

SUPPLEMENT 1: GasSim Lite Release Version 1.54.2

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1. REVISIONS TO GASSIM Lite

This supplement to the GasSim manual covers revisions to the model in release version 1.54.2. The previous version available from the GasSim web site was 1.53.3. Interim versions were internal test versions trialled before releasing this latest version. Revisions are associated with changes to the PI Reporting screen.

PI Reporting Changes

The PI Reporting screen has been improved in several ways. The list of the species has been changed to more closely match that expected for current PI Reporting. A new column has been added containing the CAS number of the species. Gases not modelled now have a reported value of 'n/a' rather than 'Not Modelled'. Figures can now be copied from the grid and a new 'Copy' button copies the entire grid to the clipboard so that it can subsequently be pasted into a spreadsheet. The grid now resizes when the form is resized by the user.

Gas	CAS	Reporting Threshold	Value to Report	(25%)	(75%)
Inorganics					
Ammonia	7664-41-7	1,000.00 kg	n/a		
Asbestos	1332-21-4	1.00 kg	n/a		
Carbon Dioxide - 'chemical'	124-38-9	10,000,000.00 kg	2,310.00 t	2,130.00 t	2,490.00 t
Carbon Dioxide - 'thermal'	124-38-9	10,000,000.00 kg	13,100.00 t	12,600.00 t	13,400.00 t
Carbon disulphide	75-15-0	1,000.00 kg	326.00 g	178.00 g	890.00 g
Carbon monoxide	630-08-0	100,000.00 kg	82.50 t	62.30 t	104.00 t
Hydrogen chloride	7647-01-0	10,000.00 kg	318.00 kg	51.20 kg	1.55 t
Hydrogen cyanide	74-90-8	100.00 kg	n/a		
Nitrous oxide	10024-97-2	10,000.00 kg	n/a		
Phosgene	75-44-5	10.00 kg	n/a		
Sulphur hexafluoride	2551-62-4	10.00 kg	n/a		
Organics					
Acetaldehyde (Ethanal)	75-07-0	100.00 kg	2.14 kg	962.00 g	6.87 kg
Acrolein	107-02-8	10.00 kg	n/a		
Acrylamide [2-Propenamide]	79-06-1	10.00 kg	n/a		
Acrylonitrile [2-Propenenitrile]	107-131	1,000.00 kg	1.17 kg	597.00 g	3.89 kg
Aldrin	309-00-2	1.00 kg	n/a		
Allyl alcohol [2-Propen-1-ol]	107-18-6	10.00 kg	n/a		
Amitrole [3-Amino-1,2,4-triazole]	61-82-5	1.00 kg	n/a		
Aniline [Benzeneamine]	62-53-3	10.00 kg	n/a		
Anthracene	120-12-7	10.00 kg	n/a		
Benzene	71-43-2	1,000.00 kg	643.00 g	188.00 g	2.33 kg
Benzo(a)pyrene	50-32-8	1.00 kg	26.50 g	1.95 g	390.00 g
Benzo(b)fluoranthene	205-99-2	1.00 kg	n/a		
Benzo(g,h,i)perylene	191-24-2	1.00 kg	n/a		
Benzo(k)fluoranthene	207-08-9	1.00 kg	n/a		
Benzo butyl phthalate (BBP)	85-68-7	10.00 kg	n/a		
Benzyl chloride	100-44-7	10.00 kg	32.00 kg	3.59 kg	210.00 kg
Bromoethene	593-60-2	10.00 kg	n/a		
Butadiene [1,3-Butadiene]	106-99-0	100.00 kg	1.45 kg	810.00 g	2.48 kg
Butene - all isomers	-	1,000.00 kg	152.00 g	67.00 g	365.00 g
Carbon tetrachloride [Tetrachloromethane]	56-23-5	10.00 kg	600.00 g	153.00 g	2.60 kg

The printing has been altered to reflect the changes to the grid.

The current list of PI gases, their associated CAS numbers and the reporting thresholds are provided in Table 1, below.

