GASSIM V1.02

Contents

Summary of changes since V1.01

A) Additional error checking of data entered into the source module. If you include a waste type for any specific year for which there is not a waste breakdown description you are warned as you exit the Source window.

B) Ability to plot multiple outputs on the same graph. The model now allows up to 3 different outputs from the results menu to be plotted on the same graph provided the units are compatible. For example it is possible to plot landfill gas generation, engine emissions of carbon dioxide and flare emissions of carbon dioxide on the same graph (see Figure 1). Users need to decide which percentile to plot and which outputs to select. It is not possible to select two outputs with differing units such as bulk gas generation (m^3/h) and trace gas output (g/h).

C) Co-incident with this release, a new and updated version of the trace.dat file has been released. This pulls together more recent information on the composition of landfill gas, flare and engine emissions. It remains important that users update the composition data of their models with site specific data rather than relying solely on this default data.

D) A bug in the Global Impact module that reported incorrect results for the "sum of all years" the first time the results window was opened has now been repaired.

E) A bug in the Human Health Exposure module that gave incorrect exposure results for the first use of Commercial Land Use if residential land use had not been previously run has been corrected.

F) A bug in the atmospheric dispersion module which used trace gas generation rate data rather than surface emission rate data as the input to the dispersion model has been fixed.

ADDITIONS TO THE USER MANUAL FOR VERSION 1.02

Additional Error Checking within the Source Model

The model allows a very flexible definition of the gas source term. However comments received from users has highlighted the fact that it is easy to define waste types within the waste "Breakdown" part of the source window and then overlook that the composition of these wastes have not been defined within the composition editor. The impact of not defining the waste within the composition editor is that the model then assumes that the undefined waste portion is inert (thus underestimating the gas generation).

For this reason, additional error checking has been added to the model to ensure that if waste types have been activated within the waste breakdown input column, then corresponding composition data exists for each year that waste composition is defined. If no such definition is found then warning messages are generated for each waste type and for each year that there is no definition. These warnings will not stop the running of the model, but users are urged to deal with the warning issues prior to running the model if you intend to rely upon the results.

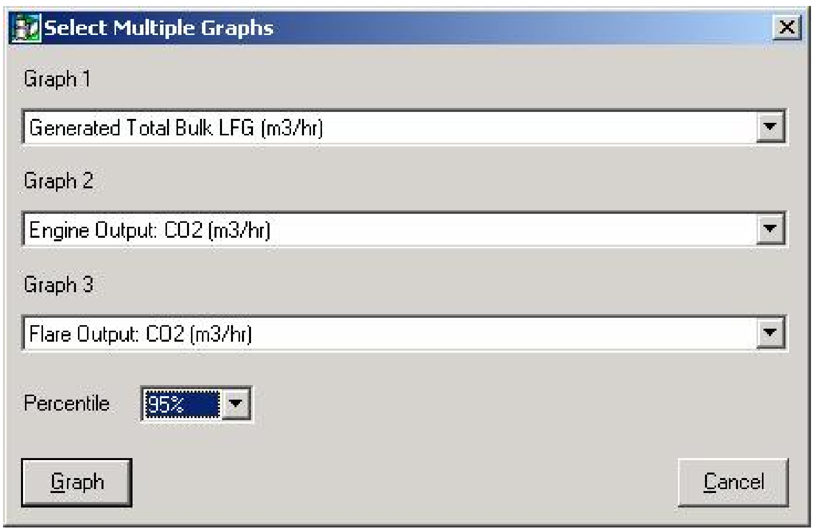
In order to check existing models developed in version 1.01 or earlier releases, you will need to open the model, open the source window then close the source window. The error checking is activated as the source window is closed.

An example of the warning message is shown below.

Plotting Multiple Graphs

Version 1.02 of GasSim will allow up to three outputs of the gas generation and emissions modules to be plotted on the same graph. There is a restriction that the selection should have the same units and users must specify a percentile to plot. This option is available under the Results menu item and is called Multiple Graphs.

Selecting two or more outputs with different units will generate a warning message but a



graph will still be generated as the units being plotted will not be applicable to all of the outputs. It is not necessary to plot three outputs - plotting just two is a valid option.

