sister applications LandSim (Landfill Performance Simulation by Monte Carlo Method, 2001) and ConSim (Contaminated Land Simulation by Monte Carlo Method, 1999). The model has been encoded using Microsoft's Visual Basic and C++ programming language, therefore users with experience of Microsoft Windows will find the program easy to navigate. The program follows all Windows conventions in terms of using the mouse, the appearance of input dialogue boxes and results screens.

In short, GasSimLite enables LFG generation and emissions for PI reporting purposes to be assessed by those without in-depth knowledge of programming.

The main screen shows a cartoon, which guides you along the process of defining the source term, the gas management options, details of the contaminant transport pathways (from the source to the various receptors). At each stage along the pathway pop-up dialogue boxes are accessed by clicking on active areas of the cartoon or from drop-down menus. These are used to enter data that enables GasSimLite to make the PI reporting estimates. The dialogue boxes are customised to the chosen landfill design and probability distributions for the default parameters are provided to prevent unnecessary data entry.

GasSimLite is a probabilistic model, which uses the Monte Carlo simulation technique to select randomly from a pre-defined range of possible input values to create parameters for use in the model calculations. Repeating the process many times gives a range of output values, the distribution of which reflects the uncertainty inherent in the input values and enables you to ascertain the likelihood of the estimated output levels being achieved.

How this Manual is Organised

This section presents a brief introduction to GasSimLite, its aims, structure and how it can be used.

Chapter 2 gives a guide to installing GasSimLite and getting started. The chapter also provides some background to the dialogue boxes, probabilistic risk assessment, and touches on quality assurance issues.

Chapter 3 shows how to enter parameters in order to set up and run a GasSimLite simulation. The chapter also details simplifying assumptions behind the model that must be borne in mind when assigning input parameters values and ranges.

Chapter 4 describes what GasSimLite predicts, how to interpret the results and how the output graph can be customised. The chapter also describes the important elements of a performance assessment and how to deal with modelling errors.

Chapter 5 contains suggested ranges of input parameters such as trace gases, engine and flare destruction efficiencies, etc.

Chapter 6 is a reference chapter which outlines the theory behind GasSimLite and presents equations used and assumptions made. Although you will probably not need to consult this chapter regularly it is recommended that you familiarise yourself with the assumptions made.

Your Experience

Don’t let GasSimLite’s ease of use deceive you. This program is intended solely for use by experienced professionals with a sound background in landfill engineering, landfill gas contaminant transport and risk assessment.

Your approach will be the key to obtaining useful results. Crucial to their validity will be your thoroughness when developing models, assessing the input parameters and working out uncertainties in the system. GasSimLite requires that you justify all expressed uncertainties and the output and printed record are locked together with a filename/timestamp system. Therefore you must be able to justify each input parameter. Your justifications are held in these records for subsequent audit.

What You Will Need

To run GasSimLite you will need an IBM compatible PC with a Pentium Processor with a speed of at least 300 MHz with 64 Mbytes of RAM. The software has been developed to run under Windows 95/98/2000. It is unlikely that NT users will have difficulty installing and using the Software, but

GasSimLite has not been specifically developed for NT and installation problems are not supported. Users will need 15 Mbytes of hard disk space for installation. Hard disk space required for temporary files during simulation may vary from 10 Mbytes upwards depending on the complexity of the simulation. Complex simulations involving multiple trace gases and human exposure may require up to 50Mb of storage or more.

On-Screen Help

For problems running the program or for technical enquiries, help files are available within GasSimLite either from the Main Menu or through buttons in each input window.

For further guidance on use of GasSimLite contact the Environment Agency on 08708 506 506.
Email pollution.inventory@environment-agency.gov.uk

You should also check the web site (www.gassim.co.uk) regularly to check for updates to the PI list, manual and model.

CHAPTER 2: GETTING STARTED WITH GASSIMLITE

2.0 GETTING STARTED WITH GASSIMLITE

The chapter aims to show you how to install and use the GasSimLite program, and provides a brief introduction to the philosophy of risk and risk assessment. The key principles behind risk, risk assessment, performance assessment and the issues of uncertainty are described. This chapter should be read even by those familiar with the concepts of risk assessment and the section describing the choice of input parameters is likely to be extremely useful.

How to Install GasSimLite

GasSimLite is supplied on mini CD or via the internet. To install the software, close any open applications and place the CD in the CD-ROM drive.

Click OK to start installing the program and follow the on-screen instructions. If the installation does not start automatically and the Setup program is not activated, run the Setup program on the CD to manually start the setup process.

You must use the Setup program to install GasSimLite. The files on the installation CD are compressed and cannot be copied directly to your hard drive. To uninstall GasSimLite you should use the Add/Remove Programs application in the Control Panel. If you wish to install further updates to the GasSimLite software that may be issued from time to time, it is essential that you uninstall the current version of the model prior to installing the update.

Keying Convention, Mouse Use and Windows Standards

GasSimLite follows the usual Windows conventions:

- ☐ mouse action;
- ☐ drop down menus triggered by the <Alt> key with navigation by arrow keys;
- ☐ drop down menus triggered by <Alt> key with navigation by key letters (which are capitalized and underscored on the menu names);
- ☐ accelerator key sequences (e.g. Ctrl + S to save a file, indicated on the drop down menu item).

This manual has been written around mouse driven use, which is likely to be the most convenient way for most people. However, an experienced user may find the keyboard short cuts faster. In terms of mouse use, the standards used by Microsoft in developing Excel have been our guide, and if you are in doubt anywhere in GasSimLite, try an Excel mouse operation. For example, double clicking (two fast clicks) on the scale of a graph will open a scale change dialogue. We have also built in a number of pop-up features and in several instances you will find the appropriate menu items available with a single click of the right mouse button.

To exit the dialogue boxes without making or saving changes use the Cancel buttons available. It is not possible to damage the GasSimLite program by any combination of events with the program.

Starting the Program

To start the program double click the GasSimLite icon, or select GasSimLite from the start menu.

During loading GasSimLite will display a graphic showing the software version.

To continue click the New Project or Open

Project options. Selection of the New Project option will open the project data file and Open Project will request that you select the existing project file. These options are described in Chapter 3. To exit GasSimLite select Exit.

Closing GasSimLite

To close down GasSimLite select the Exit option from the File menu. You will be prompted to check that you have saved your work. If you wish to close the program without saving select No, otherwise choose Yes, and GasSimLite will close down.

On-line Help

GasSimLite is supplied with full on-line help, which can be accessed through either the main menu, through the buttons on each input window or by pressing the F1 key.

REPRESENTING UNCERTAINTY AND INPUT DISTRIBUTIONS

The basic idea in all probabilistic assessments is that a probability can represent a judgement about uncertainty. Many of the model inputs have a wide range of uncertainty due to measurement techniques and natural variations. Parameter uncertainty (and to some extent model uncertainty) is dealt with by allowing specification of a range of values for each input parameter rather than a single number, using probability density functions (PDFs).

GasSimLite allows most of the inputs to be defined as single values or a number of distributions, e.g.

- Uniform Distribution. Where it is possible to specify a minimum and maximum possible value for a parameter and where there is an equal chance of all the values in between (or where there is no further information), a uniform distribution is appropriate e.g. a range in waste inputs, leachate heads or waste densities;

- Triangular Distribution. Where, in addition to minimum and maximum values, it is possible to identify a value that is most likely to occur, a triangular distribution may be used appropriate e.g. a range in waste inputs, leachate heads or waste densities;

- Log Uniform or Log Triangular Distribution. When parameter values vary by orders of magnitude, the specification of a log uniform or log triangular distribution (uniform or triangular distribution of the logs of values) avoids skewing the distribution towards the upper or lower values e.g. a range in trace gas values or cap/liner hydraulic conductivities;

- ☐ Normal or Log Normal Distribution. Many natural parameters follow a statistically normal/log normal distribution, that is described using a mean value and a standard deviation from the mean e.g. a range in trace gas values;

- ☐ Other Distribution Types. GasSimLite permits the definition of input distributions other than those specified above. If there are sufficient available data fitting these distributions, then they are available to you, although it is anticipated that in the majority of cases the simpler distributions will be appropriate.

The choice of input distribution may have a profound effect on the predicted results and it is important that the distribution type you use is justified based on the available data.

There will be instances where there is a large base of data, and a distribution may be defined that closely represents the data. A number of commercially produced software packages (such as Palisade Corporation's "Bestfit" and the latest version of Decisioneering's "Crystal Ball") are available to help you determine the most appropriate distribution of a data set. Further guidance on assessing appropriate PDFs for use in environmental risk assessments are provided in Environment Agency (2001).

Uncertainty Versus Variability

Many properties and processes are naturally variable. You would expect, for example, trace gas concentrations to vary from place to place within the waste mass. When looking at a range of monitoring data, it should be remembered that this data includes both true uncertainty (caused by test error, interpretation etc.) and true variability. Variability is also important because it does not automatically follow that the average case realistically represents reality – sometimes the weakest point in the chain may be the controlling factor.

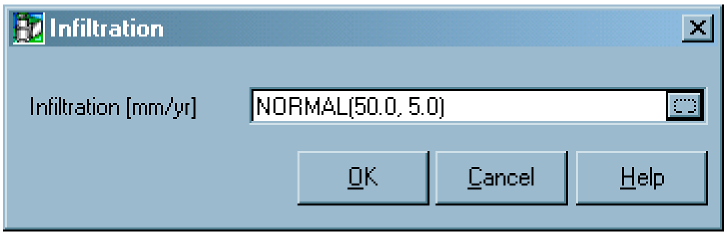
CHAPTER 3: SETTING UP AND RUNNING A SIMULATION

3. SETTING UP AND RUNIING THE SIMULATION

This chapter will explain how to input data into the model and run a GasSimLite program. The theory and equations behind the model are described in Chapter 6.

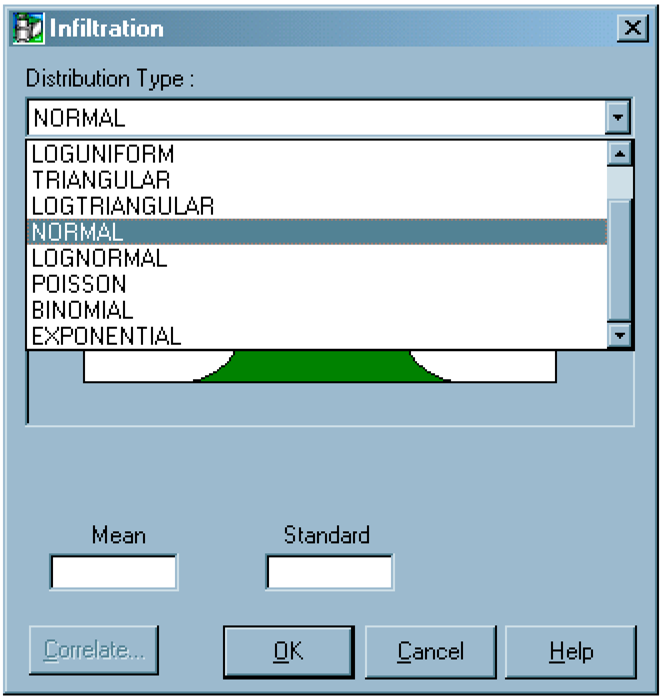
Entering PDFs

A large number of the individual inputs in the Infiltration, Source, Gas Utilisation, and Landfill Characteristics elements of the model, can be entered as **p**robability **d**ensity **f**unctions (PDFs). There are a number of methods of entering these inputs. Where a PDF can be entered in the input into a field, a small grey box with dots at the far right of the field will appear (as indicated by the arrow in the screen below).



Infiltration [mm/yr] NORMAL(50.0, 5.0)

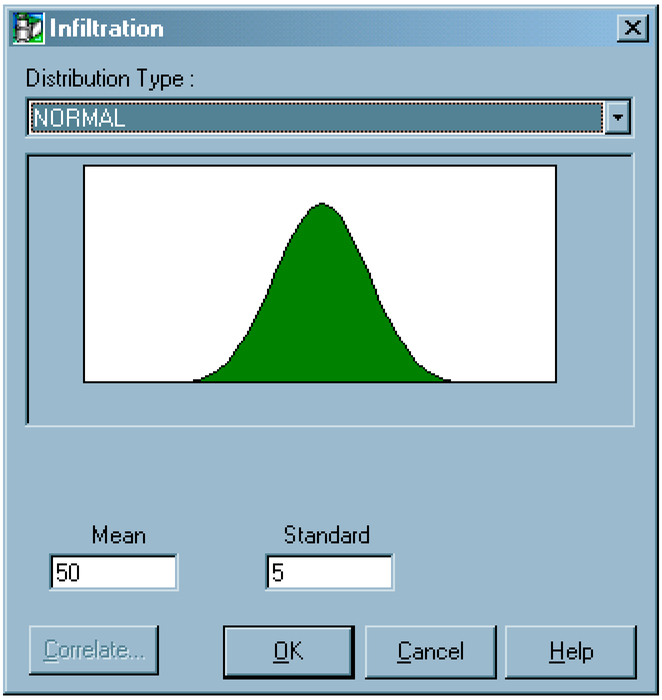
The values of individual Input Distributions may be edited in three ways:



Distribution Type : NORMAL

- ❑ You can input parameter distributions in a structured manner through an input distribution window (select the input parameter you require and click on the grey box at the right hand end of the parameter space.

- You can then select the appropriate distribution type from a drop down menu, and type in the values required.



Distribution Type : NORMAL

Mean 50

Standard 5

- You can type the parameter distribution, in words and figures, into most of the parameter spaces. (However, this function is not available when distributions are being entered into GasSimLite input tables.) You will find that if you type 'un', GasSimLite will automatically complete the word 'uniform', and you will only need to add the required values, separated by a comma. Similarly, 'tr' brings up a triangular distribution etc. As you become more familiar with the use of the model, you will decide the method that best suits you. See below for a full list of the distribution types and abbreviations.

- In addition to the above, it is also possible in most cases to use the cut and paste facility (CTRL-C and CTRL-V) on existing parameter distributions. This function is again not available when distributions and being entered into GasSimLite input tables.

Where input distributions are impossible (e.g. minimum value greater than maximum) or outside a defined range then GasSimLite will highlight the values in red and will not accept the input.

The following distributions are available:

Distribution	**Abbreviation (and syntax)**
Single(value)	None - just enter value
Uniform	UN (min, max)
Triangular	TR (min, most likely, max)
Normal	NO (mean, standard deviation)
LogUniform	LOGU (min, max)
LogTriangular	LOGT (min, most likely, max)
LogNormal	LOGN(mean, standard deviation)
Binomial	BI (No. of trials, Prob)
Exponential	EX (mean)
Poisson	PO (average)

Within GasSimLite, you will be expected to input data in commonly accepted units (for example, infiltration as mm/year, trace gas concentrations as mg/m^3). Input fields indicate the units you should use.

Retrieving (Opening) an Existing Model

Previously saved models (files with extension .gss) can be retrieved using the 'Open' option under the 'File' menu on the main GasSimLite toolbar or by selecting Open Project from the GasSimLite start menu. In order to find your previously saved file you should ensure that the drive and directory are set correctly. Only files with the extension '.gss' in the current directory will be listed.

Click on the name of the model you wish to retrieve and choose the 'OK' button. The current simulation will then revert to that saved. You cannot have more than one model open at once and you will be prompted to save the previous model before the new model is opened.

A productive way of using GasSimLite is to develop a model with the required configuration, which can then be saved with several file names. Retrieving each of these files allows minor changes to be made, e.g. changing the flare and engine capacities to represent the effect of increasing or reducing gas utilisation, with other aspects of the model remaining intact. Remember to change the notes about your simulation (if appropriate) through the 'Edit' and 'Project Details’ menus.

Each simulation file stores its complete file path to ensure that the correct results are displayed. If a *.gss file is renamed outside of the GasSimLite program, or used on a mapped drive, when you run a simulation you will get the error message "Either the Model name or time of last save has been changed. Statistics cannot be reloaded." To resolve this problem, save and rerun the simulation.

GasSim Files

You not will be able to read existing GasSim (Chapter 1) files into GasSimLite.

Project wizard (Starting a new project)

If you are creating a new project/model you will be lead through a number of input screens. The initial screen asks you to provide a file name in which to store the data (all GasSimLite files must have the suffix .gss, which is added automatically when using the Save As option from the file menu The next input screen requires the project details, described below.

The remaining stages cover the input screens for the source and emissions modules (Infiltration, Source, Landfill Characteristics and Gas Utilisation). These can also be accessed during normal editing from the main menu.

Once you have provided a file name to store the model input parameters, you can move forward and backwards (Next and Previous buttons) though the various screens. You also have the option to exit the Project Wizard (Finish button) at any time. This option allows data entry/editing in any order and it is likely that as you become more familiar with the software you will use this option more regularly.

Menu System

The data input boxes are opened by clicking the mouse button and you are encouraged to experiment with the various menus and input screens to find your optimum means of navigation around the model.

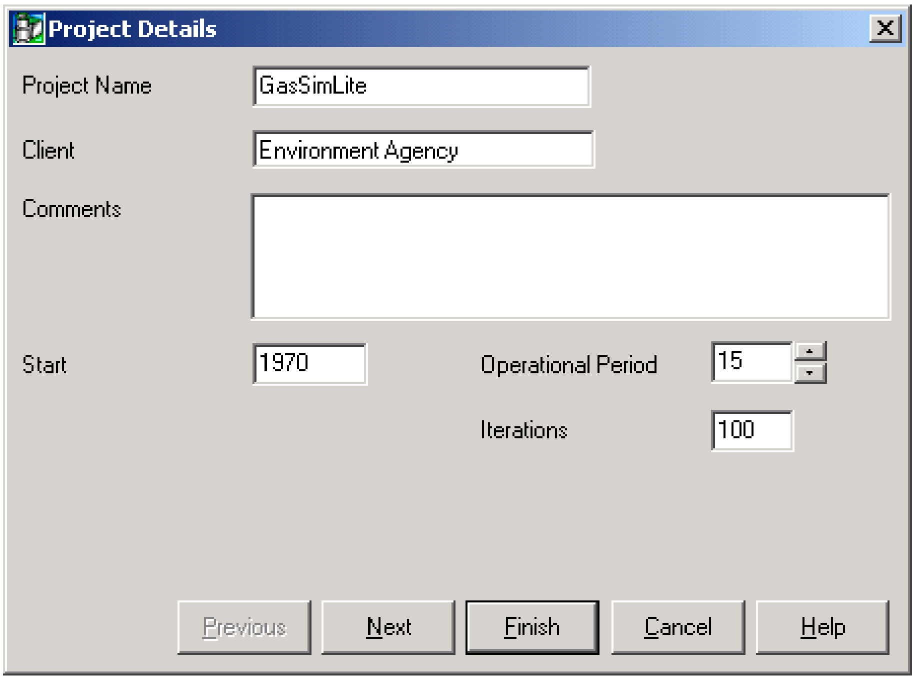
To exit the dialogue box and save the information you should click OK. To exit without saving the information can be carried out by clicking Cancel or clicking the top right hand corner of the box.

Project Details

The first information requested relates to the project/site that you wish to simulate. The ‘Project Name’. ‘Client’ and ‘Comments’ will be printed on all hardcopy outputs. The window also requires:

- ☐ the ‘Start’ year that waste deposition commenced in the landfill;
- ☐ the ‘Operation Period’ (the number of years that waste deposition occurred);
- ☐ the number of ‘Iterations’ (the number of times that the model will be run using the Monte Carlo simulation, an increased number will provide greater confidence in the results), the default value should be 100 iterations.

The window can also be assessed through Edit – Project Details on the main menu.

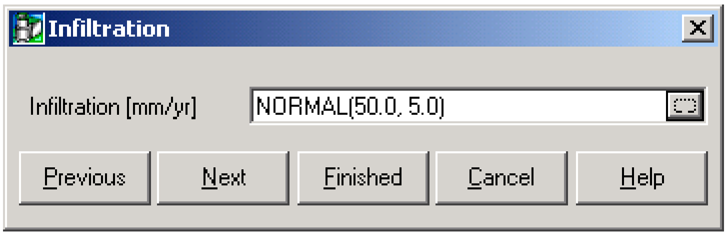


Project Name: GasSimLite
Client: Environment Agency
Comments:
Start: 1970
Operational Period: 15
Iterations: 100

It should be noted that after the Project Details are set and you have started entering data in the source model increasing the number of operation years will add years after the initial end of the filling life. Therefore you cannot add years prior to the initial filling data. Reducing the number of operational year may lead to the loss of data.

Infiltration

The 'Infiltration' term can be entered by either clicking the cartoon icon on the screen or via the project wizard. The infiltration option allows you to define the rate of water entering the landfill through the capped and uncapped areas annually (mm/yr), per unit area.



Infiltration [mm/yr]: NORMAL(50.0, 5.0)

The infiltration is effective rainfall entering the waste (i.e. rainfall less runoff, evaporation and transpiration). This information can be entered as a PDF, as described in the section above. This is usually entered as a normal PDF.

