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Soil Guideline Values for xylene in soil

Science Report SC050021 / xylene SGV

This technical note is one in a series that describe Soil Guideline Values (SGVs) for individual, or groups of similar, chemicals to assist in the assessment of risks from land contamination.

SGVs are an example of generic assessment criteria (Defra and Environment Agency, 2004) and can be used in the preliminary evaluation of the risk to human health from long-term exposure to chemicals in soil. Specifically, this note provides SGVs for xylenes in soil.

The SGVs and additional advice found here should be used only in conjunction with the introductory guide to the series entitled *Using Soil Guideline Values* (Environment Agency, 2009a), the framework documents *Updated technical background to the CLEA model* (Environment Agency, 2009b) and *Human health toxicological assessment of contaminants in soil* (Environment Agency, 2009c), and *Contaminants in soil: updated collation of toxicological data and intake values for humans. Xylene* (Environment Agency, 2009d).

Supplementary information on xylenes is also available and is referenced in this technical note.

All notes in the SGV series, the introductory guide and further supplementary information can be downloaded from our website (<http://www.environment-agency.gov.uk/clea>).

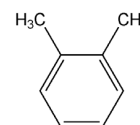
Xylenes

"Xylenes" (CAS No. 1330-20-7) is the common name for a mixture of three isomers of dimethylbenzene and ethylbenzene, which is also known commercially as "mixed xylenes". The composition of mixed xylenes varies, but the range of each constituent is illustrated in Table 1.

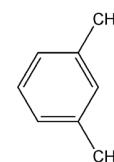
The three structural isomers are 1,3-dimethylbenzene or *meta*-xylene (CAS No. 108-38-3), 1,2-dimethylbenzene or *ortho*-xylene (CAS No. 95-47-6) and 1,4-dimethylbenzene or *para*-xylene (CAS No. 106-42-3). These isomers are shown in Figure 1 and are referred to in this technical note as xylene.

Xylene is a naturally occurring aromatic hydrocarbon compound with two methyl group substitutions on a benzene ring (ATSDR, 2007). It is its similarity to benzene that gives xylene its characteristic aromatic chemical behaviour.

meta-xylene
(1,3-dimethylbenzene)
CAS No. 108-38-3



ortho-xylene
(1,2-dimethylbenzene)
CAS No. 95-47-6



para-xylene
(1,4-dimethylbenzene)
CAS No. 106-42-3

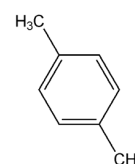


Figure 1 Structure of xylene isomers

Table 1

The general composition of mixed xylenes produced from coal tar and petroleum (IPCS, 1997; ATSDR, 2007)

Compound	Coal tar (%)	Petroleum (%)
<i>Ortho</i> -xylene	10–15	20
<i>Meta</i> -xylene	45–70	44
<i>Para</i> -xylene	23	20
Ethylbenzene	6–10	15

Benzene, toluene, ethylbenzene and xylene are often referred to collectively as BTEX because they have closely related chemical structures, and have similar fate and transport properties. They are often used together in industrial and petroleum products, and commonly occur together in the environment as a result of related pollution. In the past xylene has been known by a variety of names including methyltoluene and xylol (IPCS, 1997; ATSDR, 2007).

Xylene is a colourless, flammable liquid at normal room temperature and does not mix readily with water (IPCS, 1997; ATSDR, 2007). It has an aromatic odour (IPCS, 1997), sometimes described as sweet (ATSDR, 2007). Although readily miscible with most organic solvents, xylene has a low solubility in water (IPCS, 1997; ATSDR, 2007) and much less so than benzene (Environment Agency, 2008). Xylene is a light non-aqueous phase liquid (LNAPL) and will float on water. It will also disperse into the atmosphere (because of its vapour pressure) where it is degraded by photo-oxidation reactions (IPCS, 1997; ATSDR, 2007).

Xylene occurs naturally in forest fires and is found as a constituent of crude oil and coal tar (ATSDR, 2007). Before 1940, mixed xylenes was manufactured from coal tar; thereafter it was produced during petroleum refining (IPCS, 1997; ATSDR, 2007).

Individual xylene isomers are isolated from mixed xylenes by crystallisation, fractionation, distillation and/or solvent extraction or adsorption (ATSDR, 2007).