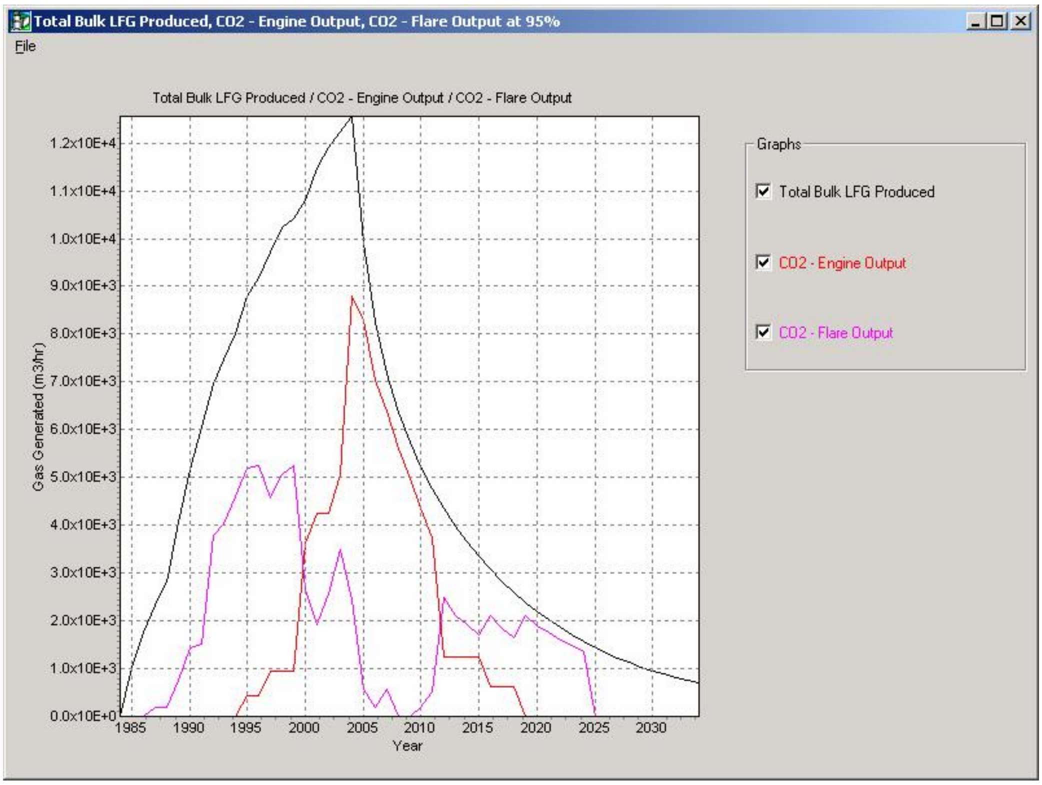


Figure 1: Multiple Output Plot

Trace.dat file

The "trace.dat" file has been comprehensively updated to reflect the availability of new data on landfill gas trace component concentrations and combustion plant emissions data. Environment Agency R&D Project P1-438/TR entitled Investigation of the Composition and Emission of Trace Components in Landfill Gas (2002a) has been used to update the default trace gas composition.

Furthermore, details of trace component compositions of engine and flare emissions have become available recently (Haigh et al 2002, Leonard et al 2002, IDGTE, 2003, Environment Agency, 2003) and these data have also allowed the updating of default data within the model. As a result the following tables have been updated.

Risk assessors should note that the data in the following tables relate to all landfill types and the forecast of emissions may not be representative of emissions from a particular landfill. Furthermore, the data in the tables are for current combustion plant, with the emissions normalised to standard reporting conditions in the Environment Agency's draft guidelines (2002b,c). It is recommended that a site specific approach is adopted for any risk assessment which is carried out.

Table 5.4: Trace Gas Default Values for General Components of Raw LFG (mg/m^3) ***(note that this replaces Table 5.4 in the manual)***

Species	Distribution and Values
1,1,1,2-Tetrafluorochloroethane	LOGTRIANGULAR(2e-3, 0.2, 2)
1,1,1-Trichlorotrifluoroethane	LOGTRIANGULAR(5e-3, 0.4, 8)
1,1,2-Trichloroethane	LOGTRIANGULAR(4e-3, 1, 10)
1,1-Dichloroethane	LOGTRIANGULAR(1e-3, 0.1, 61800)
1,1-Dichloroethene	LOGTRIANGULAR(1e-3, 0.01, 1516)
1,1-Dichlorotetrafluoroethane	LOGTRIANGULAR(0.05, 0.25, 6.4)
1,2-Dichlorotetrafluoroethane	LOGTRIANGULAR(0.01, 9.8, 300)
1-Chloro-1,1-difluoroethane	LOGTRIANGULAR(0.04, 0.57, 31)
2-Chloro-1,1,1-trifluoroethane	LOGUNIFORM(0.05, 1.5)