When selecting an infiltration rate you should considered other fluid flowing into the landfill i.e. the inflow of groundwater or disposals of liquid waste. The volume of leachate recirculated and the leachate head can be ignored at this stage, as these can be input directly into the waste moisture content dialogue box.

The infiltration rates will depend on the proportion of the landfill that is capped, the nature and age of the cap, i.e. older caps may be more permeable as a result of deterioration.

Source Term Inputs

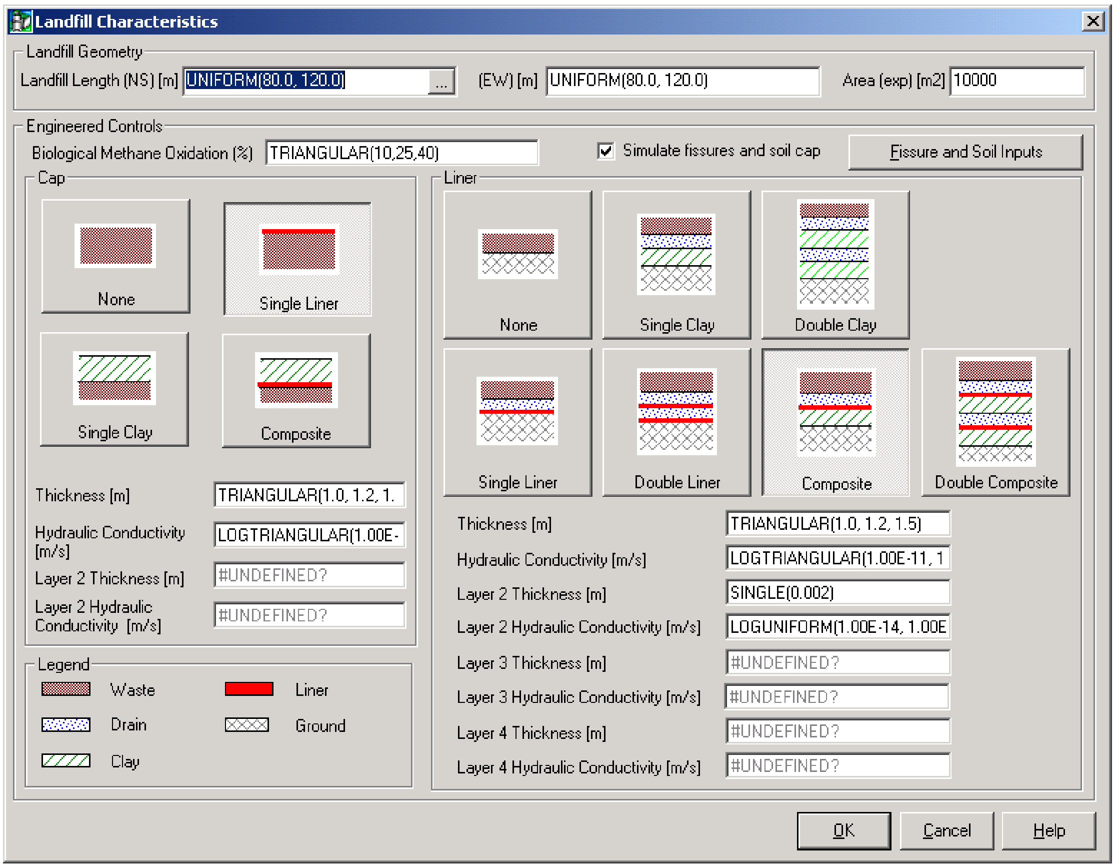
The source term has been divided into three sections:

- 'Source';
- 'Waste Moisture Content';
- 'Trace Gas Inventory'.

GasSimLite used parameters from these three dialogue boxes along with the data in the 'Infiltration' and 'Landfill Characteristics' dialogue boxes to calculate the LFG generation.

Landfill Characteristics Inputs

The Landfill Characteristics term is split into two sections, the Landfill Geometry and the Engineered Controls.



Landfill Geometry
Landfill Length (NS) [m] UNIFORM(80.0, 120.0)
(EW) [m] UNIFORM(80.0, 120.0)
Area (exp) [m2] 10000

Engineered Controls
Biological Methane Oxidation (%) TRIANGULAR(10,25,40)
☑ Simulate fissures and soil cap

Cap
Thickness [m] TRIANGULAR(1.0, 1.2, 1.
Hydraulic Conductivity [m/s] LOGTRIANGULAR(1.00E-
Layer 2 Thickness [m] #UNDEFINED?
Layer 2 Hydraulic Conductivity [m/s] #UNDEFINED?

Liner
Thickness [m] TRIANGULAR(1.0, 1.2, 1.5)
Hydraulic Conductivity [m/s] LOGTRIANGULAR(1.00E-11, 1
Layer 2 Thickness [m] SINGLE(0.002)
Layer 2 Hydraulic Conductivity [m/s] LOGUNIFORM(1.00E-14, 1.00E
Layer 3 Thickness [m] #UNDEFINED?
Layer 3 Hydraulic Conductivity [m/s] #UNDEFINED?
Layer 4 Thickness [m] #UNDEFINED?
Layer 4 Hydraulic Conductivity [m/s] #UNDEFINED?

Landfill Characteristics

The 'Landfill Characteristics' section allows you to define the landfill 'Length', assumed to be a north to south direction, and 'Width', assumed to be an east to west direction. These dimensions defined the area in which the waste has been placed. GasSimLite assumes that the entire landfill is a single phase, with vertical sides, which is reasonable as normal cell construction is designed to prevent the flow of leachate but is normally permeable to gas. GasSimLite uses these to determine the surface 'Area' and volume of the landfill. Therefore, the landfill length and width should be measured at the surface of the landfill. The surface area is used to determine the water content of the landfill from the infiltration rate and the leachate head, and is used to determine the proportion of emission released through the cap. GasSimLite calculates the depth of the landfill surface area, the waste volume and the waste density by assuming that the landfill is a 3-Dimensional rectangle (Parallelepipede) with vertical sides. GasSimLite uses the depth of unsaturated waste, (the waste depth minus the leachate head) to determine the proportion of emissions released laterally through the liner.

Methane emissions can be reduced as they pass through the landfill cap by microbes. The proportion of the methane that is converted to carbon dioxide by 'Biological Methane Oxidation' should be defined on a site-specific basis, as the quantity of methane oxidation is dependant on a number of factors including the cap thickness and permeability. GasSimLite simulates the reduction of methane using two approaches. The simplest is the reduction of methane by the proportion suggested in DEFRA policy of 10%, which is based on the IPPC guidelines, and is used by the AEAT UK emissions estimation model (AEAT, 1999), in the absence of site specific information 10% should be used.

The second approach calculates the methane oxidation rates for the different cover materials. This can be simplified to a methane oxidation range of between 10-46%, with a mean of 25%, occurring if the soil above thickness the cap (entered) is greater than 300mm. If the soil thickness is less, it is assumed that no methane oxidation will occur. Additionally you are required to enter the percentage of fissures, discrete features, on the site, GasSimLite assumes that LFG will pass through the features without methane oxidation occurring. The default number of fissures is set at 10% based on the measurements obtained using the Environment Agency's methane emissions measurements procedures (2001a). To selected this option click the 'Simulate Fissures and Soil Cap' and then select the 'Fissures' button. This will produce the 'Biological Methane Oxidation' dialogue box where the 'Soil depth' and '% of area occupied by fissures' can be defined.

Engineered Controls

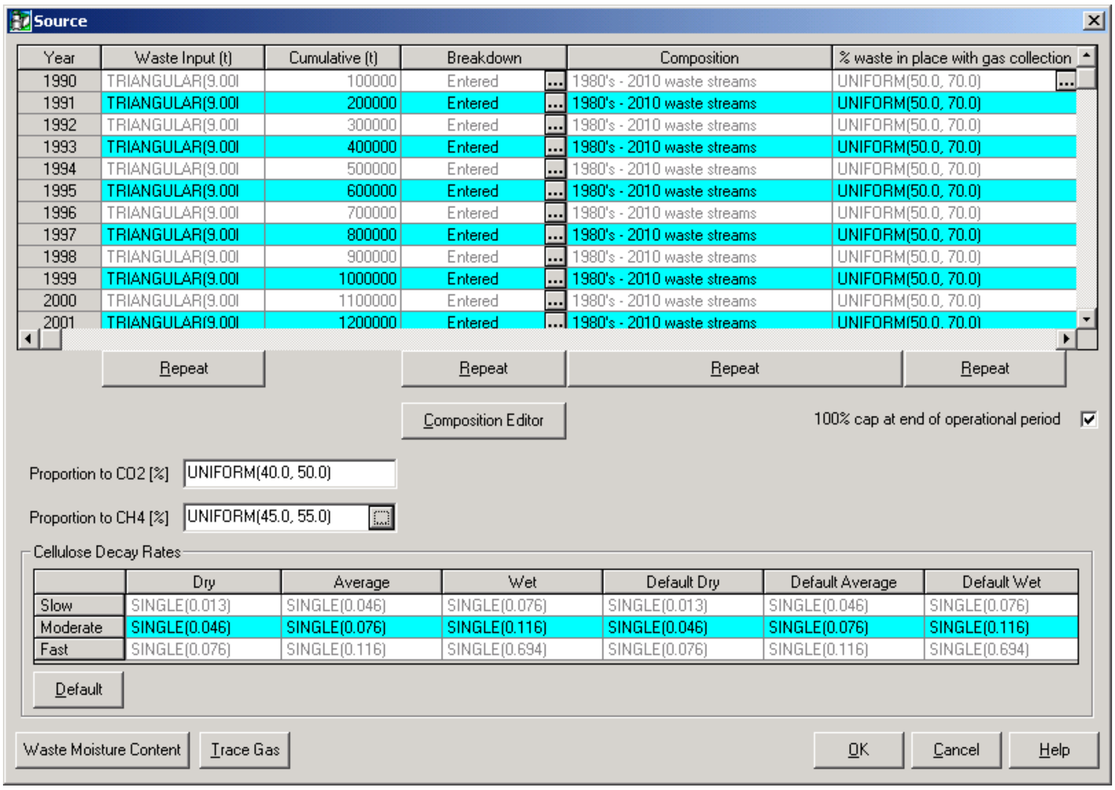
This section allows you to define the engineered controls, installed during the construction of the landfill, to prevent the uncontrolled release of LFG. These are principally the 'Cap' and 'Liner' constructions, which are important inputs as GasSimLite assumes that any gas unutilised is lost uncontrollably via these routes.

You are required to select the picture of the cap and liner design that represents the landfill that is being simulated. GasSimLite will then require the 'Thickness' and 'Hydraulic Conductivity' for each layer to be defined. Inputs that are not required will be in grey. The permeability of the cap and the liner are entered as hydraulic conductivities as this information should be readily available. GasSimLite determines the gas conductivity of these materials. GasSimLite then uses this information to determine the cap and liner gas conductivity which are assumed to be controlled by the least permeable layers.

Source

The ‘Source’ input screen requires the quantity and composition of waste deposited for the each operation year. The year that waste deposition commenced and the number of operation years are defined in the ‘Project Details’.

The ‘Waste Input’, rate (in tonnes), is required for each operation year. If this value is not known precisely then a PDF can be used to represent the uncertainty. In most cases there will be a good record of the initial void space and current void available, so a reasonable estimate of the inputs can be made.



Year	Waste Input (t)	Cumulative (t)	Breakdown	Composition	% waste in place with gas collection
1990	TRIANGULAR(9.00I	100000	Entered	1980's - 2010 waste streams	UNIFORM(50.0, 70.0)
1991	TRIANGULAR(9.00I	200000	Entered	1980's - 2010 waste streams	UNIFORM(50.0, 70.0)
1992	TRIANGULAR(9.00I	300000	Entered	1980's - 2010 waste streams	UNIFORM(50.0, 70.0)
1993	TRIANGULAR(9.00I	400000	Entered	1980's - 2010 waste streams	UNIFORM(50.0, 70.0)
1994	TRIANGULAR(9.00I	500000	Entered	1980's - 2010 waste streams	UNIFORM(50.0, 70.0)
1995	TRIANGULAR(9.00I	600000	Entered	1980's - 2010 waste streams	UNIFORM(50.0, 70.0)
1996	TRIANGULAR(9.00I	700000	Entered	1980's - 2010 waste streams	UNIFORM(50.0, 70.0)
1997	TRIANGULAR(9.00I	800000	Entered	1980's - 2010 waste streams	UNIFORM(50.0, 70.0)
1998	TRIANGULAR(9.00I	900000	Entered	1980's - 2010 waste streams	UNIFORM(50.0, 70.0)
1999	TRIANGULAR(9.00I	1000000	Entered	1980's - 2010 waste streams	UNIFORM(50.0, 70.0)
2000	TRIANGULAR(9.00I	1100000	Entered	1980's - 2010 waste streams	UNIFORM(50.0, 70.0)
2001	TRIANGULAR(9.00I	1200000	Entered	1980's - 2010 waste streams	UNIFORM(50.0, 70.0)

100% cap at end of operational period ☑

Proportion to CO2 [%] UNIFORM(40.0, 50.0)

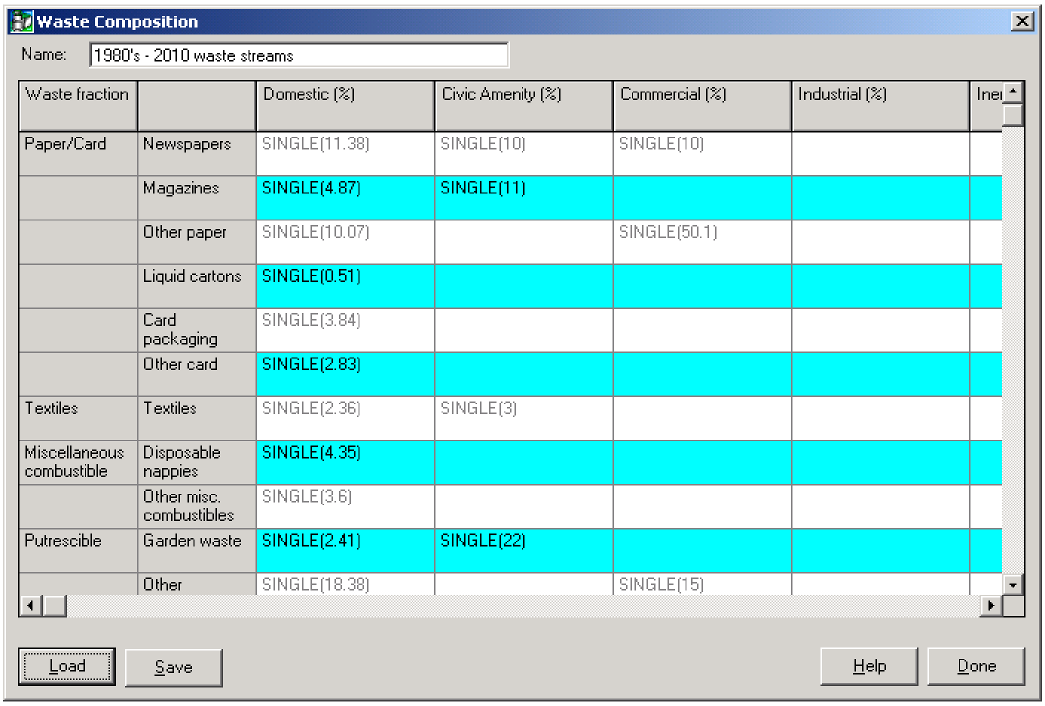
Proportion to CH4 [%] UNIFORM(45.0, 55.0)

Cellulose Decay Rates

	Dry	Average	Wet	Default Dry	Default Average	Default Wet
Slow	SINGLE(0.013)	SINGLE(0.046)	SINGLE(0.076)	SINGLE(0.013)	SINGLE(0.046)	SINGLE(0.076)
Moderate	SINGLE(0.046)	SINGLE(0.076)	SINGLE(0.116)	SINGLE(0.046)	SINGLE(0.076)	SINGLE(0.116)
Fast	SINGLE(0.076)	SINGLE(0.116)	SINGLE(0.694)	SINGLE(0.076)	SINGLE(0.116)	SINGLE(0.694)

The type of the waste (i.e. the percentage of the waste deposited that is domestic, commercial, industrial, inert waste etc.) is entered by clicking on the box containing 3 dots, to the right hand side of the waste ‘Breakdown’ box. This opens the Waste Breakdown box, which requires the percentage of waste in each stream. Once this data has been defined ‘entered’ will appear in the breakdown cell of the table for that year. If a PDF is used to describe uncertainty in one or more of the streams then the percentage will no longer equal 100%. To avoid losing or gaining mass unintentionally, the figures are normalised back to 100% on each iteration of the model.

The ‘Composition’ of each waste stream is defined by using the drag down box located on the right hand side of the composition input. This will display the default waste compositions. The composition available can be viewed and edited by clicking the Composition button. However, it should be noted that changing the name of the composition in the ‘Waste Composition’ dialogue box will not change compositions selected in the table. Therefore the new files will have to selected as described below.



Name: 1980's - 2010 waste streams

Waste fraction		Domestic (%)	Civic Amenity (%)	Commercial (%)	Industrial (%)	Ine
Paper/Card	Newspapers	SINGLE(11.38)	SINGLE(10)	SINGLE(10)		
	Magazines	SINGLE(4.87)	SINGLE(11)			
	Other paper	SINGLE(10.07)		SINGLE(50.1)		
	Liquid cartons	SINGLE(0.51)				
	Card packaging	SINGLE(3.84)				
	Other card	SINGLE(2.83)				
Textiles	Textiles	SINGLE(2.36)	SINGLE(3)			
Miscellaneous combustible	Disposable nappies	SINGLE(4.35)				
	Other misc. combustibles	SINGLE(3.6)				
Putrescible	Garden waste	SINGLE(2.41)	SINGLE(22)			
	Other	SINGLE(18.38)		SINGLE(15)		

The ‘Waste Composition’ defines the fractionation of different materials within the waste streams along with percentages for ‘Water Content’, ‘Cellulose’, ‘Hemi-Cellulose’ and ‘Decomposition’ for each waste fraction/material. The proportion of the waste in different fractions has been determined from literature sources (Chapter 5). However, the user can edit these using site specific information by clicking on the percentage that they wish to change and then selecting the button with three dots, that will bring up a PDF input screen. This information is used to calculate the quantity of carbon that is available for slow, moderate and fast degradation and thus quantity and rate of LFG production. The waste ‘Composition’ screen also provides the user with the option to Save their own composition files and Load previously saved and other default compositions to do this you mush change the name of the file and the waste composition ‘Name’ in the top left hand corner of the dialogue box. To exit the waste composition screen click the Done button or the cross in the top right hand corner of the box. If alterations have been made to the waste Composition files that have not been saved a dialogue box will appear giving you warnings to indicate where additional information/data is required. If a PDF is used to describe uncertainty in one or more of the waste components then the percentage will no longer equal 100%. To avoid losing or gaining degradable carbon unintentionally, the figures are normalised back to 100% on each iteration of the model.

The ‘Percentage Waste in Place Capped’, for each operational year, allows GasSimLite to determine the quantity of the LFG available for utilisation, as GasSimLite assumes that LFG generated in the uncapped/operation area will only be emitted to the atmosphere and not collected. The percentage of the waste in place capped vs. uncapped should be based on a tonnage to represent the proportion of the waste that is uncapped rather than an area term that will assume a uniform thickness. GasSimLite also requires the user to indicate if the site is 100% capped after the operation period. If this box is not selected, GasSimLite will assume that the proportion of site capping will remain at the level defined in the last operation year. The percentage waste in place capped is not the percentage area of the final completed landfill, but the areas capped at that time in the landfills life. For example, if the site has a total area of 20 ha, but in year 5 only covers 5 ha and 2 ha are capped, then the percentage waste in place covered would be 40%.

Once the 'Waste Input', 'Breakdown', 'Composition' and 'Waste in Place Capped' have been entered for the first operation year, GasSimLite contains a short cut that allows each these inputs to be repeated for all operational years. To select highlight the relevant cell in the column which you wish to copy to the bottom of the table and select the Repeat button. This is a useful short cut as the waste composition and breakdown may not change significantly during the operational period. However, alterations to the "waste composition", "breakdown" and "percentage waste in place capped" can still be made by editing the inputs for individual years.

GasSimLite can simulate landfills that are left uncapped or party capped for a number of years prior to full capping by extending the operation life of the landfill, and entering zero tonnes of disposed waste each year.

