



9.3 Computer Simulation of Soil Vapour Generation Potential

A theoretical analysis of soil vapour generation potential at the Former Gasworks site has been undertaken using the Johnson and Ettinger (1991) one-dimensional analytical solution to convective and diffusive vapour transport into spaces. The solution calculates the vapour generated from sources of soil and groundwater contamination and provides an estimated attenuation coefficient that relates the vapour concentration in the indoor space to the vapour concentration at the source of contamination. The analysis performed in this study has used the spreadsheet model developed for the US EPA (February 2004), which is available on their website.

The model can be constructed as both a steady-state solution to vapour transport (infinite or non-diminishing source) or as a quasi-steady-state solution (finite or diminishing source). Inputs to the model include chemical properties of the contaminant, saturated and unsaturated zone soil properties and structural properties of the building. The model has been used to estimate soil vapour concentrations in the area where the soil vapour tests were conducted in March 2005.

The Johnson and Ettinger (1991) one-dimensional analytical solution is able to account for soil vapours generated by both soil and groundwater contamination. The source vapour concentration (C_{source}) for groundwater contamination is given by the equation:

$$C_{\text{source}} = H'_{\text{TS}} C_w \quad \dots\dots\dots(1)$$

where:

- C_{source} = Vapour concentration at the source of contamination ($\text{g}/\text{cm}^3\text{-v}$)
- H'_{TS} = Henry's law constant at the system (groundwater) temperature (dimensionless)
- C_w = Groundwater concentration ($\text{g}/\text{cm}^3\text{-w}$)

The dimensionless form of the Henry's law constant at the system temperature (ie. at the average soil/groundwater temperature) is estimated using the Clapeyron equation:

$$H'_{\text{TS}} = \{ \exp [-(\Delta H_{\text{v,TS}} / R_c) (1/T_s - 1/T_R)] H_R \} / (R \times T_s) \quad \dots\dots\dots(2)$$

where:

- $\Delta H_{\text{v,TS}}$ = Enthalpy of vapourisation at the system temperature (cal/mol)
- T_s = System temperature ($^{\circ}\text{K}$)
- T_R = Henry's law constant reference temperature ($^{\circ}\text{K}$)
- H_R = Henry's law constant at the reference temperature ($\text{atm}\cdot\text{m}^3/\text{mol}$)
- R_c = Gas constant ($=1.9872 \text{ cal}/\text{mol} \cdot ^{\circ}\text{K}$)
- R = Gas constant ($=8.205\text{E-}05 \text{ atm}\cdot\text{m}^3/\text{mol} \cdot ^{\circ}\text{K}$)



The enthalpy of vapourisation at the system temperature is calculated from the Lyman equation given in the US EPA (February 2004) manual.

The source vapour concentration (C_{source}) for soil contamination is given by the equation:

$$C_{\text{source}} = (H'_{\text{TS}} C_R \rho_b) / (\theta_w + K_d \rho_b + H'_{\text{TS}} \theta_a) \dots\dots\dots(3)$$

where:

C_{source}	=	Vapour concentration at the source of contamination ($\text{g}/\text{cm}^3\text{-v}$)
H'_{TS}	=	Henry's law constant at the system (soil) temperature (dimensionless)
C_R	=	Initial soil concentration (g/g)
ρ_b	=	Soil dry bulk density (g/cm^3)
θ_w	=	Soil water-filled porosity (cm^3/cm^3)
K_d	=	Soil-water partition coefficient (cm^3/g)
θ_a	=	Soil air-filled porosity (cm^3/cm^3)

The stratigraphic model used in the computer analysis has been based on average conditions that occur across that part of the former gasworks site where elevated volatile concentrations have been measured in the soils and groundwater. The boreholes located within this area are SB03, SB04, SB06, SB18, MW03S, MW06S, MW07S, MW20S and MW30-MW34. These boreholes show that the average depth to the shallow aquifer water table is approximately 1.5m, which is comparable to the depth reached by the soil gas wells MW30-MW34 sampled in March 2005. Furthermore, the volatile contaminants present in the unsaturated shallow soils can occur throughout the shallow soil profile. This means that the soil-gas monitoring wells that were tested in March 2005 should have measured the source concentration of volatile gases given off by the shallow groundwater (C_{source}). As previously explained, the deeper aquifer and deeper soils are not considered in this vapour analysis since any vapours generated by these materials should be reflected by the water quality in the shallow aquifer.