2-Propanol	LOGTRIANGULAR(5e-3, 2, 34)
Acetaldehyde (ethanal)	LOGTRIANGULAR(0.1,0.2, 52)
Acetone	LOGTRIANGULAR(5e-3, 0.1, 50)
Acrylonitrile	LOGTRIANGULAR(0.02, 0.4, 38)
Benzene	LOGTRIANGULAR(0.001, 0.1, 114)
Benzo(a)pyrene	UNIFORM(2e-6, 6e-6)
Butadiene (modelled as 1,3-Butadiene)	LOGTRIANGULAR(0.05, 1.45, 6)
Butane	LOGTRIANGULAR(0.19, 1.0, 709)
Butene isomers	LOGTRIANGULAR(0.001, 0.2, 1.8)
Carbon disulphide	LOGTRIANGULAR(0.01, 0.1,11)
Carbon monoxide	LOGTRIANGULAR(0.11, 1.1, 5000)
Carbon tetrachloride (tetrachloromethane)	LOGTRIANGULAR(2e-4, 0.2, 152)
Carbonyl sulphide	LOGTRIANGULAR(6e-3, 0.2, 4.4)
Chlorobenzene	LOGTRIANGULAR(2e-3, 0.01, 7466)
Chlorodifluoromethane	LOGTRIANGULAR(5e-3, 0.1, 9900)
Chloroethane	LOGTRIANGULAR(1e-3, 0.01, 6146)
Chlorofluorocarbons (CFCs) (Total)	LOGTRIANGULAR(0.06, 102.3, 1230)
Chlorofluoromethane	LOGTRIANGULAR(8e-3, 0.2, 110)
Chloroform (trichloromethane)	LOGTRIANGULAR(1e-3, 0.2, 70)
Chlorotrifluoromethane	LOGTRIANGULAR(0.1, 0.2, 49)
Dichlorodifluoromethane	LOGTRIANGULAR(0.01, 9, 790)
Dichlorofluoromethane	LOGTRIANGULAR(1e-3, 0.01, 602)
Dichloromethane (methylene chloride)	LOGTRIANGULAR(1e-3, 0.02, 1524)
Diethyl disulphide	LOGTRIANGULAR(1e-3, 0.02, 2.6)
Dimethyl disulphide	LOGTRIANGULAR(1e-3, 0.02, 40)
Dimethyl sulphide	LOGTRIANGULAR(1e-3, 0.01, 60)
Ethane	LOGTRIANGULAR(5e-3, 6.25, 200)
Ethanethiol (ethyl mercaptan)	LOGTRIANGULAR(0.01, 0.01, 41.9)
Ethanol	LOGTRIANGULAR(5e-3, 0.2, 810)
Ethyl toluene (all isomers)	LOGTRIANGULAR(1e-3, 0.01, 8.3)
Ethylbenzene	LOGTRIANGULAR(1e-3,1e-3, 875)
Ethylene	UNIFORM(0.2,5.8)
Ethylene dichloride	LOGTRIANGULAR(6e-3, 0.01, 1820)
Fluorotrichloromethane	LOGTRIANGULAR(1e-3, 0.01, 1000)
Formaldehyde (methanal)	LOGTRIANGULAR(0.2, 0.2, 52)
Freon 113	LOGTRIANGULAR(0.013, 4.8, 125)
Hexane	LOGTRIANGULAR(1e-3, 9.6, 44)
Hydrochlorofluorocarbons (HCFCs) (Total)	LOGTRIANGULAR(0.02, 128.8, 916.2)
Hydrogen sulphide	LOGTRIANGULAR(5.7e-4, 2.4, 5570)
Limonene	LOGTRIANGULAR(1e-3, 0.1, 240)
Methanethiol (methyl mercaptan)	LOGTRIANGULAR(5e-3, 0.01, 87)
Methyl chloride (chloromethane)	LOGTRIANGULAR(6e-3, 0.2, 10)
Methyl chloroform (1,1,1-Trichloroethane)	LOGTRIANGULAR(1e-3, 180, 1600)