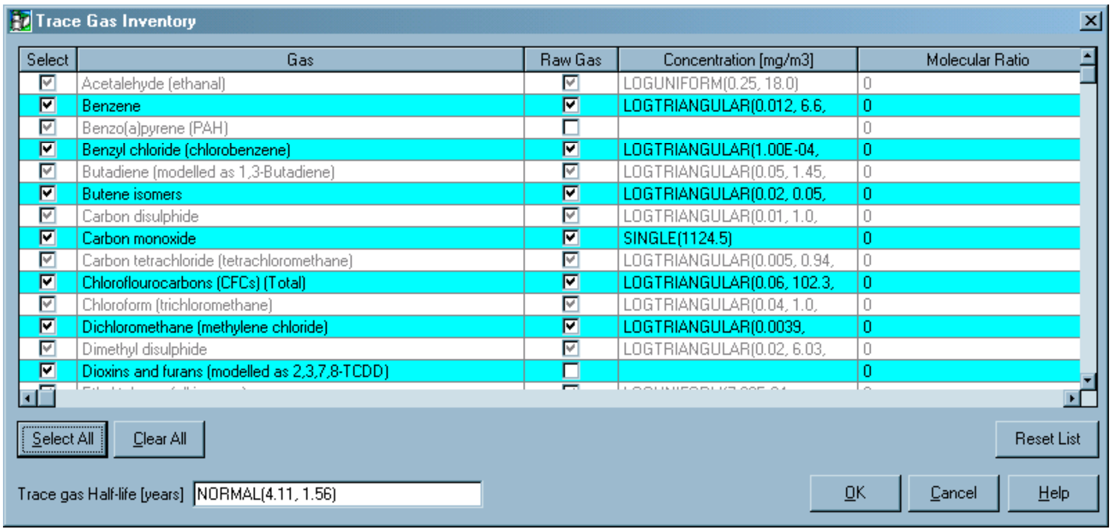
The 'Proportions of Methane' (CH_4) and 'Proportions of Carbon Dioxide' (CO_2) allow the user to define the LFG composition anticipated over the simulation period. These can be entered as percentages either as single values or PDF files. The proportions are normalised to 100% for each iteration.

The 'Cellulose Decay Rates' for 'Dry', 'Average' and 'Wet' waste, for 'Slow', 'Moderate' and 'Fast' degrading carbon determines the rate of cellulose (waste) decay. Clicking the Default button will set the simulated values to the default values provided on the right hand side of the table. Alternatively, by clicking on the required box on the left hand side of the table and selecting the button containing three dots allows user defined PDFs of these values to be entered. These values should be altered with care as they determine the rate of waste decay and thus the generation of LFG.

The cartoon contains two additional data entry points in the bottom left hand corner of the 'Source' dialogue box, the 'Trace Gas Inventory' and, 'Waste Moisture Content', clicking on the text open the dialogue box for the relevant input data.

Trace Gas Inventory

Clicking the Trace gas button produces the flowing dialogue box.



Select	Gas	Raw Gas	Concentration [mg/m3]	Molecular Ratio
☑	Acetalehyde (ethanal)	☑	LOGUNIFORM(0.25, 18.0)	0
☑	Benzene	☑	LOGTRIANGULAR(0.012, 6.6,	0
☑	Benzo(a)pyrene (PAH)	☐		0
☑	Benzyl chloride (chlorobenzene)	☑	LOGTRIANGULAR(1.00E-04,	0
☑	Butadiene (modelled as 1,3-Butadiene)	☑	LOGTRIANGULAR(0.05, 1.45,	0
☑	Butene isomers	☑	LOGTRIANGULAR(0.02, 0.05,	0
☑	Carbon disulphide	☑	LOGTRIANGULAR(0.01, 1.0,	0
☑	Carbon monoxide	☑	SINGLE(1124.5)	0
☑	Carbon tetrachloride (tetrachloromethane)	☑	LOGTRIANGULAR(0.005, 0.94,	0
☑	Chloroflourocarbons (CFCs) (Total)	☑	LOGTRIANGULAR(0.06, 102.3,	0
☑	Chloroform (trichloromethane)	☑	LOGTRIANGULAR(0.04, 1.0,	0
☑	Dichloromethane (methylene chloride)	☑	LOGTRIANGULAR(0.0039,	0
☑	Dimethyl disulphide	☑	LOGTRIANGULAR(0.02, 6.03,	0
☑	Dioxins and furans (modelled as 2,3,7,8-TCDD)	☐		0

Trace gas Half-life [years] NORMAL(4.11, 1.56)

This allows trace gases of interest to be entered. GasSimLite has a data base containing default distributions of trace gas concentrations for PI reporting requirements. The distributions of the default species have been determined for the literature (Section 5), which has resulted in a combination of log triangular, log normal, triangular, normal and single value distributions. The source concentrations can be edited by selecting the 'Concentration' of the gas of interest and redefining the PDF. It should be noted that selecting a 'Reset List' will reset trace gas concentrations to the GasSimLite default values. The function will also update the PI list if new trace gases have been added, in order to do this you will need to an up-to-date trace.data input file.

The species in the inventory can be viewed by scrolling up and down through the list. The gases simulated can be altered by clicking on the 'Select' box to pick or remove a gas from the simulation, a tick will appear in the box if the gas is selected.

You are required to select the 'Gas' species that you wish to simulate, whether these are species present within the LFG or present only as combustion products from flares and engines. Some combustion products can be determined from their Parent Species i.e. HF from F and HCl from Cl. Where this is the case, the parent product should be selected. The selection is made by clicking on the 'Select' box to the left to the species required, a tick will then appear to show that the option has been activated. Additionally all species displayed can be selected by clicking the Select All button, and all species can be deselected by clicking the Clear All button.

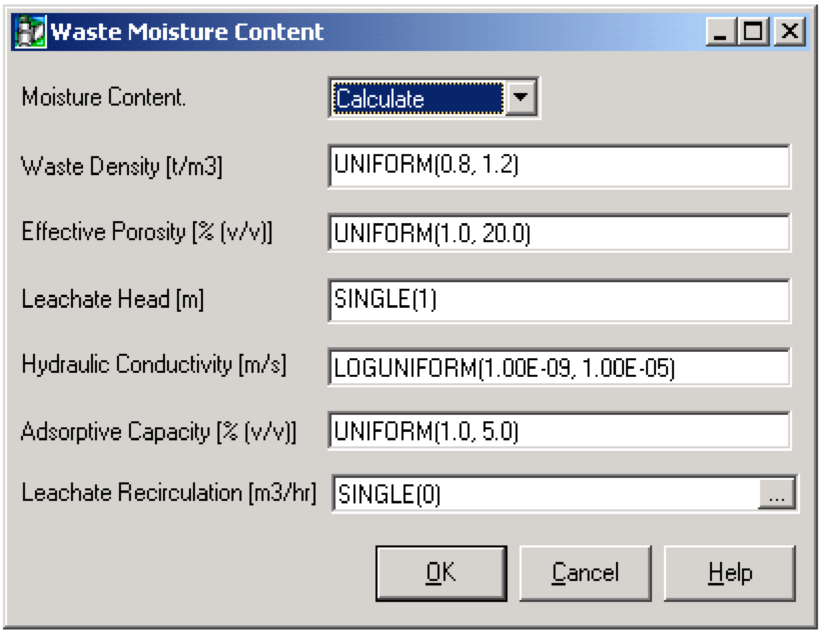
The determination of the trace gas species that are present with the LFG or the Parent Species that are present is carried out by clicking the box to the right of the species required 'Raw Gas', a tick will appear. These species will require a concentration. Species that are not selected will be defined as combustion products, the concentration of which will be defined in the Gas Utilisation dialogue box. When a parent product is used to define a combustion product you are also required to define the ‘Molecular Ratio’, i.e. the ratio of the Parent to the Daughter Species based on the molecular weights, e.g. F to HF is 1.05.

To define the distributions of the new species or edit the distributions of the default species, you should click on the species concentration box and then click on the grey button with three dots. This will bring up the distribution type box where you can define the distribution as described above.

A further option on the ‘Trace Gas Inventory’ dialogue box enables you to define a declining source term for the trace gases by entering a Half-Life. This allows all the trace gases to decay at the rate defined by the PDF. If you wish to run the simulation where the concentration of trace components effectively remains constant you should enter a very large half-life i.e. 10,000 years.

Waste Moisture Content

You are required to select ‘Waste Moisture Content’ of the waste using the pull down box. You can select ‘Moisture Content’ as ‘Dry’, ‘Average’ or ‘Wet’ moisture contents or to ‘Calculate’ the moisture content. However, the estimation of the Waste Moisture Content should be carried out with care, as this is a key factor controlling the waste degradation and thus LFG production, by determining the waste degradation constants.


Waste Moisture Content

Moisture Content: Calculate
Waste Density [t/m3]: UNIFORM(0.8, 1.2)
Effective Porosity [% (v/v)]: UNIFORM(1.0, 20.0)
Leachate Head [m]: SINGLE(1)
Hydraulic Conductivity [m/s]: LOGUNIFORM(1.00E-09, 1.00E-05)
Adsorptive Capacity [% (v/v)]: UNIFORM(1.0, 5.0)
Leachate Recirculation [m3/hr]: SINGLE(0)

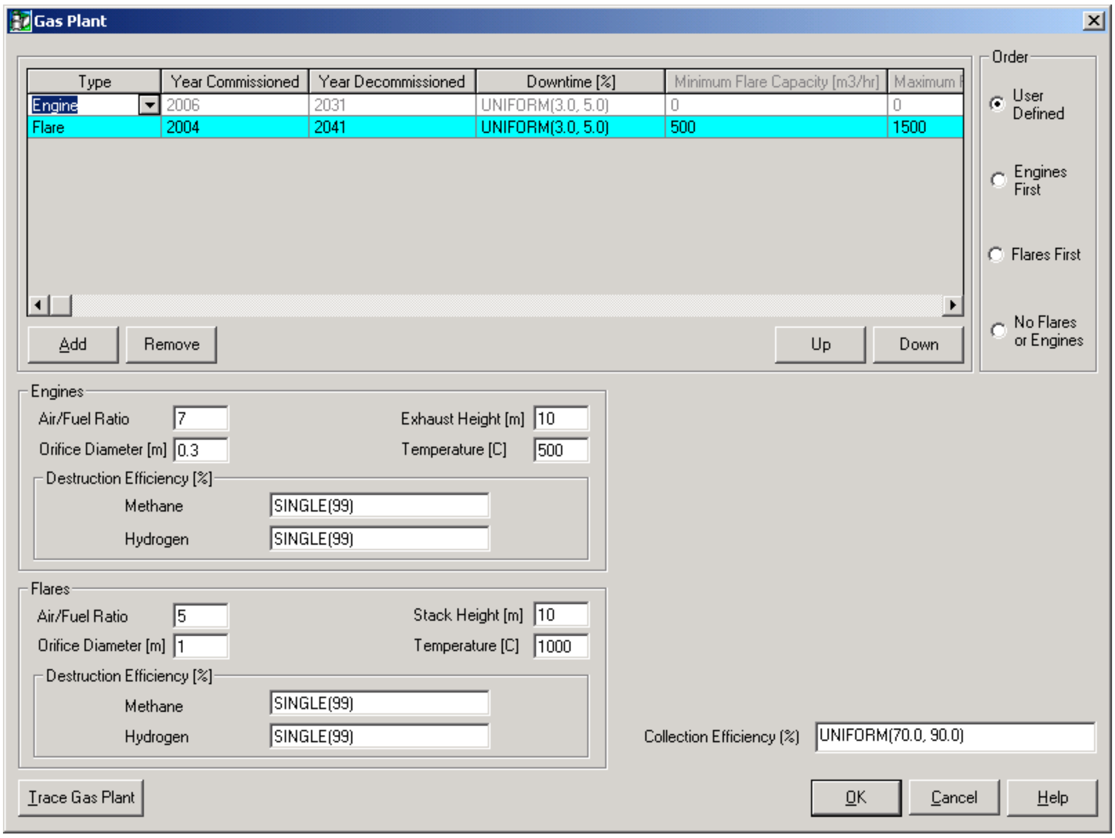
Calculation of the Waste ‘Moisture Content’ requires inputs from the volume of ‘Leachate Recirculate’, the depth of the ‘Leachate Head’, the ‘Effective Porosity’, ‘Adsorptive Capacity’, ‘Waste Density’ and ‘Waste Hydraulic Conductivity’, along with the ‘Infiltration’ rate (defined from the main screen). GasSimLite assumes that the water is derived from infiltration through the landfill cap, leachate conditions, the waste hydraulic properties and hydrogeological characteristics, and the infiltration rate and leachate level, which are constant across the entire area of the landfill. This data can be entered by clicking on the relevant box and then the grey box with three dots and entering the value as a PDF.

The ‘Leachate Recirculate’, ‘Effective Porosity’, and ‘Adsorptive Capacity’ are only used to calculate the Waste ‘Moisture Content’ and therefore these are disabled unless this is calculated. The Leachate Head, ‘Hydraulic Conductivity’ and Waste Density are required by other modules and therefore must be defined here.

GasSimLite does not allow for daily or seasonal variations in infiltration or leachate head. The model’s minimum time step is one year so all short term variations can only be accounted for via selection of appropriate input PDFs. Output values should never be used to interpret short term effects. For existing sites the actual depth of leachate (or its range) should be entered. For a new site the leachate level will either be defined in the licence, or it can be calculated on the basis of the drainage blanket configuration using a model like LandSim. The infiltration rate through the landfill cap is dependant on the effective rainfall and cap design. The determination of this is beyond the scope of GasSimLite.

Gas Plant

The ‘Gas Plant’ option allows the gas flaring and utilisation, by engines, at the site to be defined. GasSimLite uses this information, along with the LFG source/generation results, to calculate the emissions from flares, engines, the cap and through the liner. Clicking the words ‘Gas Plant’ allows access to this option and the flowing dialogue box will be displayed:



Type	Year Commissioned	Year Decommissioned	Downtime [%]	Minimum Flare Capacity [m3/hr]	Maximum
Engine	2006	2031	UNIFORM(3.0, 5.0)	0	0
Flare	2004	2041	UNIFORM(3.0, 5.0)	500	1500

Order
● User Defined
○ Engines First
○ Flares First
○ No Flares or Engines

Engines
Air/Fuel Ratio 7
Orifice Diameter [m] 0.3
Exhaust Height [m] 10
Temperature [C] 500
Destruction Efficiency [%]
Methane SINGLE(99)
Hydrogen SINGLE(99)

Flares
Air/Fuel Ratio 5
Orifice Diameter [m] 1
Stack Height [m] 10
Temperature [C] 1000
Destruction Efficiency [%]
Methane SINGLE(99)
Hydrogen SINGLE(99)

Collection Efficiency (%) UNIFORM(70.0, 90.0)

The ‘Gas Plant’ box allows you to define the number and capacity of the flares and spark ignition engines. You enter engines and flares by clicking the Add button to add engines/flares, and the Remove to remove them. For each type of gas plant you should select whether it is a ‘Flare’ or ‘Engine’ by clicking the ‘Type’ box and using the pull down menu. You must then define the ‘Year Commissioned’ and 'Year Decommissioned' for each flare/engine, by clicking in the boxes and typing the year. For 'Flares' you define the 'Maximum Flare Capacity' and 'Minimum Flare Capacity', i.e. the operational range of the flare. For 'Engines' you enter the 'Engine Capacity'. This is carried out by clicking the relevant box and entering the value.

This table allows the 'Downtime' of the individual engines and flares to de defined to allow the yearly capacity to be calculated for PI reporting. The 'Downtime' accounts for the percentage of time the engines/flares are not in operation due to routine maintenance and breakdowns.

There are various options that allow you to define the order that the engines and flares will be utilised :

- ☐ commission the engine and flares in the order that they are displayed on the screen ('User Defined');
- ☐ commission the engines first with GasSimLite determining the optimum order, with excess LGF being flared ('Engines First');
- ☐ commission the flares first with GasSimLite determining the optimum order, with excess LGF being utilised by the engines ('Flares First');
- ☐ run the simulation without gas utilisation by selecting ('No Flares or Engines').

However, it should be remember that GasSimLite will only use engines and flares that are available. Care should be taken when selecting the ordering of engines and flares as GasSimLite uses the available gas utilisation capacity to determine the quantity of gas that is combusted and thus the quantity of gas that is emitted through surface or laterally.

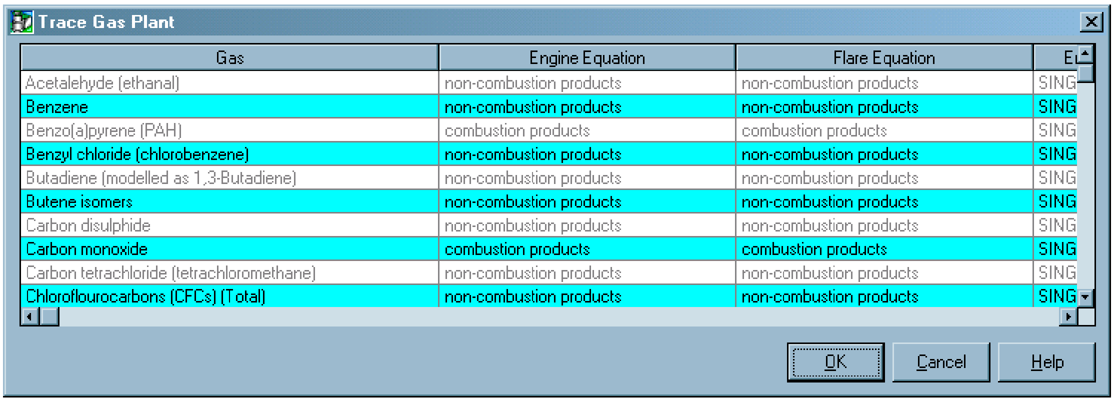
Where multiple flares/engines have been defined GasSimLite will commission additional flares/engines when sufficient LFG is available. The decommissioning date determines the latest date that the flare/engine will be operated, however the model will remove the engine/flare if the LFG generation is below the minimum capacity. GasSimLite will also trim the flaring operation to follow the gas production curve.

The gas 'Collection Efficiency', defined as a PDF, should be defined based on your experience of the landfill. However, a value of 100% should not be entered, as this is unrealistic that any collection efficiency will be 100% efficient.

The final set of inputs required are the 'Air to Fuel Ratio', the 'Stack Height', 'Orifice Diameter' and 'Temperature' of the flare, and the 'Air to Fuel Ratio', 'Exhaust Height', 'Orifice Diameter' and 'Engine Exhaust Height' of the engine. The Flare 'Orifice Diameter' is the diameter of the flare stack, as GasSimLite assumes that all flares are enclosed to reflect best practice. These parameters are used primarily in the GasSim atmospheric dispersion model, not include in GasSimLite, to calculate the release height and rate of release of the gases. However, the air to fuel ratio is also used to determine the trace gas emissions of combustion products. GasSimLite assumes that the air to fuel ratio is the same for all engines and all flares on site. The Flare 'Stack Height' and Engine 'Exhaust Height' and initially set to zero. All of these inputs except the 'Air to Fuel Ratio' are included information purposed and should be changed to the site-specific heights before running the Atmospheric Dispersion module if the file is imported into GasSim.

Combustion within flares and engines results in the destruction of the bulk gases methane and hydrogen, and the creation of carbon dioxide. You enter the 'Destruction Efficiencies', the proportion of methane and hydrogen that are destroyed in the engine and the flare, by clicking the relevant input box and entering the values or the range using a PDF. However, these should not be set at 100%, as it is unrealistic that any flare or engine will be 100% efficient. The generation of carbon dioxide is determined from the destruction of methane and VOCs.

The final option on the 'Gas Plant' dialogue box is a link to the 'Trace Gases' dialogue box. Selecting this option will open the following box:



Gas	Engine Equation	Flare Equation	E
Acetalehyde (ethanal)	non-combustion products	non-combustion products	SING
Benzene	non-combustion products	non-combustion products	SING
Benzo(a)pyrene (PAH)	combustion products	combustion products	SING
Benzyl chloride (chlorobenzene)	non-combustion products	non-combustion products	SING
Butadiene (modelled as 1,3-Butadiene)	non-combustion products	non-combustion products	SING
Butene isomers	non-combustion products	non-combustion products	SING
Carbon disulphide	non-combustion products	non-combustion products	SING
Carbon monoxide	combustion products	combustion products	SING
Carbon tetrachloride (tetrachloromethane)	non-combustion products	non-combustion products	SING
Chloroflourocarbons (CFCs) (Total)	non-combustion products	non-combustion products	SING

Trace gases can be destroyed or created by the combustion process, with some trace gases like PAHs undergoing both, due the break down of PAHs entering the flare/engine and the formation of PAHs by the breakdown of other compounds. Therefore, the emissions of these species have to be calculated using different equations and parameters. Emissions of species that are destroyed by the combustion process are determined in a similar way to methane and hydrogen. However, the emissions of combustion products (those formed in the flare or engine) require either the concentration of the species emitted to be monitored, or the concentration of the parent substance destroyed to form the daughter species to be entered e.g. chlorine forms hydrogen chloride.