World production of mixed xylenes in 1984 was estimated as 15.4 million tonnes (IPCS, 1997). In 1983, world production of *p*-xylene was estimated as 3.9 million tonnes, of which Europe accounted for 23 per cent (IPCS, 1997). World production for *o*-xylene in 1983 was estimated as 1.3 million tonnes, of which western Europe accounted for 30 per cent (IPCS, 1997). No recent data giving UK or European Union production levels of xylene or mixed xylenes were found.

According to IPCS (1997), almost all xylene produced is used as an additive in petrol. However it is also used: as an industrial solvent in paints and printing inks; to produce perfumes, pesticide formulations, pharmaceuticals and adhesives; and in the rubber, plastics and leather industries (IPCS, 1997; Environment Canada, 2004; ATSDR, 2007). The average concentration of xylene in petrol is around 10.6 per cent (CONCAWE, 1997).

Of the uses for individual isomers (excluding its use in petrol), the most commonly used is *p*-xylene, which is used to produce polyester fibre, film, insecticides, vitamins and pharmaceuticals (IPCS, 1997; ATSDR, 2007). *o*-xylene is used to produce phthalate-based plasticisers, polyimide polymers, insecticides, vitamins and pharmaceuticals, and *m*-xylene is used in the manufacture of polyester resins (IPCS, 1997; ATSDR, 2007).

Potential harm to human health

The principles behind the selection of Health Criteria Values (HCVs), and the definition of concepts and terms used, are outlined in *Human health toxicological assessment of contaminants in soil* (Environment Agency, 2009c). Specific information on the toxicity of xylene is reviewed in *Contaminants in soil: updated collation of toxicological data and intake values for humans. Xylene* (Environment Agency, 2009d) and only a brief summary is presented here.

Toxicity to the central nervous system (CNS) is the main human health concern following long-term inhalation exposure. There is a lack of human studies regarding oral toxicity. Effects to the kidneys and reduced bodyweight gain have been reported following oral exposure in experimental animals.

The inhalation tolerable daily intake (TDI) in Table 2 is based on CNS effects seen in workers exposed to xylene.

The oral TDI in Table 2 is based on doses that did not cause adverse effects (reduced bodyweight gain) in rats administered higher doses in long-term studies.

No authoritative assessments of the health risks posed by dermal exposures have been identified for xylene

Table 2

Recommended Health Criteria Values and background adult intakes for xylene (Environment Agency, 2009d)

Parameter	Xylene
TDI _{oral} , $\mu\text{g kg}^{-1} \text{ bw day}^{-1}$	180
MDI _{oral} , $\mu\text{g day}^{-1}$	11
TDI _{inh} , $\mu\text{g kg}^{-1} \text{ bw day}^{-1}$	60
MDI _{inh} , $\mu\text{g day}^{-1}$	140

bw = bodyweight

MDI = mean daily intake

TDI = tolerable daily intake

(Environment Agency, 2009d). Information on dermal toxicity and skin absorption is limited. Dermal absorption is supported by available literature information, but occurs to a lesser extent than either oral or pulmonary absorption. On this basis, it would not seem unreasonable to assume that the oral HCV value could be used for conservative screening of dermal risk (Environment Agency 2009c, d).

Taking into account the differences between indoor and outdoor air concentrations, the mean inhalation exposure for people living in the UK can be estimated as being about $140 \mu\text{g day}^{-1}$. It thus represents a minor proportion of the inhalation TDI (Environment Agency, 2009d).

Xylene has been detected in nuts, meat and fish, but was not generally detected in other food groups and its presence in water is low. Background oral exposure to xylene from its presence in food and water can be

estimated as $11 \mu\text{g day}^{-1}$. The oral MDI occupies only a very small fraction of the oral TDI (Environment Agency, 2009d).

Sources not included in the MDI estimations include: mainstream cigarette smoke; household consumer products such as insecticides, lacquers; and air at localised areas of higher concentrations such as petrol stations and areas of industrial solvent manufacture / storage.

Exposure assessment

Occurrence in soil

Although individual xylene isomers occur naturally in the environment, their contribution to soil levels is considered much smaller than anthropogenic sources (ATSDR, 2007).

Mixed xylenes and xylene isomers are widely released into the environment due to their widespread use in petrol and as an industrial solvent (IPCS, 1997; ATSDR, 2007). The majority of xylene released enters the atmosphere directly (IPCS, 1997; ATSDR, 2007). Xylene can enter the environment at production sites, but also as a result of the use, storage and transport of petroleum products or from waste disposal (ATSDR, 2007). Highly elevated concentrations in soil can occur as a result of localised spills of petroleum and solvent products from historical and poor management practice (which can result in persistent contamination over a wide area). Xylene is often a component of complex and weathered mixtures of hydrocarbon compounds and may exist in soil as degradation by-products of more complex hydrocarbons.