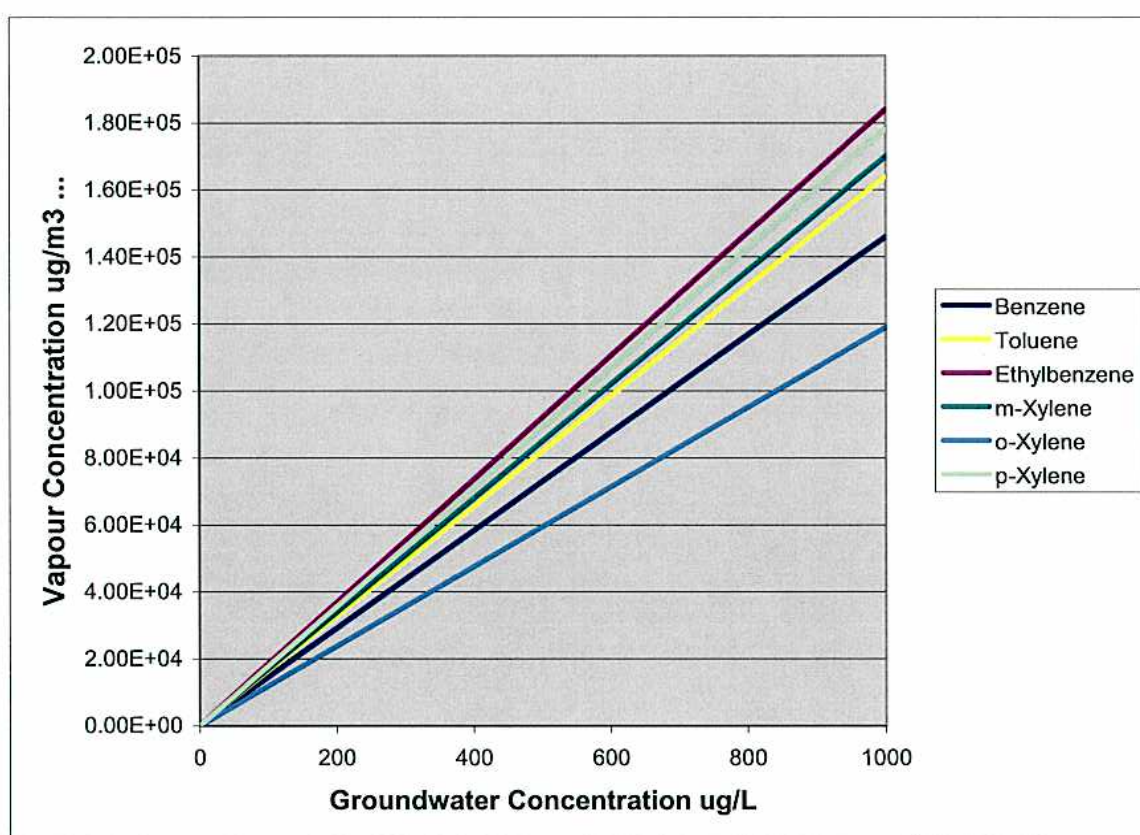
The input parameters used in the model are:

- Depth below grade to water table = 1.5m
- Soil profile = Clay
- Average soil/groundwater temperature = 15°C
- Vadose zone soil dry density = 1.5t/m³ (program default value)
- Vadose zone soil total porosity = 0.43 (program default value)
- Vadose zone soil water-filled porosity = 0.215 cm³/cm³ (program default value)