The default species have been defined with equations depending on their behaviour during combustion, described in Section 6. Additionally the emissions of VOCs, hydrogen chloride, hydrogen fluoride and sulphur dioxide can be defined using different equations depending on the parameters entered (Table 3.1). If you enter additional species GasSimLite requires you to determine the equation that will be used to calculate the emissions after combustion by selecting the relevant equations for each trace gas in the 'Engine Equation' and 'Flare Equation' column. The additional inputs that you require depend on the equation selected (a list of equations and parameters required) is provided in Table 3.1.

Table 3.1 Combustion Equations And Input Parameters Required

Equation used	Species	Parameters required
'Non-Combustion Products'	All species that are not formed by combustion, i.e. not carbon dioxide, hydrogen chloride, hydrogen fluoride, dioxins & furans, nitrogen oxides, sulphur dioxide, nitric acid, total phosphates, carbon monoxide and PAHs. Species included are vinyl chloride, CFCs, chloroform etc.	Destruction efficiency, LFG concentration generated in the source model.
'Carbon Dioxide Generation'	Carbon dioxide only.	Destruction efficiency of methane and where present VOCs, Methane and VOCs concentrations generated in the source model.
'Combustion Products'	Combustion products i.e. hydrogen chloride, hydrogen fluoride, dioxins & furans, nitrogen oxides, sulphur dioxide, nitric acid, total phosphates, carbon monoxide, PAHs and non methane VOCs.	Engine/flare air: fuel ratio, Flare stack or engine exhaust concentration.
'Combustion Products from Parent Species'	Combustion products formed from Parent LFG species hydrogen chloride, hydrogen fluoride and sulphur dioxide.	Destruction efficiency, Molecular weight correction, LFG concentration or Parent Species generated in the source model, i.e. chlorine, fluorine, sulphur.

The source concentrations of the non-combustion product trace gases or the parent trace gases and the 'Molecular Ratios' are determined by the 'Source', 'Trace Gas Inventory' dialogue box as described above. This ratio correctly balances the mass of the 'Parent' and 'Daughter' species. You are required to enter the 'Destruction Efficiencies' for these species, as PDFs in the 'Trace Gas Utilisation' 'Engine

Destruction Efficiency' and Flare 'Destruction Efficiency' columns. The destruction efficiency determine the proportion of the species that is destroyed in the flare/engine, which can be determined by on-site monitoring, or the proportion of a 'Parent' species that is converted into a 'Daughter' species.

The 'Destruction Efficiency' should be defined for VOCs, when these are simulated, even if these species are defined as 'Combustion Products' to allow the quantity of Carbon Dioxide to be calculated.

GasSimLite determines the emissions of trace gas combustion products from the 'Engine Exhaust Concentration' and/or 'Flare Stack Concentration' and the Air to Fuel Ratio. Therefore if the 'Combustion Products' equation has been selected you will be required to enter the 'Engine Exhaust Concentration' and/or Flare Stack Concentration', as a PDF in mgm^{-3}, in the relevant column for each species. These concentrations can be obtained from on-site monitoring and used to determine the emissions of 'Combustion Products' bases on the quantity of exhaust leaving the flare or engines.

Pollution Inventory (PI) Reporting

The reporting of annual emissions will become necessary for most operational landfills by June 2003, under the requirements of the PPC Regulations, 2000. Reported data may derive from measurement, calculation or estimation techniques and GasSimLite provides the capability to calculate the annual emissions of compounds previously detected in landfill gas and report them in a format suitable to meet PI requirements. The results are reported at the 25%ile, 50%ile and 75%ile levels for the year after last simulation year and the 50%ile should be used for PI reporting. The results can be viewed after simulating the model using Results –PI Reporting

The emissions of CFCs, HCFCs, HFCs, PFCs, Halons, VOCs are reported as sums of the groups of compounds as at the time of publication insufficient data was available on the individual species within these groups. GasSimLite simplifies the emission of PAHs and dioxins (PCDDs and PCDFs) by simulating these as benzo(a)pyrene and 2,3,7,8-TCDD, respectively.

The Pollution Inventory for each year of the model can be viewed after running the simulation by selecting Results _PI reporting.

Preparing to Run the Model

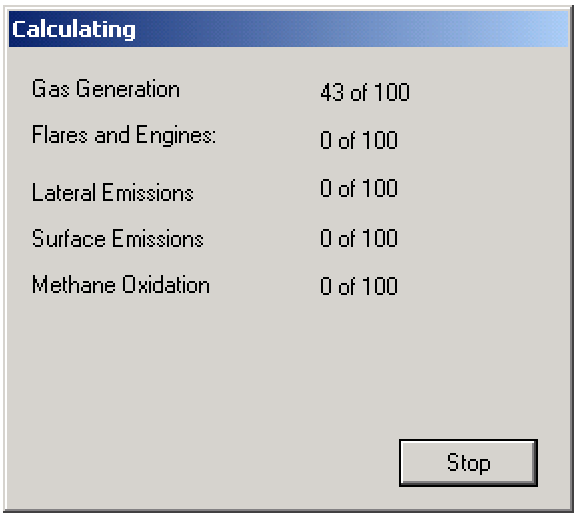
If values are invalid or if there are still input parameters that GasSimLite needs before a model can be run then a list of the dialogue boxes where additional data input are required will be shown. e.g. the message simply says 'Gas Plant'.

Before running the source and generation module you should select or check the number of iterations required for the simulation in the 'Project Details' dialogue box, accessed by Edit – Project Details. The number of iterations selected will affect the accuracy of the predictions made by GasSimLite and will also increase the time required to run the simulation. The number of iterations used for the Monte Carlo simulation determines the numbers of times that the model is run and thus the number of scenarios that are tested. It is recommended 100 iterations are used, further details regarding the number of iterations are discussed in Chapter 6.

Running the Model

Once you have selected the options you wish you can then run the model by selecting Simulate from the menu and then select Source Gases;

Alternatively, to simulate the source gases you can simply press the F5 key. If the model has been recently edited and not yet saved you will be prompted to allow GasSimLite to save the file prior to running using the current file name. If you wish to change the file name you can abort the run process by pressing the 'No' button and use the File menu to save the file to a new name using the Save As option. If you are happy to continue press the 'OK' button. The following screen will then appear.



Gas Generation	43 of 100
Flares and Engines:	0 of 100
Lateral Emissions	0 of 100
Surface Emissions	0 of 100
Methane Oxidation	0 of 100

The message that appears gives a brief summary of the model run, gives details of the model's progress through the requested number of iterations for the source and emissions modules. On completion of the model run the Results menu will become available.

Other Model Output

The PI and bulk gas production outputs are discussed in Chapter 4.

Printing Your Model

GasSimLite has been developed around the concept that printed output should be suitable for your records and audit purposed. To this end, considerable effort has been spent on print layout and quality assurance issues. You can define the printer and its set up under the Printer Set-Up option.

The Print option on the File menu allows you to send details of the model construction and the results of the landfill simulation to a printer.

Having selected 'Print', there is a further option - 'Model'. Clicking on the 'Model' option sends a summary of the model input parameters to the printer. Records of this type are essential to document your work and for quality assurance purposes.

Traceability and Quality Assurance

Approach

Because GasSimLite has been designed for use in a quality assured environment, you will have to save a model before printing a record and save a record of your model before you can run a simulation. By ensuring all your printed output is linked to the time and date stamp of the saved model, this feature provides an audit trail where output corresponds to input. Obviously, once you have run a simulation for a decision you should not overwrite your saved data file and you should keep it on a floppy disk with the project file.

Project Information

Information relating to the project should be entered on the 'Project Details' dialogue box described above.

Parameter Justification

GasSimLite, like GasSim, prompts for justification by displaying the 'Justifications' dialogue window every time a parameter is changed. This box allows the source of any parameter values entered into the model to be referenced. Information entered into the justification text box will appear in the 'Justifications' section of the model summary report attached to the relevant parameter. You should make your description clear. Think of this text as a note to an auditor. Rather than just giving the name of a report, give a figure number, page number or reference to a table. The parameter justifications can also be viewed and edited by selecting View – Justifications.

Data Input

During the initial stages of a GasSimLite desk study a considerable amount of site-specific data may be collected from a variety of sources. It is recommended that the source of data is fully documented. The justification boxes assist you in this process

CHAPTER 4: INTERPRETING THE RESULTS

4. INTERPRETING THE RESULTS

This chapter to will explain what GasSimLite predicts, the results and formats of outputs available and gives some guidance on the interpretation.

What GasSimLite Predicts

The GasSimLite output can be split into two groups:

- Total LFG generation (m^3/hr) as a time series;
- PI reporting.

Probabilistic output, e.g. different values for the PI reporting at the reported value, the 25% and 75% percentiles, will only be available if a number of realisations or iterations have been run. Running a single iteration should be avoided unless all of the inputs have been defined as single values.

The LFG generation output is intended to help you understand the behaviour of the waste degradation and thus the gas production within the landfill. These results should be studied first to ensure that the simulation is responding correctly, before proceeding to the PI reporting.

Getting To Your Results – Graphical Output

When a simulation has been run, the results can be viewed by clicking the Results option on the main menu GasSimLite toolbar. A maximum of 2 items will be visible, depending on the options that have been selected during the simulation set up. Other options will be greyed out and will not respond to the mouse, i.e. if the simulation has been run without engines and/or flares the emissions from these will not be visible:

- PI Reporting;
- Plot Bulk Gas Production.

Results Menu

Results Menu – PI Reporting

The emissions for PI reporting from flares, engines and the surface are listed 25th, 50th and 75th percentiles for the year after last operational year. The table also lists the PI reporting threshold for each species. These results are viewed by selecting Results-PI Reporting. These results can be printed using the Print button.

Plot Bulk Gas Production

This reports the total amount of LFG, the sum of CH_4, CO_2, H_2, that is generated to provide an indication of the gas that is available to be collected and flared/utilised. These graphs show the amount of gas that should be managed/controlled to minimise the environmental impact.

Loading (importing) Results Without Running the Model

After you have carried out a simulation once, the results will be saved and it is not necessary to rerun the simulation to view the results. Therefore, assuming that you have not altered any of the input parameters, the results can be imported into the model by selection File- Load Results.

Customising Your Results – Graphs

GasSim provides a number of options for viewing and printing your graphs. These are accessed through the File menu, in the top left had corner of each graph.

Plot

This option allows you to view different available plots i.e. different amounts of available carbon for operational years.

Zoom

You can zoom in on the graph (File - Zoom - In) up to three times. This will zoom into the centre of the graph and you will therefore need to alter the axis (described below) to ensure the relevant section of the graph is displayed. You can either return to the full graph in stages (File – Zoom - Out up to three times) or all at once (File - Zoom - All). The option File - Zoom – Last, displays the view before the current view.

Selecting File - Zoom - Window allows you to specify a particular area of the graph to examine in more detail. This may be done by Clicking and holding the left mouse button in the top left hand corner of the area you are interested in, dragging the window outline until you have covered the desired area, and then releasing the button. You can return to the full graph using (File - Zoom - All).

You can also zoom in on a particular area using File - Zoom- Scale. This optional allows you to change the scale of the graph axes. This option produces an additional dialogue box.

You should type in the maximum and minimum axis values you require, and when each value has been set click on the 'OK' button. The graph will immediately be rescaled. To exit the dialogue box without making changes you can click on 'Cancel' or click on the top right hand corner of the box. Built-in error checks prevent values being entered that are outside of the capabilities of the code and values beyond this range are ignored.

Individual axis can be altered, in the same way, by double-clicking on the axis you wish to edit.

You are also given the option to plot using a log scale, on the y axis, which you can use if the results span a large range. .

This facility is useful for determining the emissions during the operation period or the years just after the operational period when the gas generation peaks.

Options

Under this sub-menu you can turn the graph grid lines on and off (File - Options - Grid). By clicking and holding the left mouse button on the graph, cross hairs appear and the co-ordinates of the cross point are displayed at the top of the graph. This feature is extremely useful for determining the probability of particular values where the grid lines do not give enough detail. The feature can be turned on and off by selecting (File - Options - Co-ordinates).

Copy

This option allows you to put a copy of the current graph on the clipboard as a bitmap so that it can be incorporated in another Windows application such as Microsoft Word or Excel. You can also copy the current graph or active Window to the clipboard by pressing the Alt and PRINT SCREEN keys together. Older keyboards may not recognise Alt + PRINT SCREEN, so try Shift + PRINT SCREEN instead. To paste information from the Clipboard into a Windows application, start the destination application and place the insertion point where you want the information from the Clipboard to appear. Choose Paste from the destination application's Edit menu, and Windows will copy the information automatically to the insertion point. To capture the entire screen (not just the current graph or active window) press the PRINT SCREEN key on the keyboard. Older keyboards may require you to use Alt and PRINT SCREEN or Shift and PRINT SCREEN. Refer to your Microsoft Windows manual for more general tips on editing the clipboard contents.

Print

This option allows you to print the current graph.

Percentiles

The percentile selection boxes on the right hand side of the dialogue box allows the option to show the curves for the calculations at different percentiles. Selecting the desired percentile will draw the line on the graph for this percentile and a tick will appear in the box. To deselect, click the box again.

Exit

Clicking (File – Exit) closes the current graph

CHAPTER 5: DEFAULT VALUES AND SUGGESTED INPUTS

5. DEFAULT PARAMETERS AND SUGGESTED INPUTS

Introduction

Each time a new model is created in GasSimLite default values are assigned to some parameters and others are required to be entered before the model will run. Adopted default values are saved as part of the model and are over-written when an existing model is retrieved. This chapter explains the basis on which default values have been assigned to various parameters and also provides a reference source for other suggested input values.

Assumptions and Limitations of Default Parameters

Generally the defaults and suggested input values have been derived from UK and US sources. Consequently the uncertainty representing some of the suggested input ranges may extend over a number of orders of magnitude. The default and suggested input parameters are not intended to be mean values which may be applied to a site, but rather a range of values which may be narrowed with site-specific knowledge and data. For these reasons, it is emphasised that wherever possible site-specific values should be used as input parameters or the suggested range of values should be tightened to reflect site conditions.

Default Values

Broadly, there are three classes of defaults in GasSimLite:

- ☐ values which are project specific and which you will change in every instance;
- ☐ values of chemical and physical constants that will rarely (if ever) need to be changed;
- ☐ values for which you are unlikely to have any better information.

Examples from the classes are as follows. Project specific parameters include the landfill dimensions, the cap thickness and engine or flare capacities. Properties such as molecular weights, gas densities and viscosities have been taken from reliable sources so there should be little need to change these. Parameters for which you are unlikely to have better information, which might include engine and flare destruction efficiencies, deposition velocities and air diffusion coefficients.

Project Details

The ‘Project Details’ dialogue box requires information on the project and the client, and the ‘Start’ date that the waste deposition commences, the ‘Operational Period’ the number of years for which deposition continues, the ‘Simulation Period’ the number of years for which that you wish to run the simulation, and the number of ‘Iterations’. These should also be changed for each new model using information obtained from the site operator and the task to be undertaken. The maximum filling time has been limited at 40 years. We recommend that you run the simulation for 100 iterations.

Infiltration

Infiltration through the cap should be determined from the effective rainfall (obtained for the site) and the capping type and status. This information on rainfall should be obtained from either an on-site weather station, the Meteorological Office or literature sources.

Source

The 'Source' dialogue box is divided into three sections including the waste input table, gas and leachate composition details, and 'Cellulose Degradation Rates'. This dialogue box also contains links to the 'Waste Moisture Content', and 'Trace Gas' inputs. These are used to determine the rate and quantity of bulk gas (CH_4, CO_2 and H_2) generation and the trace gas generation using an independently defined declining source term.

Waste Input (Filling Volumes and Streams)

The dates on which the waste deposition commences and the number of years for which deposition continues are used by GasSimLite to produce a matrix in which the yearly 'Waste Input', i.e. deposition rate (in tonnes), must be defined. These should be obtained from the site operator, and therefore no defaults have been provided. Where this information is not known, an estimate of the filling rate each year should be made even if this is simply dividing the total waste mass filled by the filling time. However, the use of estimations will affect the outputs and therefore should be taken into account when interpreting the data.

The nature of the waste deposited should be defined by the 'Breakdown', the proportion of the waste from each stream i.e. percentage of domestic, inert, industrial waste etc. This influences the quantity of carbon available for degradation and therefore a default is not provided. This information should be available from the site operator.

Each waste stream is defined by the fractionation of material found within the waste, i.e. the amount of newspapers, card, garden waste etc. GasSimLite contains default waste streams for commonly deposited waste materials filled between 1980 and 2010, from HELGA (Gregory *et al.,* 1999) and an estimation of the changes in the composition of 'Domestic' and 'Civic Amenity' waste in the future with the implementation of the Landfill Directive (Table 5.1a to d). The new waste streams have been calculated assuming that the Implementation of the landfill Directive will reduce the biodegradable fraction on 'Domestic' and 'Civic Amenity' waste to 75%, 50% and 35% of its 1995 level, by 2010, 2015 and 2020, respectively.

GasSimLite provides defaults for the percentages 'Water Content', 'Decomposition', 'Cellulose' and 'Hemi-Cellulose' for each waste fraction (Gregory *et al*, 1999). Additionally GasSimLite is highly flexible to allow you to redefine or edit a waste stream, using site-specific data, by altering the PDFs defining the fraction of the material and percentages for the 'Water Content', 'Decomposition', 'Cellulose' and 'Hemi-Cellulose' for each waste fraction. GasSimLite contains four waste streams, which require defining using this process 'Waste Sorted at MRF', 'Recycling Schemes', 'Chemical Sludges', and 'Industrial Liquid Waste'. These are not defined due to their site-specific nature and users need to enter this data in order to include these options.

The ‘Percentage of Waste in Place’ is site-specific and should change from each simulation using information obtained from the site operator.

Bulk LFG Composition

The ‘Proportion of CH_4‘ to ‘CO_2’ generated by methanogenic decay has been set at a default of 50% for each. However, this ratio is very site specific and therefore the ratio measured at the site should be used, if available. It is recommend that this information is obtained from dynamic monitoring points, with the values obtained normalised to 100%, i.e. measurements should be taken from the gas collection system as biological methane oxidation can occur in passive monitoring points.

To determine the volume of hydrogen produced GasSimLite assumes that 1% of the carbon deposited in the year of deposition undergoes acetogenic decay to produce hydrogen and carbon dioxide. This assumed value has been validated during the HELGA framework (Gregory *et al*., 1999) and produces a maximum concentration of H_2 in LFG of around 10%, which fits with the work of Farquhar and Rovers (1973). Acetogenic decay will also slightly increases the CO_2 generation.

Cellulose Decay Rates

The default decay constants are used to determine the degradation of carbon for the three different waste moisture levels and the three rates of degradability (rapid, K_1, moderate, K_2, and slow, K_3). These are listed in Table 5.2. These have been obtained for the HELGA framework (Gregory *et al*., 1999).