IPCS (1997) estimates that 99 per cent of the xylene released into the air remains in the atmosphere; the remaining 1 per cent is likely to partition in water and soil.

A review of the literature identified no data regarding background levels of xylene in UK soils. A similar conclusion was drawn by Paterson *et al.* (2003) in work commissioned by the Scottish Environment Protection Agency (SEPA). Neither ATSDR (2007) nor IPCS (1997) located any international studies of xylene levels in urban or rural soils. According to Wolverhampton City Council (personal communication, 2009), average background concentrations of xylene in glacial drift deposits on a large housing estate in an urban area of the West Midlands were below the detection limit of $1 \mu\text{g kg}^{-1}$.

Behaviour in the soil environment

Recommended values for chemical data used in the exposure modelling of the three xylene isomers are provided in Table 7. There are slight differences in the properties of each isomer. Further information about the selection of chemical properties can be found in Environment Agency (2008). *Supplementary information for the derivation of SGVs for xylene* (Environment Agency, 2009e) provides additional information about the review and recommendations for the soil-to-plant concentration factors for xylene.

The xylene isomers are considered by most authoritative organisations to be relatively mobile in the soil environment (IPCS, 1997; ATSDR, 2007).

Upon release into soil, xylene will tend to sink through the unsaturated zone until it reaches the saturated zone (Environment Agency, 2003). It is a light non-aqueous phase liquid (LNAPL) and will tend to collect at the water table if present in sufficient concentrations.

Xylene can easily leach from soil given its aqueous solubility, molecular weight, and octanol–water partition coefficient (K_{ow}) (Environment Agency, 2003). Xylene has a relatively low tendency to adsorb to soil organic matter (SOM) reflected by its organic carbon water partition coefficient (K_{oc}). Nonetheless, in general, adsorption to soil will increase as SOM increases (ATSDR, 2007) and adsorption to SOM can control the potential of xylene to leach. The sorption potential also varies with other soil properties (e.g. water content, number of available adsorption sites and porosity) and environmental conditions (e.g. temperature) (IPCS, 1997; Environment Agency, 2003; ATSDR, 2007).

Most surface soils are likely to contain very little, if any, xylene. Xylene will volatilise readily from surface soil given its vapour pressure, air–water partition coefficients and K_{oc} , but less rapidly than benzene and toluene (Environment Agency, 2003; ATSDR, 2007). Volatilisation to air is the most important of the transport processes for xylene, although the rate of volatilisation will decrease at greater depths (IPCS, 1997; ATSDR, 2007). Xylene will volatilise more readily from soils with a high air-filled porosity such as sands and gravels (Environment Agency, 2003).

Key aspects of xylene's behaviour in the soil environment will be influenced by the presence of other compounds. The solubility and volatility of xylene have been reported to decrease when present with other hydrocarbon compounds and after weathering of the compounds has taken place (TPHCWG, 1998).

Xylene in soil has also been shown to undergo microbial degradation under both aerobic and anaerobic conditions. *m*-Xylene and *p*-xylene are readily biodegradable; *o*-xylene is more persistent. However, there is often "no clear relationship between the initial concentration and 'degradation' rate" (IPCS, 1997).

Biodegradation rates are dependent on several factors including: the presence of sunlight; the type and population of microbes present; initial concentration of xylene; soil temperature; soil oxygen content; and the potential presence of other electron receptors¹ (Environment Agency, 2000a, 2003).

¹ Electron acceptors are compounds which are capable of accepting electrons during oxidation–reduction reactions. Microbes obtain energy by transferring electrons from electron donors such as xylene to an electron acceptor (Environment Agency, 2000a). Typical electron acceptors found in soil include dissolved oxygen, nitrate, sulphate, iron, manganese and carbon dioxide (Environment Agency, 2000a).

The reported range of half-life values for xylene in soil is wide, from as little as 7 days to 510 days² under aerobic and anaerobic conditions (USEPA, 1999; Environment Agency, 2003; Mackay *et al.*, 2006; ATSDR, 2007). Although limited data were located regarding half-lives in soil, similar rate constants were reported by USEPA (1999) for each of the three isomers. Mackay *et al.* (2006) cites a range of aerobic degradation half-life values for xylene in soil from 7 to 28 days and ATSDR (2007) cite a range of soil degradation half-life values from 0.3 to 7.6 days.