Methyl ethyl ketone (2-butanone)	LOGTRIANGULAR(5e-3, 5e-3, 73)
Methyl isobutyl ketone	LOGTRIANGULAR(5e-3, 0.2, 9.9)
Odour Units (Predicted)	TRIANGULAR(50000, 125000, 250000)
PAH (reported as Naphthalene)	LOGTRIANGULAR(1e-3, 0.2, 17)
para-Dichlorobenzene (modelled as 1,4-Dichlorobenzene)	LOGTRIANGULAR(6e-3, 0.05, 2.7)
Pentane	LOGTRIANGULAR (0.02, 0.3, 105)
Pentene (all isomers)	LOGTRIANGULAR(1e-3, 0.2, 11)
Propane	LOGTRIANGULAR (1e-3, 1.9, 12.9)
Propanethiol	LOGTRIANGULAR(0.2, 0.2, 2.1)
Sulphide, total simulations with H2S	LOGTRIANGULAR(1e-3,2.4,5575)
Sulphide, total simulations without H2S	LOGTRIANGULAR(5e-4,8e-3,3.5)
Sulphur reduced (reported as SO2)	LOGUNIFORM(30.8, 430.5)
t-1,2-Dichloroethene	LOGTRIANGULAR (6e-3, 1.0, 41)
Tetrachloroethane (modelled as 1,1,2,2-Tetrachloroethane)	LOGUNIFORM(1e-3, 50)
Tetrachloroethylene (Tetrachloroethene)	LOGTRIANGULAR(1e-3, 0.01, 7700)
Toluene	LOGTRIANGULAR(0.01, 0.1, 1250)
Total chloride (reported as HCl)	LOGTRIANGULAR(14.7, 79.5, 850)
Total fluoride (reported as HF)	LOGTRIANGULAR(5.6, 251.2, 735)
Total non-methane volatile organic compounds (NMVOCs)	LOGUNIFORM(0.05,1473)
Trichlorobenzene (all isomers)	LOGTRIANGULAR(0.01, 0.01, 0.13)
Trichloroethylene (trichloroethene)	LOGTRIANGULAR(0.01, 2.0, 608)
Trichlorofluoromethane	LOGTRIANGULAR(1e-3, 0.01, 1000)
Trichlorotrifluoroethane	LOGTRIANGULAR(1e-3, 4.8, 24)
Trimethylbenzene (all isomers)	LOGTRIANGULAR(1e-3, 0.01, 187)
Vinyl chloride (chloroethene, chloroethylene)	LOGTRIANGULAR(1e-3, 0.01, 7660)
Xylene (all isomers)	LOGTRIANGULAR(1e-3, 1e-3, 61784)

Table 5.5: Trace Gas Default Inputs for Odorous Components of LFG (mg/m^3) ***(note that this replaces Table 5.5 in the manual)***

Species	**Distribution and Values**
Carbon disulphide	LOGTRIANGULAR(0.01, 0.1, 11)
Diethyl disulphide	LOGTRIANGULAR(1e-3, 0.02, 2.6)
Dimethyl disulphide	LOGTRIANGULAR(1e-3, 0.02, 40)
Dimethyl sulphide	LOGTRIANGULAR(1e-3, 0.01, 60)
Ethanethiol (ethyl mercaptan)	LOGTRIANGULAR(0.01, 0.01, 41.9)
Hydrogen sulphide	LOGTRIANGULAR(5.7e-4, 2.4, 5570)
Limonene	LOGTRIANGULAR(1e-3, 0.1, 240)
Methanethiol (methyl mercaptan)	LOGTRIANGULAR(5e-3, 0.01, 87)
Propanethiol	LOGTRIANGULAR(0.2, 0.2, 2.1)
Sulphide, total simulations with H2S	LOGTRIANGULAR(1e-3,2.4,5575)
Sulphide, total simulations without H2S	LOGTRIANGULAR(5e-4,8e-3,3.5)

Toluene	LOGTRIANGULAR(0.01, 0.1, 1250)
Xylene (all isomers)	LOGTRIANGULAR(1e-3, 1e-3, 61784)
Odour Units (Predicted)	TRIANGULAR(50000, 125000, 250000)

Table 5.6: Trace Gas Default Inputs for Global Impact Species of LFG(mg/m^3) ***(note that this replaces Table 5.6 in the manual)***