TABLE 5.1A COMPOSITION OF 1980'S - 2010 WASTE STREAMS

Degradable		Domestic	Civic Amenity	Commercial	Industrial	Inert	Liquid Inert	Sewage sludge	Composted organic material	Incinerator ash	Waste sorted at MRF	Recycling schemes	Chemical sludges	Industrial liquid waste	Water content (%)	Cellulose (%)	Hemi-cellulose (%)	Decomposition (%)
Paper/Card	Newspapers	11.38	10	10											30	48.5	9	35
	Magazines	4.87	11												30	42.3	9.4	46
	Other paper	10.07		50.1											30	87.4	8.4	98
	Liquid cartons	0.51													30	57.3	9.9	64
	Card packaging	3.84													30	57.3	9.9	64
	Other card	2.83													30	57.3	9.9	64
Textiles	Textiles	2.36	3.0												25	20	20	50
Miscellaneous combustible	Disposable nappies	4.35													20	25	25	50
	Other misc. combustibles	3.6													20	25	25	50
Putrescible	Garden waste	2.41	22												65	25.7	13	62
	Other putrescible	18.38		15											65	55.4	7.2	76
Fines	10mm fines	7.11	15												40	25	25	50
Sewage sludge	Sewage sludge							100							70	14	14	75
Composted organic material									100						30	Tri 0.5, 0.7,1.5	Tri 0.5, 0.7,1.5	57
Incinerator ash										100					30	Un 7.47, 9.59	Un 7.47, 9.59	57
Non-Degradable	Total	28.86	39	24.6	0	100	-	0	0	0					-	-	-	-

The proportion of different material in waste have been taken from the HELGA framework (Gregory *et al.*, 1999) ,

TABLE 5.1B PREDICTED COMPOSITION OF 2010 WASTE STREAMS (REDUCTION TO 75% OF THE BIODEGRADABLE FRACTION IN DOMESTIC AND CIVIC AMENITY WASTE)

Degradable		**Domestic**	**Civic Amenity**	**Commercial**	**Industrial**	**Inert**	**Liquid Inert**	**Sewage sludge**	**Composted organic material**	**Incinerator ash**	**Waste sorted at MRF**	**Recycling schemes**	**Chemical sludges**	**Industrial liquid waste**	**Water content (%)**	**Cellulose (%)**	**Hemi-cellulose (%)**	**Decomposition (%)**
Paper/Card	Newspapers	8.5	7.5	10											30	48.5	9	35
	Magazines	3.7	8.3												30	42.3	9.4	46
	Other paper	7.6		50.1											30	87.4	8.4	98
	Liquid cartons	0.4													30	57.3	9.9	64
	Card packaging	2.9													30	57.3	9.9	64
	Other card	2.1													30	57.3	9.9	64
Textiles	Textiles	1.8	2.3												25	20	20	50
Miscellaneous combustible	Disposable nappies	3.3													20	25	25	50
	Other misc. combustibles	2.7													20	25	25	50
Putrescible	Garden waste	1.8	16.5												65	25.7	13	62
	Other putrescible	13.8		15											65	55.4	7.2	76
Fines	10mm fines	5.3	11.3												40	25	25	50
Sewage sludge	Sewage sludge							100							70	14	14	75
Composted organic material									100						30	Tri 0.5, 0.7,1.5	Tri 0.5, 0.7,1.5	57
Incinerator ash										100					30	Un 7.47, 9.59	Un 7.47, 9.59	57
Non-Degradable	Total	46.2	54.3	24.6	-	100	-	0	0	0								

The proportion of different material in waste have been taken from the HELGA framework (Gregory *et al.*, 1999),

TABLE 5.1C PREDICTED COMPOSITION OF 2015 WASTE STREAMS (REDUCTION TO 50% OF THE BIODEGRADABLE FRACTION IN DOMESTIC AND CIVIC AMENITY WASTE)

Degradable		**Domestic**	**Civic Amenity**	**Commercial**	**Industrial**	**Inert**	**Liquid Inert**	**Sewage sludge**	**Composted organic material**	**Incinerator ash**	**Waste sorted at MRF**	**Recycling schemes**	**Chemical sludges**	**Industrial liquid waste**	**Water content (%)**	**Cellulose (%)**	**Hemi-cellulose (%)**	**Decomposition (%)**
Paper/Card	Newspapers	5.7	5.0	10											30	48.5	9	35
	Magazines	2.4	5.5												30	42.3	9.4	46
	Other paper	5.0		50.1											30	87.4	8.4	98
	Liquid cartons	0.3													30	57.3	9.9	64
	Card packaging	1.9													30	57.3	9.9	64
	Other card	1.4													30	57.3	9.9	64
Textiles	Textiles	1.2	1.5												25	20	20	50
Miscellaneous combustible	Disposable nappies	2.2													20	25	25	50
	Other misc. combustibles	1.8													20	25	25	50
Putrescible	Garden waste	1.2	11.0												65	25.7	13	62
	Other putrescible	9.2		15											65	55.4	7.2	76
Fines	10mm fines	3.6	7.5												40	25	25	50
Sewage sludge	Sewage sludge							100							70	14	14	75
									100							Tri 0.5,	Tri 0.5,	
Composted organic material															30	0.7,1.5	0.7,1.5	**57**
										100						Un	Un	
Incinerator ash															30	7.47, 9.59	7.47, 9.59	**57**
Non-Degradable	**Total**	**64.1**	**69.5**	**24.6**	**-**	**100**	**-**	**0**	**0**	**0**								

The proportion of different material in waste have been taken from the HELGA framework (Gregory *et al.*, 1999),

TABLE 5.1D PREDICTED COMPOSITION OF 2020 WASTE STREAMS (REDUCTION TO 35% OF THE BIODEGRADABLE FRACTION IN DOMESTIC AND CIVIC AMENITY WASTE)

Degradable		**Domestic**	**Civic Amenity**	**Commercial**	**Industrial**	**Inert**	**Liquid Inert**	**Sewage sludge**	**Composted organic material**	**Incinerator ash**	**Waste sorted at MRF**	**Recycling schemes**	**Chemical sludges**	**Industrial liquid waste**	**Water nt (%)**	**Cellulose (%)**	**Hemi- se (%)**	**Decomposition (%)**
Paper/Card	Newspapers	4.0	3.5	10											30	48.5	9	35
	Magazines	1.7	3.9												30	42.3	9.4	46
	Other paper	3.5		50.1											30	87.4	8.4	98
	Liquid cartons	0.2													30	57.3	9.9	64
	Card packaging	1.3													30	57.3	9.9	64
	Other card	1.0													30	57.3	9.9	64
Textiles	Textiles	0.8	1.1												25	20	20	50
Miscellaneous combustible	Disposable nappies	1.5													20	25	25	50
	Other misc. combustibles	1.3													20	25	25	50
Putrescible	Garden waste	0.8	7.7												65	25.7	13	62
	Other putrescible	6.4		15											65	55.4	7.2	76
Fines	10mm fines	2.5	5.3												40	25	25	50
Sewage sludge	Sewage sludge							100							70	14	14	75
									100							Tri 0.5,	Tri 0.5,	
Composted organic material															30	0.7,1.5	0.7,1.5	57
										100						Un	Un	
Incinerator ash															30	7.47, 9.59	7.47, 9.59	57
Non-Degradable	Total	74.9	78.7	24.6	-	100	-	0	0	0								

The proportion of different material in waste have been taken from the HELGA framework (Gregory *et al.*, 1999),

Very wet (i.e. waterlogged) landfills where the moisture content is probably >70% should be simulated as dry landfills or site-specific degradation rates should be used (rather than use the calculation approach) because under such conditions, degradation is actually retarded and gas generation can be slowed significantly. Similar retardation of degradation rates have been observed after capping but this mechanistic approach is not specifically considered in GasSim. Recirculation of leachate can also enhance degradation rates and the user is recommended to calibrate the model with site specific data in these cases.

Table 5.2 Degradation Rate Constants for the Three Fractions of the Degradable Cellulose in the Waste are Dependent on the Waste Saturation Level (from Gregory *et al.*, 1999).

Waste moisture level (water filled porosity)	Degradation rate constant	Degradation half-life, t½
Dry less than 30% (vol./vol.) moisture	k_1= 0.076 k_2= 0.046 k_3= 0.013	t ½ $_{(1)}$ = 9 t ½ $_{(2)}$ = 15 t ½ $_{(3)}$ = 53
Average greater than 30% (vol./vol.) and less than 60% (vol./vol.) moisture	k_1= 0.116 k_2= 0.076 k_3= 0.046	t ½ $_{(1)}$ = 6 t ½ $_{(2)}$ = 9 t ½ $_{(3)}$ = 15
Wet greater than 60% (vol./vol.) moisture	k_1= 0.694 k_2= 0.116 k_3= 0.076	t ½ $_{(1)}$ = 1 t ½ $_{(2)}$ = 6 t ½ $_{(3)}$ = 9

Waste moisture

The ‘Waste Moisture Content’ can be entered a ‘Dry’, ‘Average’ or ‘Wet’ or can be calculated using the inputs of ‘Infiltration’, ‘Leachate Recirculated’, ‘Leachate Head’, ‘Adsorptive Capacity’, ‘Effective Porosity’, ‘Waste Density’, and waste ‘Hydraulic Conductivity’.

The volume of ‘Leachate Recirculate’ will be site specific and should be obtained from the site operator, if this operation occurs at the site. GasSimLite assumes that this rate is constant for the simulation period.

The depth of the ‘Leachate Head’ is site specific and therefore should also be obtained from the site operator. However, in practice the leachate head is normally maintained at 1m, therefore this value has been suggested as a default.

‘Effective Porosity’, ‘Adsorptive Capacity’, ‘Waste Density ‘and waste ‘Hydraulic Conductivity’ should all be obtained on a site-specific basis, however, suggested ranges have been tabulated below(Table 5.3).

Table 5.3 **Source model default input parameters from Gregory *et al.* (1999)**

Parameter	Default range
Effective porosity (%)	1 – 20
Adsorptive capacity (%)	1 – 5
Waste density (t/ m^3)	0.8 – 1.2
Waste hydraulic conductivity (m/s)	10^{-5} – 10^{-9}

In our experience it is difficult simulate a wet site by calculating the waste moisture content without having a high leachate head. Therefore we recommend simulating wet site by selecting the 'Wet' option.

Trace Gases Inventory

Trace gas concentrations should be defined on-site by monitoring. However, default concentrations have been defined for forty-three species (Table 5.4) the reporting of which will be required for the PI reporting. The default trace gas concentrations have been derived from performing statistical analysis on the data gathered by a number of authors (AERC draft database, 2001; Derwent *et al.*, 1996; and Stoddart *et al.*, 1999)

Assumption - the concentrations of these species have been determined from literature sources. However, these concentrations are anticipated to vary with the age of the waste, the composition of the waste mass, and whether the site is capped or uncapped. Therefore site-specific data should be used when available.

The 'Trace Gases Half-Life' has been derived by examining the emissions of VOCs in landfill gas from a number of studies, described in Chapter 6, which provide a normal distribution of 4.11 ±1.56 years. However, the half-life is anticipated to vary with the LFG composition and the nature of the waste so site specific information to be used where available.

The source concentration of VOCs should be defined even when you are simulating the emissions of these as a 'Combustion Product' as GasSimLite simulates their break down to produce carbon dioxide.

Table 5.4 Trace Gas Default Inputs for PI Annual Reporting Levels for Components of LFG (mg/m^3)

Species	Distribution	Mean\ or most likely	Min.	Max.	No. of samples
Inorganic substances (not including metals)					
Carbon disulphide	Log triangular	1.0	1.0×10^{-2}	48.0	31
Carbon monoxide	Single	1124.5			1
Total chloride (reported as HCl)	Log triangular	79.5	850	14.7	21
Total fluoride (reported as HF)	Log triangular	251.2	735	5.6	7
Nitrogen oxides (except N_2O – reported as NO_2)	CE				
Sulphur reduced (reported as SO_2)	Log Uniform		430.5	30.8	6
Organic substances					
Acetaldehyde (ethanal)	Log uniform		2.5×10^{-1}	18	4
Benzene	Log triangular	6.6	1.2×10^{-2}	114	113
Benzo(a)pyrene	CE				
Butadiene (modelled as 1,3-Butadiene)	Log triangular	1.45	5.0×10^{-2}	20	34
Carbon tetrachloride (tetrachloromethane)	Log triangular	0.94	5.0×10^{-3}	2.5	18
Chlorofluorocarbons (CFCs)	Log triangular	102.3	6.00×10^{-2}	1230.0	96
Chloroform (trichloromethane)	Log triangular	1.0	4.0×10^{-2}	50	30
para-Dichlorobenzene (modelled 1,4-Dichlorobenzene)	Log triangular	$2.51\text{x}10^{-2}$	2.50×10^{-2}	14.8	11
Dichloromethane (methylene chloride)	Log triangular	77.6	3.9×10^{-3}	3000	71
Dimethyl disulphide	Log Triangular	6.03	2.0×10^{-2}	40.0	29
Dioxins and furans (modelled as 2,3,7,8-TCDD)	CE				
Ethyl toluene (all isomers)	Log uniform		7.0×10^{-4}	38	6
Ethylene	Uniform		13	42	3

Species	Distribution	Mean\ or most likely	Min.	Max.	No. of samples
Ethylene dichloride (modelled as 1,2-Dichloroethane)	Log triangular	1.41	5.0×10^{-2}	302	35
Formaldehyde (methanal)	Log triangular	1.6	5.0×10^{-2}	18	29
Halons	NA				
Hexachlorocyclohexane (all isomers)	NA				
Hydrochlorofluorocarbons (HCFCs)	Log triangular	128.8	2.00×10^{-2}	916.2	91
Hydrofluorocarbons (HFCs)	NA				
Methyl chloride (chloromethane)	Log triangular	1.0	5.0×10^{-2}	1300	26
Methyl chloroform (1,1,1 trichloroethane)	Log triangular	1.0	5.00×10^{-3}	177.0	76
Non-methane volatile organic compounds (NMVOCs) (Total)	Log uniform		5.0×10^{-2}	1473	11
Pentane	Log triangular	16	2.0×10^{-2}	613	68
Pentene (all isomers)	Log triangular	1	5.0×10^{-2}	210.0	46
Perfluorocarbons (PFCs)	NA				
Phenol	NA				
Polycyclic aromatic hydrocarbons (PAHs) (modelled as Naphthalene)	Log triangular	1.1	5.0×10^{-3}	21	36
Tetrachloroethane (modelled as 1,1,2,2-Tetrachloroethane)	Log triangular	8.91	5.00×10^{-2}	264	41
Tetrachloroethylene (tetrachloroethene)	Log triangular	26.3	7.0×10^{-4}	2200.0	79
Toluene	Log triangular	195.0	2.2×10^{-3}	1700.0	121
Trichlorobenzene (all isomers)	Single	5.0×10^{-3}			1
Trichloroethylene	Log triangular	14.13	$1.20\mathrm{x}10^{-2}$	312.0	89
Trimethylbenzene (all isomers)	Log triangular	2.51×10^{-2}	$7.0\ \mathrm{x}10^{-4}$	187	41
Vinyl chloride (Chloroethene, chloroethylene)	Log triangular	8.12	1.9×10^{-2}	264	101
Xylene (all isomers)	Log triangular	128.8	4.0×10^{-4}	1100	147

NA – Data not available CE – Combustion Emission

GasSimLite allows the simulation of a species that are produced by LFG combustion from the concentration of the Parent species, e.g. fluorine (F), concentrations can be defined to determine hydrogen fluoride (HF) emissions using the 'Combustion Product for Parent' equation. This determination requires a 'Molecular Ratio'**,** the ratio based on the molecular weight of the daughter species compared to the parent species, e.g. F to HF is 1.05. A number of commonly used correction ratios are tabulated below (Table 5.5).

Table 5.5 Molecular Weight Correction Factor

Emission of species	Species concentration in LFG	Molecular Ratio
Hydrogen chloride (HCl)	Chloride (Cl)	1.03
Hydrogen fluoride (HF)	Fluoride (F)	1.05
Sulphur Dioxide (SO_2)	Sulphur (S)	2.0

Landfill Characteristics

Landfill Geometry

The Landfill Geometry is defined by the landfill 'Length', assumed to be a north to south direction, and 'Width', assumed to be an east to west direction. These should be changed for each simulation depending on the landfill that is being simulated and should be obtained from the site operator. The area and depth of the landfill are calculated as described in Chapter 3.

Methane emissions can be reduced as they pass through the landfill cap by microbial processes. The proportion of the methane that is converted to carbon dioxide in the cap is calculated by the 'Biological Methane Oxidation' term. This can be simulated without or without fissures. Simulating this reduction without fissures requires a percentage of 'Biological Methane Oxidation', which should be defined on a site-specific basis, as the quantity of methane oxidation is dependant on a number of factors including the cap thickness and permeability. Alternatively this can be defined using the DEFRA policy default of 10% which is based on the PPC guidelines, and is used by the AEAT UK emissions estimation model (AEAT, 1999). For running GasSimLite it is recommended that the DEFRA 10% default is used if the number of fissures on the site has not been determined.

'Biological Methane Oxidation' can also be simulated by calculating the methane oxidation rates for different cover materials, based on the knowledge that caps generally have a maximum capacity for oxidation, beyond which excess methane is released. The maximum capacity is a PDF developed from lab and field measurements. This is moderated by an efficiency term which is a default triangular PDF of between 10-46%, with a mean of 25%. This calculation method also requires the 'Soil Depth' above the cap and the 'Proportion of Fissures' to be defined. Both of these parameters are site-specific and therefore information should be obtained from the site operator or by investigation. Where information relating to the proportion of fissures is not available a default number of fissures of 10% has been suggested based on the measurements obtained using the Environment Agency's methane emissions measurements procedures (2001a).

The design and construction of the engineered barriers including the 'Cap Thickness' and 'Liner Thickness' should be obtained from the site operator. The 'Cap' and 'Liner Hydraulic Conductivity' should be defined on a site-specific basis depending on their age, level of compaction, the moisture content of the cap, and the level of engineering competence i.e. the use of CQA. GasSimLite requires the definition of the hydraulic conductivities, the permeability of the strata to water, as currently very little research has been undertaken to determine the gas permeability's of natural materials. The gas conductivities are calculated within the code, using the relative density and viscosities of gas and water.

The hydraulic conductivities of mineral cap and liners should be full characterised at the source and placed to achieve a design specification, with subsequent in-situ testing. A range of typical hydraulic conductivities for mineral liners has been obtained from LandSim (Environment Agency, 2002) and is listed in Table 5.6. The hydraulic conductivities of welded membrane liner systems should be provided in the manufacturer's specifications. Where the liner is lapped, rather that welded, it is recommended that the influence of the liner is reduced, as gas will be emitted through the lapped area.

Table 5.6 Hydraulic Conductivities of the Cap and Liner

Material	Range of Water Hydraulic Conductivities (m.s^{-1})
Clay is normally engineered to a specification of	1 x 10^{-9}
Bentonite enriched sand is normally engineered to a specification of	1 x 10^{-10} – 1 x 10^{-11}
Dense Asphaltic Lining (DAC) systems is normally engineered to a specification of	1 x 10^{-11} – 1 x 10^{-12}
A Geomembrane Liner (without defects)	1x10^{-14} – 1x10^{-16}
Typical Geomembrane	1 x 10^{-12}– 1 x 10^{-14}

Gas Plant

Information relating to the number of flares and engines, the 'Year Commissioned' and 'Year Decommissioned', and the 'Order' in which they are operated is site -specific and therefore GasSimLite does not provide any defaults. This information should be obtained from the site operator.

An estimate of the 'Gas Collection Efficiency' should be obtained from the site operator or determined by the Gasfield module. However, where this is not the case GasSimLite recommends a default value of uniform range between 70-90% efficiency, as abstraction systems are never 100% efficient.

Flares

The inputs should be obtained from the flare specification or the site operator.

The flare specification and the operation will affect the 'Minimum Flare Capacity' and 'Maximum Flare Capacity' and therefore this information should be obtained from the site operator.

Bulk gas ‘Destruction Efficiencies’ (CH_4 and H_2) should be determined on-site by monitoring the concentrations in landfill gas inputted and the emitted from the flare. Allowing the determination of accurate emissions from the flare, which will depend on the flare age, capacity, temperature, air to fuel ratio, and the level of maintenance that has been carried out on the flare. Flares often have high destruction efficiencies when installed but poor maintenance and age will cause these to decline. Where site-specific data is not available, Table 5.7 provides suggested input values.

The ‘Air to Fuel Ratio’, ‘Stack Height’ of flare, flare ‘Temperature’ and flare ‘Orifice Diameter’ should be obtained from the site operator or the flare specification. GasSimLite suggests a default air to fuel ratio of 5 for flares and a flare temperature of 1000°C.

Table 5.7 Recommended Destruction Efficiency for Flares and Engines

Species	Minimum reported value (mg/m^3)	Maximum reported value (mg/m^3)	No. of samples	Recommended destruction efficiency (%)
Methane	96.0	99.6	8	99
Hydrogen				99
Hydrogen sulphide	70.6	96.9	6	99
Total VOCs				99
1,1,1-Trichloroethane	74.8	>99.99	7	99
1,2-Dichloroethane	93.8	99.99	5	99
Benzene	4.6	99.6	12	99
Carbon tetrachloride (tetrachloromethane)	71.63	>99	5	99
Benzyl chloride (chlorobenzene)	92.8	92.8	1	99
Chloroform	83.3	99.92	7	99
Dichlorodifluoromethane	97.6	98.6	2	99
Dichloromethane	93.8	99.7	5	99
Xylene isomers	92.0	99.96	14	99
Trimethybenzene	99.1	99.9	7	99
Dichloromethane (Methylene chloride)	95	>99.9	3	99
Tetrachloroethene	83.3	99.98	5	99
Toluene	92.0	99.99	12	99
Trichloroethylene (trichloroethene)	97.8	99.97	10	99
Trichlorofluoromethane	89.8	99.8	4	99
Trichlorotrifluoroethane	95.2	99.5	2	99
Chloroethene (vinyl chloride)	89.3	>99.9	4	99
Other Species				99

Trace Gas ‘Destruction Efficiencies’ should be determined on-site by monitoring the Trace LFG concentrations and the engine/flare emissions. These are required where the emissions of these species are being simulated using the ‘Non-Combustion Products’, ‘Combustion Product from Parent’ or ‘Carbon Dioxide Generation’ equations. However, where site-specific data is not available Table 5.13 provides recommended data. The ranges have been obtained from the following studies: Baldwin et al. (1993a and 1993b), Millican (1995), California State Air Resources Board (1986a and 1986b), and LQM (2002).

Additionally when using the ‘Combustion Product from Parent’ equation the ‘Destruction Efficiency’ relates to the destruction the parent species and not the generation of the daughter species i.e. Chlorine is destroyed by a 99% destruction efficiency to form 1% hydrogen chloride.