A report prepared for the US Environment Protection Agency (USEPA) describes a number of half-life studies based on laboratory investigations. These are not discussed here as the optimised conditions mean that the half-lives and thus degradation potential are not comparable with a real soil environment. Half-lives from groundwater studies are also not discussed as oxygen is often the rate limiting parameter for biodegradation. Results may therefore not be applicable to aerobic soils (USEPA, 1999).

The biodegradation half-lives reported in soil and the physical-chemical parameters of xylene indicate that it would be removed rapidly on entry into soil. However, site-specific conditions and the presence of other contaminants should be taken into account as, in some situations, xylene will remain in the soil longer than anticipated (Alvarez and Vogel, 1991).

Modelling the partitioning of volatile organic compounds (VOCs) such as xylene from the soil to ambient or indoor air is subject to a number of simplifications and limitations (CIRIA, in press). Many environmental models, including the CLEA model, predict chemical concentrations in soil systems using simple linear partitioning models. CIRIA (in press) reports empirical data from a large number of site investigations in the US and UK which illustrates that this approach is conservative for many petroleum hydrocarbons across different situations and soil types.

Although the reasons for the difference between empirical and theoretical calculations is the subject of continued debate (CIRIA, in press), reported factors include sampling technique, biodegradation in the vapour phase, and natural ground heterogeneity. As soil vapour is transported upwards towards the building, biodegradation of petroleum hydrocarbons commonly occurs which can significantly affect the amount of vapour that will enter the building. Among other factors, this is dependent on the oxygen availability in the unsaturated zone (CIRIA, in press).

Using simple linear partitioning, the concentrations of petroleum hydrocarbons in the soil gas can be over-predicted by at least a factor of 10 (and up to a factor of 1,000) (Environment Agency, 2009b; CIRIA, in press).

Given the likely level of overprediction reported in empirical studies, it is not unreasonable to include a sub-surface soil to indoor air correction factor of 10 in the derivation of SGVs for xylene. This is the lower end of the range of over-predictions reported and, therefore,

sufficiently conservative to be appropriate to use in a generic screening value.

Xylene is moderately hydrophobic based on its K_{ow} (Environment Agency, 2009e). The potential exists for the uptake of xylene into plants from soil to occur directly through passive root uptake or indirectly following volatilisation of the chemical from the soil and subsequent vapour phase sorption onto plant surfaces. On entering the leaves, xylene may be lost through transpiration or metabolised. The resulting metabolites may be retained in the leaves as bound residues or incorporated into structures, or transpired. Xylene has also been reported to accumulate in oil-containing plant structures such as the waxy layers of leaves and fruit (Environment Agency, 2009e).

Available studies indicate that xylene can cause damaging effects in plants; these are dependent on the soil type, concentration of xylene in the soil, and plant species. Data on the phytotoxicity of xylene are not widely documented, but reduced seedling emergence, shoot dry mass and root length have been reported (Environment Agency, 2009e).

In the absence of sufficient data to specify soil-to-plant concentration factors for xylene, Environment Agency (2009e) recommends that the generic CLEA models for calculating soil-to-plant concentration factors are used in the derivation of SGVs.³

A review of the literature did not identify any studies for quantifying the dermal absorption fraction for xylene. Therefore the default value of 0.1 proposed by Environment Agency (2009b) for organic compounds was used in the derivation of the SGVs.

A review of the literature found no data relevant to the concentrations of xylene in soil derived household dust. There are a number of potential sources of xylene from products used in the home and therefore xylene is likely to be present in indoor dust. But even if data were available regarding the level of xylene in household dust, it would be difficult to distinguish observed enrichment of xylene in indoor dust that has derived from non-soil sources within the home to that from soil. The default value of 0.5 g g⁻¹ dry weight (DW) for the soil-to-dust transport factor was used in the derivation of the SGVs (Environment Agency, 2009b). This is considered to be a sufficiently conservative assumption.

Soil Guideline Values

Soil Guideline Values for the three isomers of xylene are presented according to land use in Table 3 and are derived using physical-chemical data specific to each isomer. For residential and allotment land uses, SGVs are based on estimates representative of exposure of young children because they are generally more likely to have higher exposures to soil contaminants. Further information on the default exposure assumptions used in the derivation of SGVs can be found in *Updated*

² Based on a first-order rate constant.

³ In the absence of suitable models for shrub fruit and herbaceous fruit (Environment Agency, 2009b), exposure from ingestion of shrub and herbaceous fruits was not included in the derivation of the SGVs.

technical background to the CLEA model (Environment Agency, 2009b).