Species	Distribution and Values
Chlorofluorocarbons (CFCs) (Total)	LOGTRIANGULAR(0.06, 102.3, 1230)
1-Chloro-1,1-difluoroethane	LOGTRIANGULAR(0.04, 0.57, 31)
Chlorodifluoromethane	LOGTRIANGULAR(5e-3, 0.1, 9900)
Chlorofluoromethane	LOGTRIANGULAR(8e-3, 0.2, 110)
2-Chloro-1,1,1-trifluoroethane	LOGUNIFORM(0.02, 1.5)
Chlorotrifluoromethane	LOGTRIANGULAR(0.1, 0.2, 49)
Dichlorodifluoromethane	LOGTRIANGULAR(0.01, 9, 790)
Dichlorofluoromethane	LOGTRIANGULAR(1e-3, 0.01, 602)
1,1-Dichlorotetrafluoroethane	LOGTRIANGULAR(0.05, 0.25, 6.4)
1,2-Dichlorotetrafluoroethane	LOGTRIANGULAR(0.01, 9.8, 300)
Hydrochlorofluorocarbons (HCFCs) (Total)	LOGTRIANGULAR(0.02, 128.8, 916.2)
1,1,1,2 Tetrafluoro chloroethane	LOGTRIANGULAR(2e-3, 0.2, 2)
Trichlorofluoromethane	LOGTRIANGULAR(1e-3, 0.01, 1000)
Trichlorotrifluoroethane	LOGTRIANGULAR(1e-3, 4.8, 24)

Table 5.14: Trace Gas Emissions for Flares (mg/m^3) ***(note that this replaces Table 5.14 in the manual)***

Species	Distribution and Values
Dioxins and furans (modelled as 2,3,7,8-TCDD)	LOGTRIANGULAR (9e-9, 3.1e-8, 3.6e-7)
Total fluoride (reported as HF)	LOGTRIANGULAR (0.4, 2.5, 33)
Total non-methane volatile organic compounds (NMVOCs)	LOGUNIFORM(1,30)
Carbon monoxide	LOGUNIFORM (8, 2450)
Total chloride (reported as HCl)	LOGUNIFORM (1,110)
Nitrogen oxides	TRIANGULAR(27,80,170)
Sulphur reduced (reported as SO2)	LOGUNIFORM(18, 482)
Benzo(a)pyrene	LOGUNIFORM(1e-6,6e-4)
PM10s	UNIFORM(1,10)

Table 5.15: Trace Gas Emissions for Engines (mg/m^3) ***(note that this replaces Table 5.15 in the manual)***

Species	**Distribution and Values**
Dioxins and furans (modelled as 2,3,7,8-TCDD)	LOGTRIANGULAR (2e-10, 8.8e-9, 2.3e-6)
Total fluoride (reported as HF)	LOGTRIANGULAR (0.18, 7, 45)
Total non-methane volatile organic compounds (NMVOCs)	LOGTRIANGULAR(0.01, 4.5, 225)
Carbon monoxide	TRIANGULAR(180, 1660, 2770)
Total chloride (reported as HCl)	LOGTRIANGULAR (0.015, 10, 710)
Nitrogen oxides	LOGTRIANGULAR (130, 525,2132)
Sulphur reduced (reported as SO2)	LOGTRIANGULAR (1,112,540)
Benzo(a)pyrene	LOGUNIFORM (1.1e-6, 0.09)
PM10s	LOGTRIANGULAR (1, 9.3, 38)

Erratum

Equation 6.78 is shown in the manual in the form

$$V_s \qquad \frac{k}{\;} \; P_2 \quad P_1 \; d$$

This should be

$$V_s \qquad \frac{k}{\;} \; P_2 \quad P_1 \; /d \qquad 6.78$$

The model code remains correct.

Additional References

Haigh C, Cope D and Deed C. 2002, Development of Monitoring Protocols for Stack Emissions from Landfill Gas Utilisation Systems. In: Waste 2002. Integrated Waste Management and Pollution Control, Research, Policy and Practice. Stratford-upon-Avon, 24-26 September 2002, pp 375-385.

Environment Agency 2002a. Investigation of the Composition and Emission of Trace Components in Landfill Gas Project P1-438/TR

John Blowes IDGTE 2003 provision of monitoring data from Engine Emissions 2003

Pers Comm Chris Deed Environment Agency - provision of speciated PAH data for engine emissions 2003

Environment Agency 2002b. Guidelines for the monitoring of landfill gas engine emissions. Draft for consultation, December 2002

Environment Agency 2002c. Guidelines for the monitoring of enclosed landfill gas flares. Draft for consultation, December 2002

Leonard A, Dollard, G and Deed, C. Development of monitoring protocols for stack emissions from landfill flares. In: Waste 2002, pp 397-408