‘Flare Exhaust Concentrations’ are required for species that are generated by the combustion process, using the ‘Combustion Product’ equation. These concentrations should be determined on-site as the levels of emissions will depend on the flare age, capacity, residence time, temperature, air : fuel ratio and level of maintenance. If site-specific data is not available, a number of recommended values are listed in Table 5.8. The ranges have been obtained for the following studies; Valis (2000) and LQM (2002).

The destruction efficiency and source concentration of VOCs should be defined even when you are simulating the emissions of these as a ‘Combustion Product’ as GasSimLite simulates their break down to form carbon dioxide.

The flare ‘Downtime’ if the percentage of time that the flare will not operate per year due to routine maintenance and breakdown. This information should be obtained from the site operator, alternatively where this information is not available a value of Uniform distribution 3-5% should be used as a default.

Table 5.8 Trace Gas Emissions for Flares (mg/m^3)

Species	Distribution	Mean\ or most likely	St Dev	Max.	Min.	No. of samples
Oxides of sulphur (SO_X)	Uniform			38	20	2
Oxides of nitrogen (NO_X)	Uniform			87	76	2
Total VOCs	Log Uniform			990	52	2
Carbon monoxide	Uniform			650	290	2
Hydrogen fluoride	Uniform			18	1.4	2
Hydrogen chloride	Log Uniform			90.44	0.5	57
Hydrogen sulphide	Single	3				1

Engines

The inputs for engines, like flares, should be obtained from the specification or the site operator.

The ‘Engine Capacity’ will depend on a number of factors including the type of engine used and the methane to carbon dioxide ratio of the gas. Therefore these should be obtained from the operator or the engine specification.

The 'Air to Fuel Ratio', 'Exhaust Height' of the emission stack, engine 'Temperature' and Exhaust 'Orifice Diameter' are engine specific and should be obtained from the site operator. However, where this information is not available defaults of the 'Air to Fuel Ratio' of 7 and a 'Temperature' of 500°C are recommended.

'Destruction Efficiencies' for trace gases are required where the emissions of these species are being simulated using the 'Non-Combustion Products', 'Combustion Product from Parent' or 'Carbon Dioxide Generation' equations. The 'Destruction Efficiencies' of both bulk gas are always required. These should be determined on-site by monitoring the concentrations in landfill gas and the emissions from the engine, as the emissions will depend on the residence time, combustion temperature, air to fuel ratio and level of maintenance that has been carried out on the engine. It is often the case, as with flares, the destruction efficiencies of poorly maintained engines decline with time. Where site-specific data is not available Table 5.7 provides default values.

Additionally when using the 'Combustion Product from parent' equation the 'Destruction Efficiency' relates to the destruction the parent species and not the generation of the daughter species i.e. Chlorine is destroyed by a 99% destruction efficiency to form 1% hydrogen chloride.

Assumption – using the limited data available, the destruction efficiencies from engines have been assumed to be the same as flares in the absence of detailed studies on engine emissions.

'Engine Exhaust Concentrations' are required for species that are generated by the combustion process, using the 'Combustion Product' equation. These concentrations should be determined on-site as the levels of emissions with depend on the engine age, capacity, residence time, temperature, air:fuel ratio and level of maintenance. Where site-specific data is not available, a number of recommended values are provided in Table 5.9.

The 'Destruction Efficiency' and source concentration of VOCs should be defined even when you are simulating the emissions of these as a 'Combustion Product' as GasSimLite simulates their break down to form carbon dioxide.

The engine 'Downtime' if the percentage of time that the engine will not operate per year due to routine maintenance and breakdown. This information, as with flares, should be obtained from the site operator, alternatively where this information is not available a value of uniform distribution 3-5% should be used as a default.

Table 5.9 Trace Gas Emissions for Engines (mg/m^3)

Species	Distribution	Mean\ or most likely	St Dev	Max.	Min.	No. of samples
Oxides of sulphur (SO_X)	Log Triangular	90		540	18	9
Oxides of nitrogen (NO_X)	Log Uniform			1500	360	9
Total VOCs	Log Triangular	1410		5260	530	9
Carbon monoxide	Triangular	1700		1900	508	9
Hydrogen fluoride	Log Triangular	3.5		6.2	0.2	8
Hydrogen chloride	Log Uniform			9.5	0.2	8
2,3,7,8 TCDD (PCDDs & PCDFs	Log Triangular	$1.2x10^{-9}$		$1.3x10^{-9}$	$9x10^{-10}$	7
Benzo-a-pyrene	Log Triangular	0.001		0.03	0.001	7
Hydrogen sulphide	Triangular	1.5		2.5	1.5	8
Particulate matter (PM10s)	Log Uniform			33	1.9	8

CHAPTER 6: THEORY BEHIND GASSIMLITE (CALCULATIONS)

6. THEORY BEHIND GASSIMLITE (CALCULATIONS)

This chapter contains the assumptions made, the equations used and any simplifications adopted to produce GasSimLite.

Overview of the Model and Model Theory

General

A complete GasSimLite simulation is carried out using 2 modules:

- ☐ source term (source);
- ☐ emissions model (source);

GasSimLite considers the uncertainty in processes, models and parameters, focusing on the impact of landfill gas on the above. GasSimLite does not simulate the catastrophic impacts associated with inundation of floodwater, earthquake or collapse of underlying mine workings. Additionally GasSimLite has a minimum time step of one year and therefore cannot simulate acute exposure resulting in asphyxiation or other acute health effects.

This chapter discusses the processes and models that produce the equations coded into GasSimLite. GasSimLite does not consider the movement of landfill leachate or LFG dissolved in water, only LFG generation, emissions and utilisation are considered in the model. GasSimLite calculates possible concentrations of species in LFG.

The modules carry out a series of calculations:

- ☐ calculates the moisture content of the waste from the infiltration rate, leachate conditions, waste hydraulic properties and hydrogeological characteristics;
- ☐ calculates the LFG generation rate for bulk gases (CH_4, CO_2, H_2) using the waste quantity, breakdown/composition, the rate of decay, moisture content and the emission ratio of CH_4 to CO_2;
- ☐ calculates the trace gas concentrations by determining the volume of bulk gas generated, the concentration of trace gas monitored in 1 m^3 of LFG and the half-time of trace gases;
- ☐ calculates the volume of gas that is utilised by flares and engines, and thus determines the emissions from these processes and the uncontrolled emissions through the liner and cap,
- ☐ simulates biological methane oxidation including the presence of fissures;
- ☐ estimates the PI emissions.

Model Operation

GasSimLite considers the landfill as one unit as, unlike leachate, cells are rarely isolated with respect to LFG.

The source term determines the generation of LFG for an individual site based on the mass of waste deposited and the waste composition of the waste stream or streams. The waste is degraded following a first-order decay model that calculates the LFG generation for up to 200 years, using the GasSimLite multi phase equation. The emission model uses this output to calculate the LFG emission of bulk and trace gases to the environment after allowing for LFG collection, flaring, utilisation (energy recovery), and biological methane oxidation. This is undertaken by using information on the site gas collection system, flare, engine, and engineered barriers (cap and liner) if present. It is assumed that LFG generated and not collected is in equilibrium and will be emitted from the landfill cap or liner at a steady state. Additionally, the model calculates the concentrations of other major and trace gases emitted from surface, slides, flares and engines.

Source Term

Waste moisture content

GasSimLite calculations begin with the determination of the waste moisture content. GasSimLite assumes that the water is derived from infiltration through the landfill cap, leachate conditions, the waste hydraulic properties and hydrogeological characteristics (as detailed in Chapter 3). GasSimLite assumes that the infiltration rate and leachate level are constant across the entire area of the landfill. The total infiltration rate and leachate volume are obtained by multiplying the rates by the landfill area. It is not necessary to allow for daily or seasonal variations in infiltration or leachate head because the effect of these will be smoothed out over time. The determination of the effect of infiltration and drainage systems on the depth of the leachate head is beyond the scope of GasSimLite and therefore this should be determined before running GasSimLite; potentially using a model like LandSim. The infiltration rate through the landfill cap is dependant on the effective rainfall and cap design. The determination of this is also beyond the scope of GasSimLite.

Precipitation, and infiltration through the capped and uncapped area of the landfill generally follow a normal distribution, a mean value and a standard deviation are therefore required to define the distribution. Precipitation can normally be obtained form Meteorological office records or the on-site meteorological station.

The waste moisture content, free void space, and the effective saturation of the waste are determined by using a water balance calculation.

The model then defines different categories of the waste moisture:

- ☐ wet - greater than 60% (vol./vol.) moisture;
- ☐ dry - less than 30% (vol./vol.) moisture;
- ☐ average - greater than 30% (vol./vol.) and less than 60% (vol /vol.)moisture.

Alternatively if the waste moisture content is known the moisture category can be entered directly. However, the determination of the waste moisture content should be carried out with care, as this is a key factor controlling the waste degradation and thus LFG production, by determining the waste degradation constants.

Landfill Gas Generation

The Gas generation in GasSimLite is determined using the GasSimLite multi-phase first order LFG generation equation, developed by the HELGA framework (Gregory *et al.*, 1999). This was originally based on the model developed by Hoeks and Oosthoek (1981) and Zanten and Scheeps (1996). However, the GasSimLite multi-phase equation is a significant improvement on these as it can:

- ☐ define precisely the mix (breakdown), composition and moisture content of waste in the landfill site; and
- ☐ calculate LFG generation based on the degradation rates of the individual materials in the landfilled waste.

These additions make the GasSimLite multi-phase equation highly flexible and allow it to be tailored to individual landfill sites, taking account of specific waste streams, filling/deposition rates and environmental conditions.

The source model has two main processes:

- ☐ defining the waste in the landfill site; and
- ☐ calculating carbon available for decay from a specified mass of waste.

Defining the Waste Mass and Volume

GasSimLite simulates the landfilling process by the user defining the year that deposition commenced, and then entering a mass of waste disposed for each operational year. Simulating the Gas generation using the multiple phase equation also requires the breakdown of the waste using the various waste streams, described below, to be defined for each year of deposition.

Defining the Waste

The breakdown and composition of the waste within the landfill site will affect the rate of generation and total yield of LFG produced, which is determined by the mass and degradability of the cellulose and hemi-cellulose in the waste. However, the ultimate degradability of cellulose polymers differs between waste materials. Different biodegradable materials have different quantities of cellulose and hemi-cellulose, and different waste streams have different compositions (as discussed in the default data Chapter 3). Therefore, GasSimLite uses the total waste composition of the different waste streams to determine the mass and degradability of cellulose and hemi-cellulose (discussed below).

GasSimLite only models the decay of cellulose and hemi-cellulose, which are known to make up approximately 91% of the degradable fraction (Barlaz *et al.*, 1989) and ignores other potentially degradable fractions that do not contribute significantly i.e. protein and lipids.

The user characterises the waste deposited by defining the proportion/breakdown of the waste in different default waste streams or by defining their own waste streams, each year for up to 40 years (as discussed in Chapter 3).

Defining the Emissions Ratio

The ratio of methane to carbon dioxide in LFG is used to determine the quantity of methane and carbon dioxide produced by methanogenic decay. This is a site-specific parameter and is user defined.

Data manipulation

GasSim multi-phase equation

GasSimLite uses the data above to calculate the:

- percentage of each component in the waste;
- dry weight of each fraction;
- dry weight of the waste;
- cellulose and hemi-cellulose content of the waste;
- degradable carbon in the waste;
- fraction of rapidly, moderately and slowly degradable carbon in the waste;
- conversion of carbon; and
- LFG (methane, carbon dioxide and hydrogen) production from the waste (hourly, yearly and cumulatively).

This is undertaken by combining the waste streams into a yearly waste source. Each waste stream is divided into components i.e. the proportion of paper, garden waste and non-degradable waste. The composition and the waste moisture content of each fraction are then used to calculate the weight components and the total waste deposited each year.

The yearly cellulose and hemi-cellulose contents of the waste are then determined, using the make up of the waste fractions along with the proportion of the waste that can degrade. The waste is also partitioned into three fractions that are degraded at different rates (Table 6.1), depending on the degree of lignification of cellulose in the material:

- waste that degrades slowly;
- waste that degrades at a moderate rate; and
- waste that degrades rapidly.

The dry weight of carbon available for degradation for each fraction is determined for each year.

The model then assumes the each fraction degrades by first order decay at a specific rate. This allows putrescible waste to be degraded at a faster rate than wood or paper.

Table 6.1 Degradation rate assigned to each waste fraction

Degradability	Fraction
Rapid	Putrescibles Fines Garden wastes Sewage sludge
Moderate	¼ Paper (excluding newspaper) Nappies Miscellaneous combustible
Slow	¾ Paper (excluding newspaper) Newspaper Textiles

Biodegradation

GasSimLite simulates the biodegradation during the aerobic (acetogenic) and anaerobic (methanogenic) stages. This is carried out individually for each year of waste deposition with the results of all the deposition years aggregated before reporting.

To allow the generation of hydrogen to be simulated aerobic (acetogenic) degradation has been included. This is carried out by the rapid acetogenically decay of a 1% of the waste deposited in the year. The remaining 99% of the waste is degraded methanogenically, as discussed below. In the second and subsequent years this waste is only degraded methanogenically. The default value of 1% of the waste degrading acetogenically was validated using the HELGA framework (Gregory *et al.*, 1999), with this producing a maximum concentration of H_2 in LFG of around 10%, which fits with the work of Farquhar and Roveres (1973).

Under anaerobic (methanogenic) degradation, GasSimLite assumes that the degradable cellulose and hemi-cellulose are converted to carbon available for degradation.

Landfill Gas Production

The production of LFG is determined from the mass of available carbon (1 mole of carbon produces 1 mole of carbon dioxide or methane). The proportion of carbon dioxide to methane for methanogenic degradation is determined using the ratio of 1%, as described in Chapter 5. The quantity of carbon dioxide and hydrogen generated acetogenically is determined by the equation below (Equation 6.1).

$$C_6H_{12}O_6 \xrightarrow{Acetogenesis} 2CH_3COOH + 4H_2 + 2CO_2$$

or

$$6Carbon = 2AceticAcid + 4Hydrogen + 2CarbonDioxide \tag{6.1}$$

Calculating the Landfill Gas Generation

The degradation and biodegradation of organic material is carried out by a multi-phase, first order decay equation (6.2) that deals with the three degradable fractions separately and aggregates the amount of carbon converted to LFG.

$$C_t = C_0 - \left(C_{o,1}e^{(-k_1 t)} + C_{o,2}e^{(-k_2 t)} + C_{o,3}e^{(-k_3 t)}\right)$$

And $C_x = C_t - C_{t-1}$ (6.2)

where:

C_t	mass of degradable carbon degraded up to time t (tonnes)
C_0	mass of degradable carbon at time t = 0 (tonnes)
$C_{o,i}$	mass of degradable carbon at time t = 0 in each fraction (1, 2, 3, rapidly, moderately and slowly degradable fractions respectively (tonnes)
C_x	mass of carbon degraded in year t (tonnes)
t	time between waste emplacement and LFG generation (years)
k_i	degradation rate constant for each fraction of degradable carbon (per year)

The rates of decay and degradation half-lives are dependant on the waste moisture content, as a wet waste will degrade at a faster rate than a dry waste. The default decay constants used are discussed in Chapter 5.

Calculating the Trace Gas and VOC Source

The concentration of trace gas species can either be entered by the user or using the defaults (discussed in Chapter 3).

GasSimLite simulates the concentrations of gases as mg/m^3. However on-site gas concentrations are normally measured in ppm, these two units can be converted using the following equation (6.3):

$$C_P = \frac{C_{\%v/v}}{100\%} \cdot \frac{(1000 \cdot MW_P)}{(Vm)}$$

(6.3)

where:

C_p	concentration of species P (mg/m^3)
$C_{\%v/v}$	concentration of species P (%v/v)

MW_P molecular weight of species P (g)

Vm molar volume (at STP) ($2.241x10^{-2}$ m^3/mol)

Using a Declining Source Term

Examination of total VOC emissions from landfills has indicated that the concentration of trace gases emitted from landfills reduce the over time. Therefore, GasSimLite simulates the source of traces gases by assuming that these decline over time, following the decay equation (6.4).

$$C_{tg} = C_g . e^{(-k_{tg} t)} \tag{6.4}$$

where:

C_{tg} trace gas concentration t (tonnes)

C_g trace gas concentration at time t = 0 (tonnes)

k_{tg} decay constant, trace gas half life

t time between waste emplacement and LFG generation (years)

This declining source was determined by examining the emissions of VOCs in landfill gas from a number of landfills from studies carried out by Knox (1990), Scott *et al.* (1988a), Allen *et al.* (1997), Young and Parker (1983), Emberton and Scott (1987), Jones *et al.* (1988), and Scott *et al.* (1988b). The data has been analysed (Figure 6.2) using a FITCURVE directive (using Genstat 5 Release 4.1 (Third Edition) statistical package (Genstat 5 Committee, 1993)) using a standard non-linear regression model (Figure 6.1). This directive estimates the model's only non-linear parameter, r, which defines the rate of exponential decrease of VOCs with time. The other linear parameters (a and b) are estimated by linear regression at each stage of an iterative search for the best estimate of r.

This method provides the estimated parameter and error (standard error) values listed in Table 6.2 and the parameters used in Equation 6.7. This fit is statistically significant (P<0.001).

Table 6.2 Fitted parameter values for the VOC declining source term

Parameter	Estimate	Standard Error
a (mg/m^3)	0	0
b (mg/m^3)	3067	452
R	0.8449	0.054
K^* ($year^{-1}$)	0.1685	0.0639

$r^2 = 0.21$, $r = 0.46$, $n = 48$, $df = 47$, $P < 0.001$

* $k = -\ln(r)$, $\Delta k = \Delta r/r$

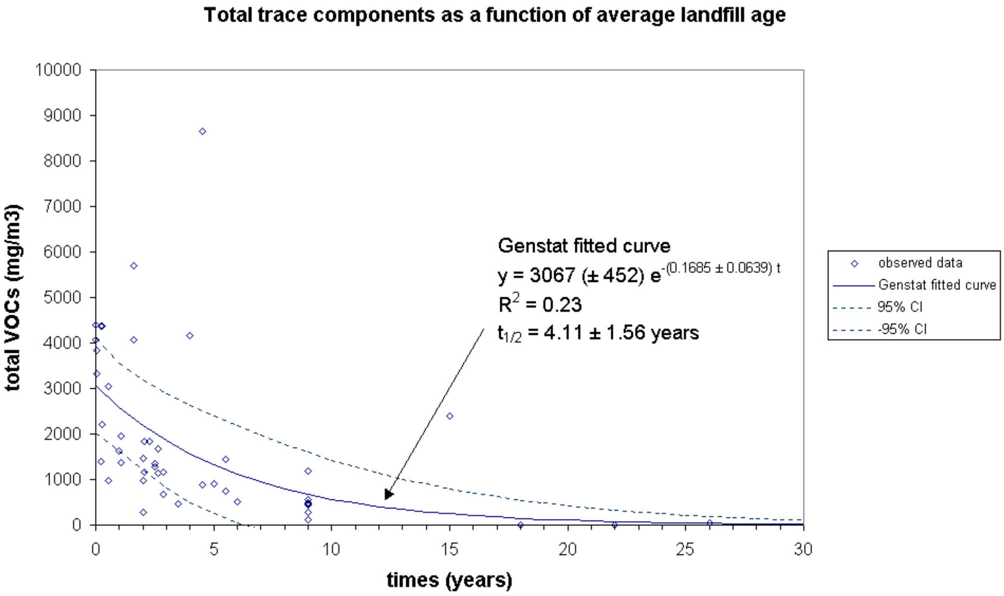


Figure 6.1 Total VOCs declining source term

Simulating a Constant Source Term

GasSimLite simulations can be undertaken using a conservative constant source term by limiting the rate of trace gas decay i.e. by defining the decay half life as a large number of years (e.g. 10,000 years).

Emission model

The emissions from a landfill are normally, but not always, controlled by engineering measures, i.e. the installation of engineered barriers (cap and liner) and gas collection system. The gas collected can then be flared or utilised, by spark ignition engines to produce electricity. GasSimLite uses the information provided on these engineering measures to determine the quantity of uncontrolled LFG releases through the surface, the cap, and/or lateral emissions, through the liner. The model assumes that any LFG generated that is not collected is in equilibrium with the rate of gas emitted through the landfill cap or liner, i.e. at a steady state conditions. Additionally, GasSimLite estimates the surface and lateral emission of trace gases, using either default or user defined values, and the atmospheric emissions from flares and engines, using destruction efficiencies or flare/engine exhaust data.

GasSimLite simulates the LFG abstraction by determining the available engine and flare capacity per year and using the collection efficiency of the system and the engine/flare down time to determine the maximum quantity of gas that can be abstracted. If this is greater than the gas generation rate, all the gas, (except for the quantity that can not be collected due to collection efficiency not being 100% or the engine/flare not operating due to downtime), will be utilised or flared. When this quantity of gas is less than the amount of gas generated, the residual gas will be lost uncontrollably.