The SGVs for xylene are based on a consideration of the oral, dermal and inhalation routes of exposure. The toxicological effects are considered to be systemic and the combined assessment criteria are presented.

An SGV is presented in Table 3 for each of the three isomers of xylene. These SGV are calculated using:

- HCV based on the intake of total xylene; and
- physical-chemical data specific to each isomer of xylene.

Mixed xylenes can consist of over 40 per cent *m*-xylene (IPCS, 1997; ATSDR, 2007). Of the individual isomers, the most commonly used is *p*-xylene (as an intermediate in the manufacture of polyester fibre, film and fabricated products) (IPCS, 1997). When assessing a fresh spill of mixed xylenes, *m*-xylene is likely to predominate and the SGV for *m*-xylene should be compared with the representative site soil concentration for total xylene.

If the composition of the xylene source is not known or the mixed xylene is weathered, the representative site soil concentration for total xylene (that is, the sum of all three isomers) should be compared with the most health protective SGV. For a residential and allotment land use, this is *p*-xylene and, for a commercial land use, it is *o*-xylene. Alternatively, Detailed Quantitative Risk Assessment (DQRA) (Defra and Environment Agency, 2004) could consider a hazard quotient approach (Environment Agency, 2009b) using site-specific information.

The percentage of exposure attributable to each individual relevant pathway for the residential and the allotment land uses is presented in Tables 4, 5 and 6 for the three isomers respectively. The ADE/HCV ratios for oral and inhalation exposures are also presented. Modelling suggests that:

- the inhalation of indoor vapour and the consumption of homegrown produce are the most significant exposure pathways at the SGV for the residential land use (both contributing similar amounts, approximately 45 per cent of total exposure, each). However, because the inhalation HCV is three times lower than that for oral exposure, the dominant exposure pathway driving the risk for the SGV for this land use is inhalation of indoor vapour;
- the consumption of homegrown produce is the most significant exposure pathway at the SGV for allotment land use;
- the exposure via dermal pathways is negligible, contributing no more than 1 per cent of total exposure at the SGVs for both residential and allotment land uses;
- the inhalation of dust is not an important exposure pathway. This is due to the combined effects of vapour pressure, air-water partition coefficient and the K_{oc} value of xylene.

Using the CLEA model to calculate SGVs for the commercial land use scenario results in an exceedance of the lower of the vapour or aqueous saturation concentration for each of the three isomers of xylene. The lower saturation limit is at a concentration much lower than the combined assessment criteria. At the lower saturation limit, the vapour pathway contributes almost 60 per cent of total exposure for any of the xylene isomers. At soil concentrations above the lower saturation limit there is potential for free phase contamination to be present. The CLEA model does not account for oral or dermal exposure via direct contact with, or inhalation exposure from vapours arising from, free phase chemicals and may under estimate the risk to health at higher soil concentrations. The SGV has therefore been set equal to the lower of the aqueous and vapour saturation limit of 3.46×10^3 (vapour limit), 2.62×10^3 (solubility limit) and 3.17×10^3 (solubility limit) mg kg⁻¹ for the *m*-, *o*- and *p*- isomers respectively.

Analytical limits of detection⁴ for *m*- and *p*-xylene are dependent on the analytical technique used and range from 0.001 to 0.014 mg kg⁻¹ DW, with limits of quantification⁵ ranging from 0.005 to 0.070 mg kg⁻¹ DW. Analytical limits of detection for *o*-xylene are dependent on the analytical technique used and range from 0.001 to 0.010 mg kg⁻¹ DW, with limits of quantification ranging from 0.005 to 0.050 mg kg⁻¹ DW. Limits of detection and quantification can vary due to the range, sensitivity, set-up of the instrumentation being used and the sample matrix. MCERTS⁶ accredited analytical methods for testing for xylene in soil are available.

⁴ The amount of a substance that can be detected, but not measured quantitatively.

⁵ The amount present of a substance that can be measured quantitatively.

⁶ Environment Agency's Monitoring Certification Scheme

Table 3

The Soil Guideline Values for xylene presented in this table should only be used in conjunction with the information contained in this technical note and with an understanding of the exposure and toxicological assumptions contained in *Updated technical background to the CLEA model* (Environment Agency, 2009b), *Human health toxicological assessment of contaminants in soil* (Environment Agency, 2009c) and *Contaminants in soil: updated collation of toxicological data and intake values for humans. Xylene* (Environment Agency, 2009d).