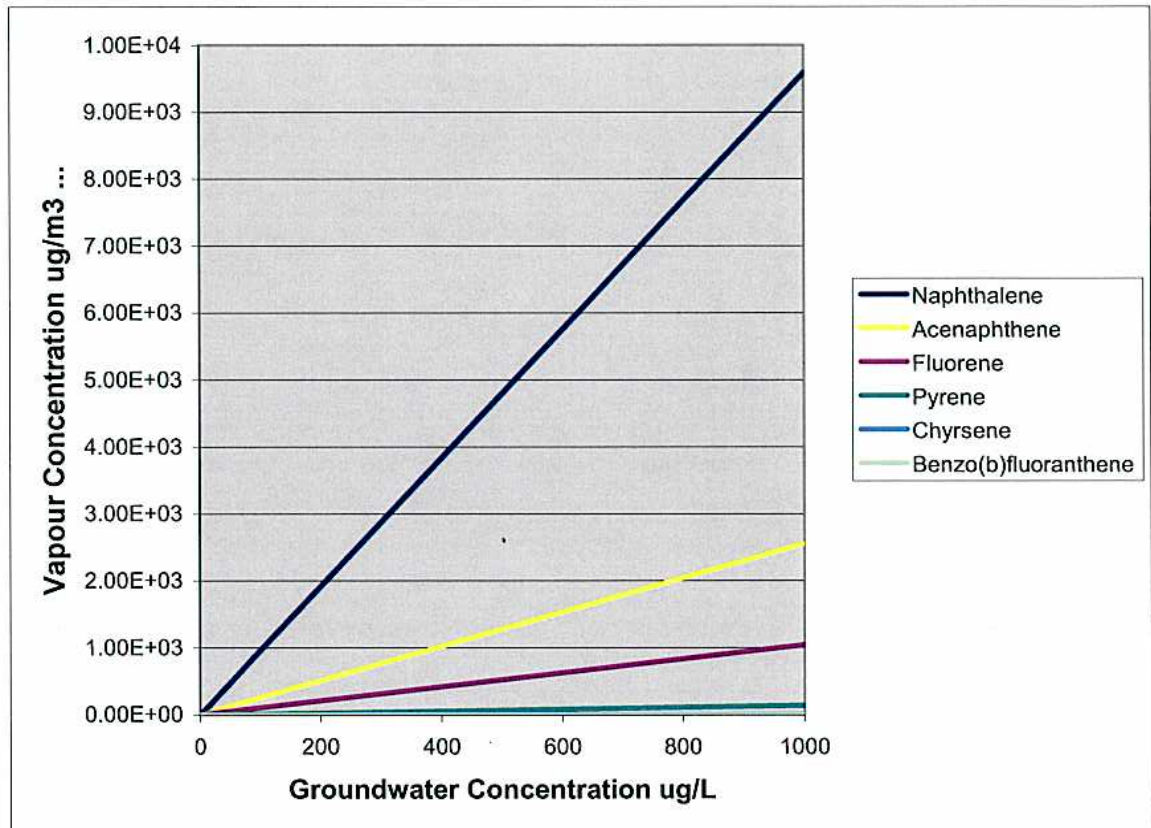
The computer model was first used to calculate the relationship between contaminant concentrations in the groundwater and the resulting source vapour concentrations. The groundwater concentrations used in the analysis cover the ranges that have been measured in the plume area for the three rounds of groundwater monitoring conducted at the site, as presented previously in **Table 17B**. The results of the analyses for BTEX are provided in **Figure 16** and for the six target PAHs in **Figure 17**.

- **Figure 16 Relationship Between Groundwater and Source Vapour Concentrations for BTEX Contamination in the Shallow Groundwater Aquifer**





- Figure 17 Relationship Between Groundwater and Source Vapour Concentrations for Target PAH Contamination in the Shallow Groundwater Aquifer



The results of the shallow groundwater analysis show:

- There is a linear relationship between volatile groundwater concentrations and the source vapour concentrations that would be measured near the water table;
- Each of the BTEX compounds generate similar source vapour concentrations, as shown by the clustered lines in **Figure 16**;
- There is a wide divergence in the vapour generating potential between the six target PAH compounds. **Figure 17** shows naphthalene to generate by far the highest vapours of all the PAH compounds, with benzo(b)fluorene and chrysene generating very little vapour; and
- The BTEX compounds are capable of generating much higher soil vapour concentrations than any of the PAH compounds. This is shown by the data provided in **Table 18C**, which provides a comparison of the predicted soil vapour concentrations that would be generated by 100µg/L of each target compound.