Table 1: PI Reporting Thresholds

Gas	CAS	Threshold
Inorganics		
Ammonia	7664-41-7	1.00 t
Asbestos	1332-21-4	1.00 kg
Carbon Dioxide	124-38-9	10,000.00 t

Carbon disulphide	75-15-0	1.00 t
Carbon monoxide	630-08-0	100.00 t
Hydrogen chloride	7647-01-0	10.00 t
Hydrogen cyanide	74-90-8	100.00 kg
Nitrous oxide	10024-97-2	10.00 t
Phosgene	75-44-5	10.00 kg
Sulphur hexafluoride	2551-62-4	10.00 kg
Organics		
Acetaldehyde [Ethanal]	75-07-0	100.00 kg
Acrolein	107-02-8	10.00 kg
Acrylamide [2-Propenamide]	79-06-1	10.00 kg
Acrylonitrile [2-Propenenitrile]	107-13-1	1.00 t
Aldrin	309-00-2	1.00 kg
Allyl alcohol [2-Propen-1-ol]	107-18-6	10.00 kg
Amitrole [3-Amino-1,2,4-triazole]	61-82-5	1.00 kg
Aniline [Benzeneamine]	62-53-3	10.00 kg
Anthracene	120-12-7	10.00 kg
Benzene	71-43-2	1.00 t
Benzo(a)pyrene	50-32-8	1.00 kg
Benzo(b)fluoranthene	205-99-2	1.00 kg
Benzo(g,h,i)perylene	191-24-2	1.00 kg
Benzo(k)fluoranthene	207-08-9	1.00 kg
Benzo butyl phthalate (BBP)	85-68-7	10.00 kg
Benzyl chloride	100-44-7	10.00 kg
Bromoethene	593-60-2	10.00 kg
Butadiene [1,3-Butadiene]	106-99-0	100.00 kg
Butene - all isomers	-	1.00 t
Carbon tetrachloride [Tetrachloromethane]	56-23-5	10.00 kg
Chlordane	57-74-9	1.00 kg
Chlordecone	143-50-0	1.00 kg
Chloroethane	75-00-3	10.00 kg
Chloroform [Trichloromethane]	67-66-3	100.00 kg
Chloroprene	126-99-8	10.00 kg
Chrysene	218-01-9	10.00 kg
Crotonaldehyde	4170-30-3	10.00 kg
Cumene hydroperoxide	80-15-9	10.00 kg
Dibutyl phthalate	84-74-2	10.00 kg
p-Dichlorobenzene [1,4-Dichlorobenzene]	106-46-7	1.00 kg
Dichlorodiphenyltrichloroethane (DDT)	50-29-3	1.00 kg
Dichloromethane (DCM) [Methylene chloride]	75-09-2	1.00 t
Dieldrin	60-57-1	1.00 kg
Diethyl aniline [N,N-Diethyl benzeneamine]	91-66-7	10.00 kg
Di(2-ethylhexyl)phthalate (DEHP)	117-81-7	10.00 kg
Diethyl ether	60-29-7	10.00 kg
Diisopropyl ether	108-20-3	10.00 kg
Dimethylaniline [N,N-Dimethyl benzeneamine]	121-69-7	10.00 kg
Dimethyl sulphate	77-78-1	1.00 kg
Dimethylformamide	68-12-2	1.00 t
Dimethyl-o-toluidine	609-72-3	10.00 kg
Dimethyl-p-toluidine	99-97-8	10.00 kg
Dioxane	123-91-1	10.00 kg
Diphenylamine	122-39-4	10.00 kg
Endrin	72-20-8	1.00 kg
2-Ethoxyethanol [Ethyleneglycol ethylether]	110-80-5	10.00 kg
2-Ethoxyethyl acetate [Ethyleneglycol ethylether acetate]	111-15-9	1.00 kg