Land use	Soil Guideline Values (mg kg ⁻¹ DW) ^{1,2,3,4,5,7}		
	o-xylene	m-xylene	p-xylene
Residential	250	240	230
Allotment ⁸	160	180	160
Commercial ⁶	2.6 × 10 ³	3.5 × 10 ³	3.2 × 10 ³

Notes

¹ Based on a sandy loam soil as defined in Environment Agency (2009b) and 6% soil organic matter (SOM). At a lower SOM, SGVs may not be sufficiently protective.

² Generic assessment criteria for xylene will vary according to SOM for all land uses.

³ Figures are rounded to one or two significant figures.

⁴ SGVs assume that free phase contamination is not present.

⁵ SGVs based on a sub-surface soil to indoor air correction factor of 10.

⁶ SGVs presented for a commercial land use have been capped at the lower of the vapour or aqueous saturation limit.

⁷ Exposure to all isomers of xylene should be considered together, because the HCV applied is based on the intake of total xylene, and not an individual isomer in isolation.

⁸ In applying the rules for non-soil background to the allotment SGV, the inhalation background ADE is limited to being no larger than the contribution of the inhalation soil ADE

It is unlikely that soil concentrations of xylene at the level of the residential or allotment SGVs will pose a significant additional risk to health from this pathway. However, where contamination is found or is suspected close to buried water services, the risk assessor should consider its implications carefully and, where necessary, investigate the likelihood of contamination of the water supply.

The potential for free phase product should be assessed at the preliminary stage of risk assessment when formulating the outline conceptual model as outlined within Defra and Environment Agency (2004). For example, maps may show the presence of tanks or anecdotal information may indicate that spills might have occurred at the site. The SGVs in Table 3 should be applied cautiously where free phase contamination is suspected (e.g. by taking into account visual and olfactory observations) and its potential presence at the surface should be considered qualitatively as part of the risk assessment. In such cases, alternative methodologies, such as those which model vapours from NAPLs, or the consideration of dermal contact with NAPLs may be more suitable (Environment Agency, 2009f).

The generic conceptual exposure models used to derive SGVs (as described in Environment Agency, 2009b) assume that:

- the source term is infinite;
- the source term is not itself reduced by biological or chemical degradation;
- xylene is present in isolation and not in a mixture with other compounds.

Assessors undertaking a Detailed Quantitative Risk Assessment (DQRA) (Defra and Environment Agency, 2004) may wish to consider the applicability of these assumptions on a site-specific basis. The actual degradation half-life of a chemical in soil is highly site-specific and dependent on a number of influences including soil temperature, oxygen availability, microbial population and the presence of other contaminants.

Ethylbenzene is a constituent of mixed xylenes and it is highly unusual for xylene to occur in isolation in a contaminated soil, although fate and transport calculations (such as those used by the CLEA model) normally assume single component behaviour. Xylenes environmental behaviour will be influenced by the presence of other compounds in the mixture (TPHCWG, 1998; ATSDR, 2007). The assessor should consider the effects of other substances on the mobility of xylene as part of a Detailed Quantitative Risk Assessment. For example, when the inhalation of vapour is a key pathway, assessors may wish to use Raoult's Law to determine the effective vapour concentration of xylene in the mixture (TPHCWG, 1999, Environment Agency, 2003).

Ingestion of drinking-water contaminated from on-site sources is not an exposure pathway included in the CLEA model (Environment Agency, 2009b). Environment Agency (2000b) and WRAS (2002) identify petroleum hydrocarbon compounds including xylene as having the potential to permeate certain types of plastic water pipes. Pipe permeation is especially likely to occur where there is prolonged contact with heavily contaminated soils including the presence of free phase. Permeation is dependent on several factors such as the chemical characteristics of xylene or the mixture present, the water content of the soil, the distribution between the soil, air and vapour phases (mobility and K_{oc}), length of exposure and temperature (DWI, 1997).

RIVM (1995) proposed a method of estimating pipe permeation, although this is highly uncertain and the assessment will depend on the type of pipe work found, water usage and the soil concentration immediately adjacent to the pipe wall.

The phytoavailability of xylene to garden produce depends on a number of complex factors. The soil-to-plant concentration factors used in the derivation of the SGVs are calculated from generic algorithms (detailed in Environment Agency, 2009b) for a generic scenario and are dependent on the K_{ow} of the individual xylene isomer (that is, the degree to which the individual xylene isomer partitions between water and plant lipids). In circumstances where the SGV is exceeded and the consumption of produce is a significant pathway, assessors may wish to adjust for the site-specific measured SOM. A higher SOM will mean that less xylene is available for plant uptake because it remains sorbed to the soil.