The emission model manipulates the data provided by the source model along with the information provided in the Gas Utilisation dialogue box to determine the following for a 200 year assessment period:

- ❑ volume of LFG that can be utilised by engines;
- ❑ volume of LFG that can be flared;
- ❑ volume of LFG lost in uncontrolled emissions:
- ❑ volume through the cap,
- ❑ volume through the liner;
- ❑ methane oxidation in the cap.

Capped and uncapped areas

The LFG generated by the source model is split into the proportions generated by the capped and uncapped areas of the landfill. This is simulated by the user defining of the percentage of the waste in place that is capped (Equation 6.5), per year. This term should be based on the tonnage of waste placed as using an area term assumes that the waste has a uniform thickness, which is unlikely to be the case during filling.

This is a slight over simplification of the actual situation and assumes that all the LFG emitted form the operation phase is through the surface and that gas generated in the capped area is not emitted through the uncapped sides with the operational area.

$$Q_{gen} = Q_{genCapped} - Q_{genUncapped} \tag{6.5}$$

where:

Q_{gen}	LFG generated by the source model
$Q_{genCapped}$	LFG generated in the capped proportion of the landfill
$Q_{genUncapped}$	LFG generated in the uncapped proportion of the landfill

Gas collection

The gas collection system is assumed to extract gas from the entire capped area of the landfill. The collection efficiency can be defined. GasSimLite assumes gas is collected and then either flared or utilised for energy recovery using spark ignition engines for electricity generation at a set efficiency and within a minimum and maximum rate.

The gas collection system is set up to simulate normal operation practices using one of the following options:

- ☐ commission the engine and flares in the order that they are displayed on the screen ('User Defined');
- ☐ commission the engines first with GasSimLite determine the optimum order, with excess LGF being flared ('Engines First');
- ☐ commission the flares first with GasSimLite determine the optimum order, with excess LGF being utilised by the engines ('Flares First');
- ☐ run the simulation without gas utilisation by selecting 'No engines and flares'.

However, it should be remembered that GasSimLite calculates the available gas removal capacity using engines and flares that are operational i.e. that have been commissioned and have not been decommissioned.

The maximum capacity of the gas collection system is then calculated using the above information along with capacity of each engine and/or flare and number of flares and/or engines, allowing for downtime. It is assumed that where multiple flares and/or engines have been specified that new engines/flares will be brought on line when sufficient gas is available and removed when insufficient gas is available. The minimum gas collection capacity is determined by the lowest abstraction rate for a flare or engine. The concept of downtime determines the yearly operation collection rate for each engine or flare by accounting for the proportion of time that they are not operational due to routine maintenance and breakdown. This involves a simple calculation of reducing the yearly capacity for each engine/flare by the downtime percentage e.g. a 500 m^3/hr engine with 10% down time will remove on average 450m^3/hr.

It is assumed when flaring if gas is produced at a level between these rates and the operation will be trimmed to follow the gas production curve. This is a fairly good assumption as in reality it is trimmed to the point at which air is drawn into the system. If gas is generated above this rate then the excess LFG will be released uncontrollably, and if gas is generated below the rate at which the flare will not operate and any gas generated will be released. It should also be noted that in practice no system is 100% efficient, and therefore a quantity of gas will always be emitted

The uncollected LFG that is emitted by uncontrolled emissions from the capped area can then be determined by equation 6.6.

$$Q_{res} = Q_{gencapped} - ((Q_{flare} + Q_{utilisation}) \text{ x } (1\text{-}CF/100) \tag{6.6}$$

where:

Q_{res}	Residual LFG production
$Q_{genCapped}$	LFG generated in the capped portion of the landfill

Q_{flare}	LFG routed to flare system
$Q_{utilisation}$	LFG routed to the energy recovery plant
CF	the LFG collection efficiency

Surface and Lateral Emission routes

The presence of uncollected gas in the capped area (Q_{res}) will result in uncollected emissions from the cap and/or the liner. The quantity of emission through both the cap and liner are determined by the permeability and thickness of the most impervious layer, of each individually. GasSimLite assumes that gas movement is via plug flow and that both the cap and liner are homogenous and isotropic, even through in practice poor cap/liner construction and maintenance can result in cracks and micro-fractures. However, although these may be locally important their net effect on the emissions will be averaged out across the site. The uncontrolled emissions are calculated in GasSimLite from the:

- ☐ cap design;
- ☐ cap hydraulic conductivity;
- ☐ cap thickness;
- ☐ waste thickness;
- ☐ waste hydraulic conductivity;
- ☐ liner thickness;
- ☐ liner hydraulic conductivity; and
- ☐ site dimensions.

In some cases the most impervious layer could be the waste itself, which is also assumed to be homogenous and isotropic, if this is the case then the waste thickness is assumed to be half the average total waste thickness.

The emissions of LFG can be calculated using Darcy's law, for a homogeneous medium. The emissions from the cap and the liner are calculated at the same time, as the excess gas (Q_{res}) will be emitted through each medium at different proportions (Equation 6.7). The equation has been modified from the original HELGA framework by the inclusion of the surface area.

$$Q_c = \frac{Q_{res}}{\left(\frac{d_c}{K_c.A_c} . \frac{K_l.A_l.}{d_l}\right) + 1}$$

$$Q_l = \frac{Q_{res}}{\left(\frac{d_l}{K_l.A_l} . \frac{K_c.A_c}{d_c}\right) + 1}$$

(6.7)

where:

Q_c	Flux from cap (l = liner)
Q_{res}	Residual LFG production
K_c	effective permeability of medium of cap (l = liner)
d_c	thickness of cap in direction of flow (l = liner)
A_c	Surface area of cap in the direction of flow (l = liner)

The surface area of the liner is determined from the landfill perimeter and the depth of the unsaturated zone within the landfill, as it is assumed that LFG is not dissolved in the landfill leachate.

The gas produced from the uncapped area ($Q_{resUncapped}$) will all be emitted through the surface as it is assumed the open surface of the waste will be far more permeable that the landfill edge, which may or may not be engineered.

Biological Methane Oxidation

Any landfill gas that is not collected by the gas collection system has the potential to migrate through the cap and lateral liner of a landfill, independent oft the design of the lining system. The lateral migration pathway does not simulate methane oxidation since offsite conditions are difficult to quantify and thus the model generates a conservative estimation of lateral methane migration. In comparison, the potential for methane oxidation in the cap is much better understood. This is a good secondary methane management system for the residual landfill gas for a site under abstraction, and also for a site generating little gas such that a gas abstraction system is not able to be used successfully because of the low rate of generation or low calorific value of the gas.

The process is a four stage bacteriological conversion of methane into carbon dioxide (Equation 6.8):

$$CH_4 \rightarrow CH_3OH \rightarrow HCHO \rightarrow HCOOH \rightarrow CO_2 \qquad (6.8)$$

methane methanol methanal methanoic acid carbon dioxide

Methanotrophic bacteria use these reactions to gain energy and carbon for their growth (Hanson and Hanson, 1996). Methane oxidation has been linked to the two main types of methanotrophic bacteria (Borjesson at al, 1998) this is soporiferous. Data on field based observations appear to show a seasonal relationship across many orders of magnitude. This relationship is also on laboratory scale observations of the conversion of methane to carbon dioxide, which are more likely to be undertaken at favourable conditions (i.e. close to the theoretical maximum which biological activity can attain in the soil medium) (Table 6.3). There are also data on the estimates of the rate of methane oxidation in cover soils using ^{13}C analysis (which gives a measure of the fraction of methane which is actually converted). GasSimLite uses known methane oxidation rates in different cover materials and in-situ conversion efficiencies to develop an empirical equation for the removal of methane from landfill gas emitting through the surface.

Alternatively, the GasSimLite model adopts the DEFRA policy option which is based on the Intergovernmental Panel on Climate Change IPCC guidelines for methane oxidation, and is used by the AEAT UK emissions estimation model (AEAT, 1999). The choice of which option is used for an assessment should be agreed with the regulator.

Both approaches are described below.

The empirical/scientific method

This is based on laboratory estimates of methane oxidation and in-situ field estimates of percentage methane oxidised. The combination of the two sets of data is considered to be a conservative approach .

Estimates of the fraction of LFG which could be oxidised by methanotrophs and which is actually oxidised, range from 10 – 46% (Borjesson et al 2000). The GasSimLite model assumes a mean value of 25% and a triangular distribution between 10 – 46% based on the data presented in (Borjesson et al 2000).

In addition, it is believed that there must be a limiting rate of methane oxidation for a given soil thickness and type. Methane oxidation occurs predominantly in the upper 50cm of soil cover where oxygen ingress is facilitated, and appears to be strongest in the zone 20 – 30cm below the surface. The default figures which are used in GasSimLite will be suitable for a soil cover >30cm thick overlying a single liner, clay or composite cap. Below 30cm thickness of soil on these engineered designs, or below 1m thickness of soil if no engineered cap is present, the GasSimLite model will switch off all methane oxidation, on the basis that the surface soil cover is insufficiently thick to permit a significant amount of methane oxidation to take place.

The measured rates of soil methane oxidation capacity are remarkably consistent in their observed range. However, the frequency per year at which the highest rates may apply is not known, and so the shape of the PDF that actually applies to the oxidising potential cannot be determined . These high values probably occur during summer conditions. A factor of 10 – 40% (discussed above) is applied to a normal distribution to give an estimate of the overall flux rate at which all the methane may be converted to carbon dioxide. The range of values in both parameters is used to help simulate seasonal variation in methane oxidation, soporiferous.

At all landfill sites, some landfill gas will escape through cracks and fissures, and joints in the landfill engineering/gas field infrastructure. The GasSimLite default for this quantity of gas lost is 10% of the total landfill gas that could be lost through the surface in any given. This value can also be measured using the Environment Agency's methane emissions measurement protocol (Environment Agency, 2001a).

If potential landfill methane emissions (methane at the base of the cap) are below the oxidising capacity of the cap under field conditions, then no methane (other than that lost through fissures etc) is released to the atmosphere. If potential landfill methane emissions exceed the oxidising capacity of the cap under field conditions, then only the methane lost through fissures and the excess methane flux through the cap is released, the remainder being converted to carbon dioxide. Table 6.3 lists the typical ranges and means recorded in the literature, and converts them to standard units.

The quantity (i.e. flux) of methane oxidised to carbon dioxide (Q_{ox}) and the calculated methane flux ($Q_{methane\ flux}$) in a given year, for >30cm soil cover above an engineered cap is defined below (Equations 6.9 to 6.11).

If

$$\Delta_{field\ efficiency} \,.\, (Q_{oxidising\ capacity} \,.\, 24 \,.\, 365) > (1-\Delta_{fissure}).(Q_{base\ of\ cap}) \tag{6.9}$$

Then

$$Q_{ox} = (1 - \Delta_{fissure}).(Q_{base\ of\ cap})$$

$$Q_{methane\ flux} = (\Delta_{fissure} \,.\, Q_{base\ of\ cap}) \tag{6.10}$$

Otherwise

$$Q_{ox} = \Delta_{field\ efficiency} \,.\, (Q_{oxidising\ capacity} \,.\, 24 \,.\, 365)$$

$$Q_{methane\ flux} = (\Delta_{fissure} \,.\, Q_{base\ of\ cap}) + (1 - \Delta_{fissure}).(Q_{base\ of\ cap} - \Delta_{field\ efficiency} (Q_{oxidising\ capacity} \,.\, 24 \,.\, 365)) \tag{6.11}$$

Where:

Q_{ox}	total quantity of methane oxidised to carbon dioxide (m^3/y)
$Q_{base\ of\ cap}$	total quantity of methane at base of cap for surface emission (m^3/y)

$Q_{\text{oxidising capacity}}$	soil oxidising capacity ($m^3/m^2/hr$)
Δ_{fissure}	empirical correction factor for fraction of methane lost directly through fissures
$\Delta_{\text{field efficiency}}$	empirical correction factor for effectiveness of oxidation under field conditions

The DEFRA/IPCC Policy method

AEAT have developed a spreadsheet model for DEFRA (and previously DETR) to estimate the emissions of methane from UK landfills (Brown et al, 1999). In line with the Intergovernmental Panel on Climate Change (IPCC) (1996a;b) view on methane oxidation in the cover materials of landfill sites, Brown et al (1999) set the methane oxidation rate (expressed as a percentage of the methane remaining after collection) for all site types in the DEFRA policy model at 10%. This is the recommended default value provided by the IPCC Expert Group on Waste. It should be noted that the Kyoto agreements are based on IPCC (1996a;b) regardless of more recent work by IPCC and/or others.

In policy mode, GasSimLite adopts the 10% value which is applied to all landfill gas not collected by the gas abstraction system.

The empirical scientific model will allow more residual methane oxidation than the policy model provided the engineering and gas collection systems are properly designed. That proviso, is the reason for the conservative value recommended by the IPCC Expert Group, and why agreement on which method is used could be sought with the regulator before performing an assessment.

Table 6.3 Methane oxidation capacity of cover materials

Conversion of methane oxidation measurements to standard terminology

Reference		Cap type and scenario		Oxidation of methane in landfill cover materials			
				Raw data from reference		Standardised data	
				$g/m^2/hr$	$litres/m^2/hr$	$mg/m^2/s$	$m^3/m^2/hr$
Hoecks	1983	Field study	max	0.23		6.39E-02	3.22E-04
			min	2.04		5.67E-01	2.86E-03
Mennerich	1986	Lab study	max	7.3		2.03E+00	1.02E-02
Whalen	1990	Lab study,	max	45		1.25E+01	6.30E-02
et al		topsoil					
Figueroa	1993	Sand cap (lab)	max		5.6	1.11E+00	5.60E-03
			min		0.7	1.39E-01	7.00E-04
Jones and	1993	Field study	max july	7.21		2.00E+00	1.01E-02
Nedwell		0-32cm	min	1.34E-05		3.72E-06	1.88E-08
Kightley	1995	coarse sand	max	6.95		1.93E+00	9.73E-03
et al							
Boeckx and	1996	soil	max	2.36		6.56E-01	3.30E-03
van Cleemput			min	0.84		2.33E-01	1.18E-03
Borjesson		Sand cap	max	6.3		1.75E+00	8.82E-03
and		0 - 80cm	min	1.9		5.28E-01	2.66E-03
Svensson	1997	Sandy loam	max	8.7		2.42E+00	1.22E-02
			min	0.14		3.89E-02	1.96E-04
		Sewage sludge	max	16.8		4.67E+00	2.35E-02
			min	1.6		4.44E-01	2.24E-03
Scharff		0-30cm	max		5.9	1.17E+00	5.90E-03
et al	2001		min		0.3	5.95E-02	3.00E-04
			mean		3.0	5.95E-01	3.00E-03
		0-100cm	max		3.8	7.54E-01	3.80E-03
			min		1.0	1.98E-01	1.00E-03
			mean		2.6	5.16E-01	2.60E-03

Trace Gas Emissions

In addition to the emission of bulk gases, GasSimLite also simulates the emissions of trace gases from surface and lateral emissions. The influence of the waste source term on the emission of these trace gases is unknown. Therefore the quantity emitted is determined by the concentration of the species per m^3 of LFG and the LFG emission rate.

The emissions from the surface can be determined by the equation 6.12:

$$R_{ps} = G \cdot G_p \tag{6.12}$$

where:

R_{ps}	release of species by surface emissions (mg/hr)
G	total landfill gas emitted via surface (Q_c) or lateral emissions (Q_l) (m^3/hr)
G_P	concentration of species P within raw landfill gas (mg/m^3)

This equation has been used for the surface and lateral emissions of all species, except for those which are created during combustion (HCl, HF, NO_x, SO_x, HNO_3 and total phosphates)and consequently will have zero emissions if no flares and engines are present.

Engines and Flare Emissions

Where gas is controlled by combustion (flaring and utilisation), the equation 6.12 is modified to account for species (P) which are assumed to be destroyed (as determined by the destruction efficiency) during the combustion process. The destruction efficiency can be user-defined or a default value. However, this should be set to 100%, as discussed in Chapter 5. Identical equations are used in GasSimLite to calculate the emissions for both flares and engines; therefore they have been discussed together here. The destruction efficiencies and other inputs are defined individually for flares and engines.

For the purposed of these equations GasSimLite assumes that all flares are enclosed, which reflects the current best practice.

The emissions are thus calculated by (Equation 6.13):

$$R_{pc} = (Q_{engine}\ or\ Q_{flare}) \cdot G_p \cdot \left(1 - \frac{DE\%}{100\%}\right) \tag{6.13}$$

where:

R_{pc}	release of species by combustion (mg/hr)
Q_{engine}	landfill gas to engine (m^3/hr)
Q_{flare}	landfill gas to flare (m^3/hr)
DE%	destruction efficiency of the gas flare or engine

G_P concentration of species P within raw landfill gas (mg/m^3)

This equation is used by GasSimLite to determine the atmospheric emissions from engines and flares of all species, except for those listed below that have modified equations.

- ☐ Major Gases:
- ☐ carbon dioxide (equation 6.14);
- ☐ hydrogen chloride (equations 6.15 and 6.16);
- ☐ nitrogen oxides (equation 6.15);
- ☐ sulphur dioxide (equations 6.15 and 6.16);
- ☐ carbon monoxide (equation 6.15).
- ☐ Organic Carbon Groups:
- ☐ dioxins and furans (equation 6.15);
- ☐ PAHs (equation 6.15).
- ☐ Named Organic Compounds:
- ☐ total non-methane VOCs (NMVOCs or VOCs) (equation 6.13 and 6.15).
- ☐ Other Individual Acid Forming Gases:
- ☐ hydrogen fluoride (equations 6.15 and 6.16);
- ☐ nitric acid (equation 6.15);
- ☐ total phosphates (equation 6.15).

Determination of carbon dioxide engine and flare emissions

GasSimLite assumes that emitted carbon dioxide arises from (1) the uncontrolled surface emissions of LFG (with methane oxidation) (discussed above), (2) the combustion of VOCs, and (3) the combustion of methane. The determination of emissions from the combustion process is dependent on the quantity and quality of gas flared or utilised and the destruction efficiency. Therefore, corrections are included to balance the mass of carbon dioxide produced per mole of methane combusted (44/16) or VOC (44/12, based on an average unit of VOC having a generic formula C_nH_{2n}). The VOC composition has been set to be conservative and to simplify the equation, as other substituted groups would reduce the average molar carbon content. Therefore the quantity of carbon dioxide emitted is(Equation 6.14):

$$R_{CO_2c} = (Q_{engine}\, or\, Q_{flare}) \cdot \left(\left[G_{CH_4} \right] \cdot \frac{44}{16} \right) \cdot \left(\frac{DE\%_{CH_4}}{100\%} \right) + \left(\left[G_{VOC} \right] \cdot \frac{44}{14} \right) \left(\frac{DE\%_{VOC}}{100\%} \right) \quad (6.14)$$

where:

R_{CO2c} release of carbon dioxide by combustion (mg/hr)

Q_{engine} landfill gas to engine (m^3/hr)

Q_{flare} landfill gas to flare (m^3/hr)

G_{CH4} concentration of methane within raw landfill gas (mg/m^3)

G_{VOC} concentration of total VOCs (as organic C) within raw landfill gas (mg/m^3)

DE% destruction efficiency of the gas flare or engine

Determination of the releases of the major combustion products (other than carbon dioxide and carbon monoxide) using post-combustion data

Hydrogen chloride, hydrogen fluoride, dioxins & furans, nitrogen oxides, sulphur dioxide, nitric acid, total phosphates, carbon monoxide, PAHs and non methane VOCs are produced by the combustion process. The emissions of these gases from engines and flares have been determined using a correction for the proportion of these species formed during the combustion process. This has been undertaken by scaling up the observed emissions from engine exhausts and/or flare stacks according to an assumed air to fuel (landfill gas) ratio of 5:1, (Chapter 5)(), with releases increasing in direct proportion to the gas combusted. Thus producing the following equation (6.15):

$$R_{pc} = \cdot(AF+1)\cdot\left(\ [F_p]\cdot Q_{flare} + [E_p]\cdot Q_{engine}\right) \tag{6.15}$$

where:

R_{pc} release of species by combustion (mg/hr)

Q_{engine} landfill gas to engine (m^3/hr)

Q_{flare} landfill gas to flare (m^3/hr)

F_P concentration of species P within flare stack (mg/m^3)

E_P concentration of species P within engine exhaust (mg/m^3)

AF air to fuel ratio

It is assumed that:

- for measured flare stack emissions, correction to standard oxygen and to dry gas has not been possible because there is no systematic reporting of the data available to allow such corrections to be made.

- for engine emissions data the reported values were expressed for reference conditions of 15% oxygen content and dry gas.