Ethyl acrylate	140-88-5	10.00 kg
Ethyl benzene	100-41-4	100.00 kg
Ethyl bromide [Bromoethane]	74-96-4	10.00 kg
1-Ethyl-3,5-dimethylbenzene	934-74-7	10.00 kg
Ethylene [Ethene]	74-85-1	1.00 t
Ethylene dichloride [1,2-Dichloroethane]	107-06-2	1.00 t
Ethylene oxide [1,2-Epoxyethane]	75-21-8	1.00 t
Ethyl toluene - all isomers	25550-14-5	10.00 kg
Fluoranthene	206-44-0	1.00 kg
Formaldehyde [Methanol]	50-00-0	10.00 kg
Heptachlor	76-44-8	1.00 kg
Hexabromobiphenyl	36355-1-8	100.00 g
Hexabromocyclododecane	25637-99-4	10.00 kg
Hexachlorobenzene	118-74-1	1.00 kg
Hexachlorocyclohexane - all isomers	608-73-1	1.00 kg
Hexane	110-54-3	10.00 kg
1-Hexene	592-41-6	10.00 kg
Indeno(1,2,3-cd)pyrene	193-39-5	1.00 kg
Iodomethane	74-88-4	10.00 kg
Isophorone	78-59-1	10.00 kg
Isophorone diisocyanate	4098-71-9	1.00 kg
Isoprene	78-79-5	10.00 kg
Lindane	58-89-9	1.00 kg
Maleic anhydride	108-31-6	10.00 kg
Methane	74-82-8	10.00 t
Methanol	67-56-1	100.00 kg
2-(Methoxyethoxy)ethanol	111-77-3	10.00 kg
2-Methoxyethanol	109-86-4	10.00 kg
2-Methoxyethyl acetate	110-49-6	10.00 kg
Methyl bromide [Bromomethane]	74-83-9	100.00 kg
2-Methyl-2-butene	513-35-9	10.00 kg
3-Methyl-1-butene	563-45-1	100.00 kg
Methyl chloride [Chloromethane]	74-87-3	1.00 t
Methyl chloroform [1,1,1-Trichloroethane]	71-55-6	10.00 kg
4,4'-Methylene-bis(2-chloroaniline)	101-14-4	1.00 kg
4,4'-Methylene dianiline	101-77-9	10.00 kg
4,4'-Methylenediphenyl diisocyanate	101-68-8	1.00 kg
Methyl isocyanate	624-83-9	1.00 kg
Mirex	2385-85-5	1.00 kg
Naphthalene	91-20-3	100.00 kg
Nitrobenzene	98-95-3	10.00 kg
2-Nitropropane	79-46-9	1.00 kg
Pentachlorobenzene	608-93-5	1.00 kg
Pentachlorophenol	87-86-5	1.00 kg
Pentane	109-66-0	100.00 kg
Pentene - all isomers	25377-72-4	1.00 t
Phenol	108-95-2	10.00 kg
Propylbenzene	103-65-1	10.00 kg
Propylene	115-07-1	10.00 t
Propylene oxide	75-56-9	100.00 kg
Styrene	100-42-5	100.00 kg
Tetrachloroethane [1,1,2,2-Tetrachloroethane]	79-34-5	10.00 kg
Tetrachloroethylene	127-18-4	100.00 kg
Tetrafluoroethylene	116-14-3	10.00 kg
Toluene	108-88-3	100.00 kg
Toluene diisocyanate - all isomers	-	10.00 kg

Toxaphene	8001-35-2	1.00 kg
Trichlorobenzene - all isomers	12002-48-1	1.00 kg
Trichloroethylene	79-01-6	1.00 t
Trichlorotoluene	98-07-7	10.00 kg
Trimellitic anhydride	552-30-7	1.00 kg
Trimethylbenzene - all isomers	25551-13-7	10.00 kg
Vinyl acetate	108-05-4	10.00 kg
Vinyl chloride	75-01-4	1.00 t
Xylene - all isomers	1330-20-7	1.00 t
Metals and compounds		
Antimony	7440-36-0	1.00 kg
Arsenic	7440-38-2	1.00 kg
Beryllium	7440-41-7	1.00 kg
Boron	7440-42-8	1.00 t
Cadmium	7440-43-9	1.00 kg
Chromium	7440-47-3	10.00 kg
Copper	7440-50-8	10.00 kg
Lead	7439-92-1	100.00 kg
Manganese	7439-96-5	10.00 kg
Mercury	7439-97-6	1.00 kg
Nickel	7440-02-0	10.00 kg
Selenium	7782-49-2	100.00 kg
Vanadium	7440-62-2	10.00 kg
Zinc	7440-66-6	100.00 kg
Other substances		
Brominated diphenylethers - penta, octa and deca	-	10.00 kg
Chlorine and total inorganic compounds - as HCl	7782-50-5	10.00 t
Chlorofluorocarbons (CFCs)	EDF-079	1.00 kg
Dioxins and furans (PCDDs/PCDFs) - I-TEQ	-	0.01 g
Dioxins and furans (PCDDs/PCDFs) - WHO-TEQ	-	0.01 g
Fluorine and total inorganic compounds - as HF	7782-41-4	1.00 t
Halons	-	1.00 kg
Hydrobromofluorocarbons (HBFCs)	-	10.00 kg
Hydrochlorofluorocarbons (HCFCs)	-	1.00 kg
Hydrofluorocarbons (HFCs)	-	100.00 kg
Nitrogen oxides - NO and NO ₂ as NO ₂	-	100.00 t
Non-methane volatile organic compounds (NMVOCs)	-	10.00 t
Particulate matter - PM _{2.5}	-	1.00 t
Particulate Matter - PM ₁₀	-	1.00 t
Particulate Matter - total	-	10.00 t
Perfluorocarbons (PFCs)	-	10.00 kg
Polychlorinated biphenyls (PCBs)	1336-36-3	100.00 g
Polychlorinated Biphenyls (PCBs) - as WHO TEQ	1336-36-3	0.01 g
Sulphur oxides - SO ₂ and SO ₃ as SO ₂	-	100.00 t