Assessors undertaking a Detailed Quantitative Risk Assessment could also carry out further investigation (including the sampling and chemical analysis of edible parts of fruits and vegetables) to determine site-specific plant concentration factors. Herbaceous and shrub fruit produce groups have not been modelled in the derivation of SGVs (Environment Agency, 2009b). In cases where these predominate the total fruit and vegetables consumed from a site, further consideration is necessary. However, the sampling and chemical analysis of edible parts of fruits and vegetables is unlikely to be an easy task.

Environment Agency (2009b) highlights some uncertainties in the Johnson and Ettinger algorithms used to estimate the concentrations within indoor air. It is recognised that the concentration of petroleum hydrocarbons within the building may be overestimated using this approach.

A number of factors contribute significantly to the amount of xylene that will partition into the soil vapour phase, including SOM (sorption to organic matter retards volatilisation). When the inhalation of indoor air is the pathway driving the risk, assessors undertaking a Detailed Quantitative Risk Assessment could carry out further assessment such as soil vapour monitoring. Further guidance and information can be found in CIRIA (in press).

As noted above, soil organic matter content may affect the vapour inhalation and plant uptake pathways significantly. SGVs are based on a SOM content of 6 per cent. At a lower SOM, they may not be sufficiently protective.

Exposure from dermal contact and direct soil ingestion pathways may be important in scenarios where the vapour pathway is actively or passively managed by, for example, the building design. Further discussion of these pathways can be found in Environment Agency (2009b).

Table 4Contribution to total exposure for the relevant pathways for *ortho*-xylene as calculated by the CLEA software

	ADE:HCV ratio	
	Residential	Allotment
Oral ADE:HCV ratio at SGV	0.25	1.0
Inhalation ADE:HCV ratio at SGV	0.75	0
	Contribution to exposure ^{1,3} according to land use (%)	
Exposure pathway	Residential	Allotment
Ingestion of soil and indoor dust ²	2.0	0.2
Consumption of homegrown produce and attached soil	45.1	99.2
Dermal contact (indoor)	0	NA
Dermal contact (outdoor)	1.0	0.1
Inhalation of dust (indoor)	0	NA
Inhalation of dust (outdoor)	0	0
Inhalation of vapour (indoor)	42.0	NA
Inhalation of vapour (outdoor)	0	0.1
Oral background	0.7	0.3
Inhalation background	9.2	0.1

Notes¹ Rounded to one decimal place.² Treated as one pathway (see Environment Agency, 2009b).³ Percentage contributions not presented for a commercial land use as the commercial SGV presented is at the vapour saturation limit.

ADE = Average Daily Exposure

HCV = Health Criteria Value

NA = not applicable (This exposure pathway is not included in the generic land use.)

Table 5Contribution to total exposure for the relevant pathways for *meta*-xylene as calculated by the CLEA software

	ADE:HCV ratio	
	Residential	Allotment
Oral ADE:HCV ratio at SGV	0.22	1.0
Inhalation ADE:HCV ratio at SGV	0.78	0
	Contribution to exposure^{1,3} according to land-use (%)	
Exposure pathway	Residential	Allotment
Ingestion of soil and indoor dust ²	2.0	0.2
Consumption of homegrown produce and attached soil	41.4	99.2
Dermal contact (indoor)	0	NA
Dermal contact (outdoor)	1.0	0.1
Inhalation of dust (indoor)	0	NA
Inhalation of dust (outdoor)	0	0
Inhalation of vapour (indoor)	45.3	NA
Inhalation of vapour (outdoor)	0	0.1
Oral background	0.7	0.3
Inhalation background	9.6	0.1

Notes¹ Values rounded to one decimal place.² Treated as one pathway (see Environment Agency, 2009b).³ Percentage contributions not presented for a commercial land use as the commercial SGV presented is at the vapour saturation limit.

ADE = Average Daily Exposure

HCV = Health Criteria Value

NA = not applicable (This exposure pathway is not included in the generic land use.)