Alternative methods for determining the emissions of HCl, HF and SO_2 from combustion

If is often the case that flare and engine emissions of hydrogen chloride, hydrogen fluoride and sulphur dioxide, daughter species, are determined using parent species, i.e. total chlorine, fluorine, and an estimated reduced sulphur content in landfill gas. The parent species are simulated missing word a trace gas, as described above, and the emissions are determined using equation 6.16, where a correction factor is applied for the molecular ratio, based on the molecular mass. These equations are base on those presented in AP-42 (US EPA, 1998).

$$R_D = \left(Q_{engine} \, or \, Q_{flare}\right) \cdot [G_P] \cdot MM \cdot \frac{DE\%}{100\%} \tag{6.16}$$

where:

R_D	release of daughter species by combustion e.g. hydrogen chloride (mg/hr)
Q_{engine}	landfill gas to engine (m^3/hr)
Q_{flare}	landfill gas to flare (m^3/hr)
G_P	total concentration of parent species within raw landfill gas e.g. Chlorine (mg/m^3)
MM	ratio of molecular mass e.g. of HCl to Cl = 1.03
DE%	destruction efficiency of the emitted from the gas flare or engine i.e. HCl (this value can not be set to 0%)

Because there are limited published data on the total sulphur content of raw landfill gas the total concentration of reduced sulphur is calculated using sulphur dioxide.

Model Confidence and number of iterations

If the results of the modelling are being examined at a specific confidence level there is a theoretical minimum number of iterations that should be made. For instance, if the results are being examined at a 95% confidence level, then for each output 10 values must occur above the 95% confidence level to ensure that these high values are representative.

By definition, there will also have to be 190 values below the 95% confidence level. To obtain reasonable results at the 95% confidence level, therefore, more than 200 iterations should be specified. If the results are to be examined at the 99% confidence level then the same argument applies and the landfill should be simulated more than 1000 times. The following table gives the number of iterations required for other confidence levels.

Confidence Level (%)	Theoretical Minimum Number of iterations
1	1001
5	201
10	101
50	21
90	101
95	201
99	1001

7 GLOSSARY

Acetogenic degradation	The aerobic degradation of waste resulting in the generation of carbon dioxide, hydrogen and fatty acids.
Adsorptive capacity	The capacity for the waste to adsorb water.
Air diffusion coefficient	The rate at which a gas will move through air.
Air: fuel ratio	The ratio of air to LFG (fuel) used by an engine or flare
Available carbon	The quantity of carbon that is available to undergo decay.
Biological methane oxidation	The conversion of methane to carbon dioxide in the soil as a result of micro-organisms.
Breakdown (of waste)	The definition of the waste mix using the waste streams i.e. 50% domestic, 40% commercial, and 10% inert.
Bulk gas	Gases that make up the majority of the LFG volume i.e. methane, carbon dioxide and hydrogen.
Cap	An engineered barrier used to cover the landfill
Capped area	The area of a landfill that has been covered by an engineered barrier.
Cellulose decay constants	The half-life values for the degradation of carbon and thus generation of LFG.
CFCs	Chlorofluorocarbons
Combustion	Burning LFG
Composition (of waste)	The fractionation or make up of the waste streams, i.e. the amount of paper, fines, putrescible etc material.
Conceptual model	A simplified representation of how a real system is believed to behave based on qualitative analysis of field data. A quantitative conceptual model includes preliminary calculations for key processes.
Conductivity	See Hydraulic Conductivity.
Daughter species	The species formed during combustion from a parent species in LFG, i.e. hydrogen fluoride (HF) is formed during the combustion process from fluorine

(F).

Decay – rapid, moderate, slow	The decomposition of available carbon to generate LFG. GasSimLite simulates waste fractions degrading at three different rates – rapid, moderate and slow (link to manual help page).
Decomposition	The decay of available carbon to generate LFG.
Default values	Generic information provided with GasSimLite that can be refined where site-specific data is unavailable.
Degradable carbon	The quantity of carbon that is degraded to generate LFG.
Degradation rate	A constant that defines the rate at which waste decomposes and thus LFG is generated.
Destruction efficiencies	The ratio of a species removed by the process of combustion by either flaring or engines.
Deterministic model	A model where all elements and parameters of the model are assigned unique values.
Discrete feature	This includes anisotropic areas of the cap e.g. fissures, passive venting wells etc.
Distributions (probability)	Defines uncertainty in a parameter in terms frequency of occurrence of a graph with either a uniform (horizontal), triangular, log triangular or normal curve. The area beneath the curve being equal to one. Distribution is used in GasSimLite to bias the random selection of the parameter input values. Thus, for a triangular distribution, values close to that most likely will be selected more frequently than values that are close to either the minimum or maximum.
Downtime	The proportion of time that engines and flares are not operating as a result of routine servicing and maintenance.
Effective porosity	The volume of void space that is available for fluid (liquid or gas) movement.
Effective rainfall	Total rainfall less evaporation, evapotranspiration, run-off and storage. This parameter has units of length/time (mm/y).
Emissions	The uncontrolled release of gas from a landfill surface, side, or from an engine/flare.

Engine	A spark ignition machine which generates electricity from the combustion of LFG
Engine capacity	The volume of gas that an engine uses at the defined methane to carbon dioxide ratio.
Engine output	The bulk and trace gas emissions from the engines.
Engineered barrier system	A containment structure designed and constructed to inhibit the migration of landfill leachate and/or gas from operating or closed landfills.
Engineering controls	Operational measures for the management of emissions of LFG.
Exhaust height	The distance above ground level of the engine exhaust (m).
Expected value	Most likely value of a forecast.
Exposure module	Assesses the risk of LFG impacting human health from atmospheric dispersion and lateral migration to on-site workers and the off site residents.
Flare	The equipment used to combust LFG.
Flare capacity	The operational range, the minimum and maximum capacity of the flare.
Flaring	The combustion of methane and gases by burning in an enclosed flare.
Flux	The emissions from an area measured as concentration per unit time.
Gas collection	The removal of gas from a landfill by vertical and horizontal gas wells. This gas is then sent to a flare or engine.
Gas collection efficiency	The percentage of gas that is removed by the gas collection system.
Gas hydraulic conductivity	This is a measure of the ability of a geological unit or engineered barrier to transmit a unit volume of fluid (Gas) through a unit cross sectional area under a unit hydraulic gradient in a unit time. The parameter is a function of both the properties of the fluid and the properties of the geological unit.
Gas plant module	Part of model which includes the specification of the LFG collection and utilisation options for conversion to energy, using spark ignition engines, or flaring.
Gas production curve	A graph of LFG volume (generated or emitted) against time.

Gas viscosity	The resistance of a gas to flow.
GasSim	A more complicated version of GasSimLite, developed for the Environment Agency, designed to allow landfill gas risk assessments. This model is available from Golder Associates. Details are available on www.GasSim.co.uk
Generated gas	The amount of bulk or trace gases that is simulated, this is used as the source term for the rest of the model.
Half-life	The time for the concentrations of a species to decay to 50%. Half-lives are used in GasSimLite to define decay of trace gasses and the cellulose degradation rates.
HCFCs	Hydrochlorofluorocarbons.
HELGA framework	The initial Environment Agency project that produced the majority of the equations that have been coded in GasSimLite, Reference - Gregory RG, Revans AJ, Hill MD, Meadows MP, Paul L and Ferguson CC, (1999), A Framework to Assess the Risks to Human Health and the Environment from Landfill Gas, *Environment Agency Technical Report P271 (CWM 168/98),* ISBN 1 85 705254 4.
Histogram	Chart showing frequency distribution of parameter values on an interval scale.
Hydraulic conductivity	Usually defined for individual geological units and is a measure of the ability of that unit to transmit a unit volume of fluid through a unit cross sectional area under a unit hydraulic gradient in a unit time. The parameter is a function of both the properties of the fluid and the properties of the geological unit. For the purposes of modelling the impact of leachate migration, however, Hydraulic Conductivity is assumed to be the same for both groundwater and leachate. Hydraulic Conductivity has units of length/time (m/s).
Infiltration (net)	The volume of water per unit area which passes into the waste mass. In GasSimLite this parameter includes both effective rainfall and any other source of water which may affect the water balance of the landfill under consideration, for example lateral inflows, leachate re-circulation (and co-disposal of liquids. This parameter has units of length/time (mm/y).
Iteration	A single run of the model, using one randomly selected value for each input parameter and generating a single realisation.

Landfill characteristics	The landfill geometry and cap/liner characteristics
Landfill gas (LFG)	Volatile species produced by the decomposition of waste.
Landfill geometry	The landfill length (north-south) and width (east-west). These are used to calculate the surface area and depth, along with the waste density.
Lateral emissions	The uncontrolled release from the sides of the landfill.
Leachate	Contaminated water generated within a landfill as a consequence of the reaction between decomposing waste materials and infiltration.
Leachate head	The height (head) of leachate above the base of the landfill .
LFG management systems	The processes used to limit the uncontrolled emissions of LFG.
Liner	The engineered medium installed in the base and side of the landfill, primarily to prevent the release of leachate.
Log normal (probability) distribution	A probability distribution defined log to the base 10 of the mean and the standard deviation of the mean.
Log triangular (probability) distribution	A distribution defined by the log to the base 10 of the minimum, most likely and maximum values expected for a given parameter.
Longitudinal dispersivity	See Dispersivity.
Maximum flare capacity	The greatest volume of gas that a flare can use at the defined methane to carbon dioxide ratio.
Mean	An arithmetically derived value calculated by dividing the sum of all of the values by the total number of values. More commonly referred to as the average and may be differentiated from both the mode (most frequent value in a distribution) and the median (central value in a distribution).
Membrane	A synthetic material manufactured and installed in the base of a landfill cell to reduce the rate of leachate and gas egress (and groundwater ingress). Can also be used as a capping system. In GasSimLite, membrane refers only to a synthetic (HDPE type) containment layer
Methanogenic degradation	The decomposition of waste under anaerobic conditions principally to produce carbon dioxide and methane.

Minimum flare capacity	The smallest amount volume of gas that a flare can use at the defined methane to carbon dioxide ratio.
Moisture content	Ratio between the mass of water present in a sample and the dry mass of the solids.
Molar volume of a gas	Molar volume (at STP) (2.241x10-2 m3/mol)
Molecular ratio	The ratio of the Parent to the Daughter Species, based on the molecular weights, i.e. F to HF is 1.05.
Monte Carlo simulation	A system that uses random numbers to repeatedly sample from within a probability distribution to measure the effects of uncertainty.
Normal (probability) distribution	A probability distribution defined by the mean and the standard deviation of the mean.
Operational area	The area of a landfill that is uncapped and/or receives waste.
Operational period	The total number of years for which a landfill site is being filled.
Orifice diameter	The size of the engine exhaust or flare stack.
PAHs	Polyaromatic hydrocarbons
Parameter	A variable, which is used in the calculations performed by GasSimLite.
Parent species	The species destroyed during combustion to generate a daughter species in LFG, i.e. fluoride (F) is destroyed during the combustion process to from hydrogen fluorine (HF).
PI reporting	Information on the Pollution Inventory, release of gases as required by the Environment Agency.
Porosity	Ratio of the volume of voids in a porous geological medium to the volume occupied by matter. Expressed as a fraction.
Pressure	The force applied to a unit area of surface.
Project details	The dialogue box that contains information on the model run along with the initial set up parameters e.g. operational period, project name and number of iterations.

Realisation	The forecast generated by a single iteration of the model.
Residual results	The amount of gas remaining after collected (flared or utilised) gas has been removed.
Simulation	Predictive model of the conditions at a site, which incorporates uncertainty in the input parameter values.
Simulation period	The period for which the modelling will be undertaken.
Single (probability) distribution	A probability distribution defined by an individual value.
Soil cap	Soil which is either placed directly on the waste or on the engineered cap.
Source depletion	The decline of a source as a result of releases or deposition.
Source term	The module used to determine the degradation of waste and thus the generation of LFG, bulk and trace gasses.
Species	Term describing elements, ions or molecules, which may be comprised of a number of different elements and/or ions.
Stack height	The distance above ground level of the flare stack.
Standard deviation	A measure of the spread of a series of values from the arithmetic mean of that series.
Surface emissions	The uncontrolled release of gas for the capped and uncapped area of the landfill.
Temperature	The emissions temperature of the flare stack or engine exhaust.
Time slices	Time series defining points in time, after the commencement of landfilling at which forecasts are made.
Trace gas	Minor species contained within LFG i.e. benzene
Trace gas inventory	The list of trace gases to be simulated.
Triangular (probability) distribution	A probability distribution defined by the minimum, most likely and maximum values expected for a given parameter.
Uncapped area	An open area of the landfill not covered by an engineered cap, but which may be covered daily cover. This area is normally the operational area of the

	landfill in which filling is taking place.
Uniform (probability) distribution	A probability distribution defined by the minimum and maximum values expected for a given parameter.
Utilisation (energy recovery)	The recover of energy from LFG using spark ignition engines.
VOCs	Volatile Organic Compounds
Volume of leachate recirculated	The quantity in m^3 of leachate that is recycled through the waste, normally by removing the leachate from the base of the landfill and reinjecting it near the top.
Waste breakdown	The proportion of different waste streams.
Waste component	The types of material contained within the waste i.e. newspaper, cardboard etc.
Waste composition file	The file containing the information on the waste streams composition.
Waste density	The mass of the waste per unit volume.
Waste deposition	The placement/filling of waste within the landfill.
Waste components	The proportions make up or composition of the waste streams, i.e. the amount of paper, fines. putrescible etc material.
Waste fraction	A group of materials of waste components that decay at a similar rate, i.e. rapidly, moderately or slowly.
Waste hydraulic conductivity	Defined for the waste as a measure of the ability of that unit to transmit a unit volume of fluid through a unit cross sectional area under a unit hydraulic gradient in a unit time. The parameter is a function of both the properties of the fluid and the geological unit.. Hydraulic Conductivity has units of length/time (m/s).
Waste input	The tonnage of waste deposited each year.
Waste moisture content	Ratio between the mass of water present in the waste and the dry mass of the waste solids.
Waste streams	The breakdown of the waste mixture i.e. domestic, commercial, inert etc waste.

Water balance	An assessment of the volume of (water) recharge, storage and discharge within a system.
Water content	Ratio between the mass of water present and the dry mass of the solids.
Year commissioned	The time that an engine or flare is made available.
Year decommissioned	The time that an engine or flare ceases to be available.

8 REFERENCES

Allen, MR, Braithwaite, A, and Hills, CC (1997). Trace organic compounds in landfill gas at seven UK waste disposal sites. Environmental Science & Technology. 31:1054-1061.

Baldwin, G, Scott, P & Cowan, L (1993a). Landfill gas flares, a study of composition and impact of emissions, Part 1. Environmental Safety Centre Harwell, Report to the DoE, AEA-EE-0055.

Baldwin, G, Scott, P, Sopp, C, Hills, KE, Waring, S & Cowan, L (1993b). LFG, a study of composition and impact of emissions, Part 2. Environmental Safety Centre Harwell, Report to the DoE, ref AEA/CS/18300004/030/1.

Balthasar, H.U., Boschi, R.A.A., and Menke, M.M., 1978. Calling the shots in R&D. Harvard Business Review, May-June.

Barlaz, M.A., Schaefer D.M. and Ham R.K. (1989) Mass balance analysis of decomposed refuse in laboratory scale lysimeters. ASCE Journal of Environmental Engineering, 115(6): 1088-1102

Borjesson G, Galle B, Samuelsson J and Svensson BH (2000). Methane emissions from landfills: options for measurement and control. In: Proceedings of the Waste 2000 Conference – Waste management at the dawn of the third millennium. 2 – 4 October 2000, Stratford-upon-Avon, Warwickshire. pp31 – 40. ISBN 0 9539301 0 6.

Brown KA, Smith A, Burnley SJ, Campbell DJV, King K and Milton MJT (1999) Methane emissions from UK landfills. Final report for The Department of the Environment, Transport and the Regions. Report AEAT-5217.

California State Air Resources Board (1986a). Evaluation test on a landfill gas flare at the Los Angeles County Sanitation District's Puente hills landfill facility. ARB-SS-87-06m (PB-87-204764).

California State Air Resources Board (1986b). Evaluation test on a landfill gas flare at the BKK landfill facility, West Covina, California. ARB-SS-87-09m (PB-87-204756).

Derwent, R.G., Jenkin, M.E., and Sanders, S.M., (1996) Photochemical ozone creation potential for a large number of reactive hydrocarbons under European conditions. Atmospheric Environment. 30 (2); 181-199

Emberton, JR and Scott, PE (1987). The use of cover materials to attenuate landfill gas odour at Ugley landfill, Essex. II. Field trials. First year monitoring. AERE Harwell Research Report no AERE R12346.

Environment Agency (1998) Annual released to air and water, Inventory of Sources and Releases – Guidance Note.

Environment Agency (2001a). Landfill Methane Surface Emissions. Measurement Procedures and Protocols. October 2001 (draft).

Environment Agency, (2001b), “LandSim, Landfill Performance Simulation by Monte Carlo Simulation”, Environment Agency R&D Publication 120.

Farquhar G.J and Rovers F.A (1973) Gas production during refuse decomposition. Water, Air and Soil Pollution, 2: 483-493

Ferguson, C.C., Krylov, V.V., and McGrath, P.T., (1995) Contamination of Indoor Air by Toxic Soil Vapours: a Screening Risk assessment Model, *Building and Environment*, Vol. 30, No. 3, pp 375-383.

Genstat 5 Committee. (1993). G*enstat 5 Release 3 Reference Manual*. Oxford : Clarendon Press.

Gregory, R. G., Revans, A. J., Hill, M. D., Meadows, M. P., Paul, L. and Ferguson, C. C., 1999, “A framework to assess the risks to human health and the environment from landfill gas”, Environment Agency Technical Report P271, under contract CWM 168/98.

Hoeks J and Oosthoek J (1981) Gaswinning uit afvalstortterreinen. Gas, 101.

Intergovernmental Panel on Climate Change (1996a). Revised 1996 IPCC Guidelines for National Greenhouse Gas Inventories: Reference Manual, Chapter 6.

Intergovernmental Panel on Climate Change, 1996a. “Revised 1996 IPCC Guidelines for National Greenhouse Gas Inventories: Reference Manual, Chapter 6”.

Intergovernmental Panel on Climate Change, 1996b. “IPCC Expert Group on Waste, Topical Workshop on Carbon Conversion and Methane Oxidation in Solid Waste Disposal Sites”, Argonne National Laboratory, Chicago, USA, 25 October 1996.

Jones, DL, Crowcroft, P, and Pritchard, BN (1988). Design of a motorway service station on a landfill site. 11th GRCDA Landfill Gas Symposium, USA. 14pp.

Kabus, I., 1976. You can bank on uncertainty. Harvard Business Review, May-June.

Karickhoff S.W. 1981 Semi-Empirical Estimation of Sorption of Hydrophobic Pollutants on Natural Sediments and Soils *Chemosphere* **10** 833-846

Knox, K (1990). Assessment of landfill gas potential using leachate and gas analyses. Environment Agency Technical Report (CWM 019/90), 1990.

LQM (2002). Landfill Gas Engine Exhaust and Flare Emissions project for the Biogas Association and EB Nationwide. Land Quality Management Limited, Client Project Reference No. M0468.

Millican, R (1995). Communications from SCAQMD, California, 29 June.

Sander, W.E., 1969. The value of subjective forecasts by R&D project managers. IEEE Transactions on Engineering Management, pp35-43.

Scott, PE, Baldwin, G, Checkley, C and Hemsworth, J (1988). The composition of landfill gas and emission from a landfill flare. Report to Department of the Environment, Harwell.

Scott, PE, Dent, CG and Baldwin, G (1988). The composition and environmental impact of household waste derived landfill gas: second report. Waste Research Unit, AERE Harwell, report. AERE G4436. Environment Agency report no. CWM 041/88.

Spetzler, C.S. & von Holstein, C.S., 1975. Probability encoding in decision analysis. Management Science 22,3, 340-358.

Stoddart, J., Zhu, M., Staines, J., Rothery, E., and Lewicki, R., (1999). Experience with halogenated hydrocarbons removal from landfill gas. Proceedings of Sardinia 99, Seventh International Waste Management and Landfill Symposium. S. Margherita di Pula, Cagliari, Italy; 4-8 October 1998.

Tversky, A. & Kahneman, D. 1973, p15. Judgement under uncertainty: heuristics and biases. Science 185, 1124-1131.

US EPA (1998). Compilation of air pollutant emission factors. AP-42, 5th edition, volume 1. Chapter 2, Solid Waste Disposal, 2.4 MSW Landfills.

Valis E., (2000) Waste Industry Air Coalition personal communication

Young, PJ and Parker, A (1983). The identification and possible environmental impact of trace gases and vapours in landfill gas. Waste Management and Research, Vol I: 213-226.

Zanten B van and Scheepers M J J (1996) Modelling of landfill gas potentials. Working paper International Energy Agency Activity.