Table 6Contribution to total exposure for the relevant pathways for *para*-xylene as calculated by the CLEA software

	ADE:HCV ratio	
	Residential	Allotment
Oral ADE:HCV ratio at SGV	0.22	1.0
Inhalation ADE:HCV ratio at SGV	0.78	0
	Contribution to exposure according to land use (%) ^{1,3}	
Exposure pathway	Residential	Allotment
Ingestion of soil and indoor dust ²	1.9	0.2
Consumption of homegrown produce and attached soil	42.0	99.2
Dermal contact (indoor)	0	NA
Dermal contact (outdoor)	0.9	0.1
Inhalation of dust (indoor)	0	NA
Inhalation of dust (outdoor)	0	0
Inhalation of vapour (indoor)	44.9	NA
Inhalation of vapour (outdoor)	0	0.1
Oral background	0.7	0.3
Inhalation background	9.5	0.1

Notes¹ Values rounded to one decimal place.² Treated as one pathway (see Environment Agency, 2009b).³ Percentage contributions not presented for a commercial land use as the commercial SGV presented is at the vapour saturation limit.

ADE = Average Daily Exposure

HCV = Health Criteria Value

NA = not applicable (This exposure pathway is not included in the generic land use.)

Table 7

Recommended physical-chemical data for xylene (at 10°C unless stated)

Chemical property	<i>o</i> -xylene	<i>m</i> -xylene	<i>p</i> -xylene	Reference
Air–water partition coefficient, $\text{cm}^3 \text{cm}^{-3}$	0.092	0.112	0.107	Environment Agency (2008)
Dermal absorption fraction, dimensionless	0.1	0.1	0.1	Environment Agency (2009b)
Diffusion coefficient in air, $\text{m}^2 \text{s}^{-1}$	7.01×10^{-6}	7.03×10^{-6}	7.04×10^{-6}	Environment Agency (2008)
Diffusion coefficient in water, $\text{m}^2 \text{s}^{-1}$	5.31×10^{-10}	5.31×10^{-10}	5.31×10^{-10}	Environment Agency (2008)
Octanol–water partition coefficient (log), dimensionless	3.12	3.20	3.15	Environment Agency (2008)
Organic carbon–water partition coefficient (log), $\text{cm}^3 \text{g}^{-1}$	2.63	2.69	2.65	Environment Agency (2008)
Relative molecular mass, g mol^{-1}	106.17	106.17	106.17	Environment Agency (2008)
Soil–water partition coefficient, $\text{cm}^3 \text{g}^{-1}$	NA	NA	NA	
Vapour pressure, Pa	386	495	475	Environment Agency (2008)
Water solubility, mg L^{-1}	173	200	200	Environment Agency (2008)
Soil-to-dust transport factor, $\text{g g}^{-1} \text{DW}$	0.5	0.5	0.5	Environment Agency (2009b)
Sub-surface soil to indoor air correction factor, dimensionless	10	10	10	Recommended in this report.
Soil-to-plant concentration factor, $\text{mg kg}^{-1} \text{FW per mg kg}^{-1}$				
Green vegetable produce	To be modelled	To be modelled	To be modelled	Environment Agency (2009e)
Root vegetable produce	To be modelled	To be modelled	To be modelled	Environment Agency (2009e)
Tuber vegetable produce	To be modelled	To be modelled	To be modelled	Environment Agency (2009e)
Herbaceous fruit produce ¹	To be modelled	To be modelled	To be modelled	Environment Agency (2009e)
Shrub fruit produce ¹	To be modelled	To be modelled	To be modelled	Environment Agency (2009e)
Tree fruit produce	To be modelled	To be modelled	To be modelled	Environment Agency (2009e)

Notes ¹Algorithms are not presented in Environment Agency (2009b) for herbaceous and shrub fruit. Exposure from these pathways was therefore not considered in the derivation of the SGVs.

DW = dry weight
FW = fresh weight
NA = not applicable

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The CLEA Guidance incorporates the following

- 1) *Science Report SC050021/SR2: Human health toxicological assessment of contaminants in soil.*
- 2) *Science Report SC050021/SR3: Updated technical background to the CLEA model.*
- 3) *Science Report SC050021/SR4: CLEA Software (Version 1.04) Handbook.*
- 4) *CLEA Software version 1.04 (2009)*
- 5) *Toxicological reports and SGV technical notes*

The CLEA Guidance can help suitably qualified assessors to estimate the risk that a child or adult may be exposed to a soil concentration on a given site over a long period of exposure that may be a cause for concern to human health. The CLEA Guidance does not cover other types of risk to humans, such as fire, suffocation or explosion, or short-term and acute exposures. Nor does it cover risks to the environment or the pollution of water.

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