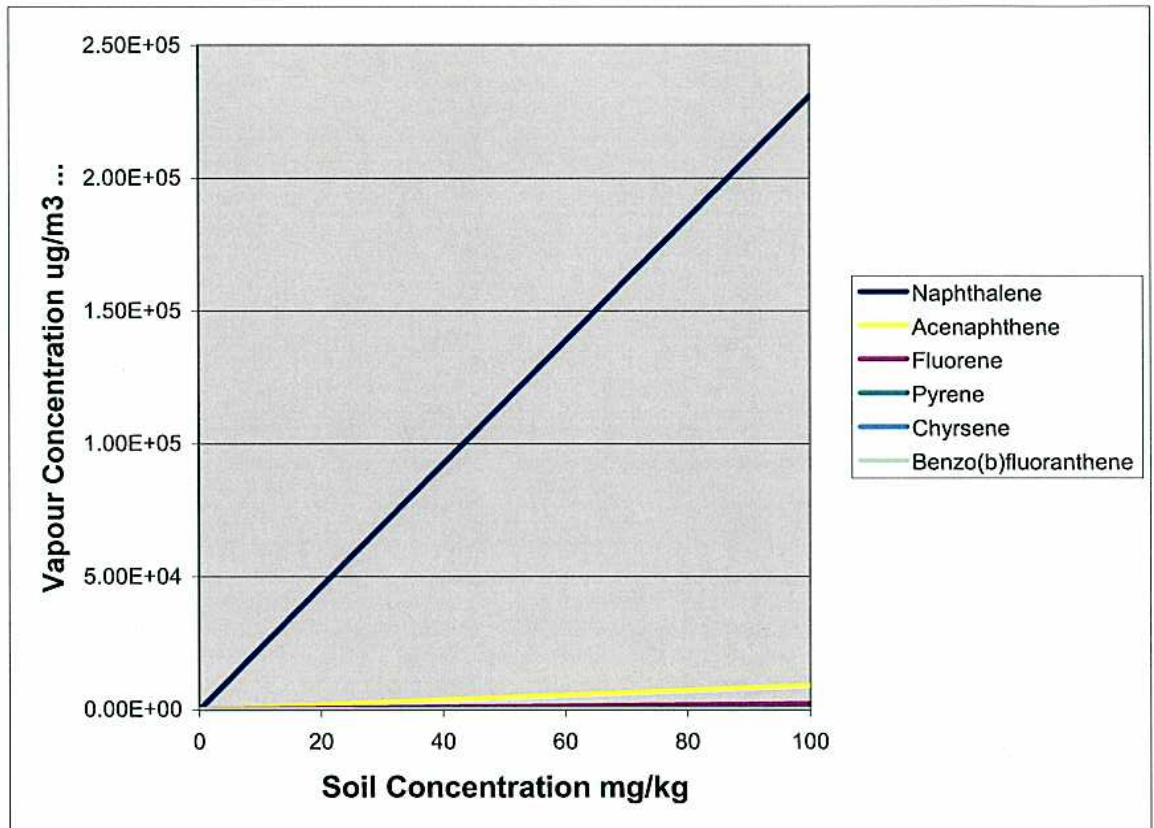


■ Table 18C Comparison of Soil Vapour Concentrations for Target Volatile Compounds at 100µg/L in Groundwater

Target Chemical	Soil Vapour Concentrations (µg/m ³)	Generation Potential Ratio (Benzene = 1)
Benzene	1.46E+04	1
Toluene	1.64E+04	1.12
Ethylbenzene	1.84E+04	1.26
m-Xylene	1.70E+04	1.16
o-Xylene	1.19E+04	0.815
p-Xylene	1.78E+04	1.22
Naphthalene	9.59E+02	0.0657
Acenaphthene	2.55E+02	0.0175
Fluorene	1.04E+02	0.00712
Pyrene	1.39E+02	0.000952
Chrysene	0.603	0.0000413
Benzo(b)fluoranthene	0.158	0.0000108

The computer model was then used to calculate the relationship between contaminant concentrations in the unsaturated shallow soils and the resulting source vapour concentrations. Only the six target PAHs were considered in this analysis since the laboratory data measured only very low BTEX concentrations in the soil samples collected from this area, as previously shown in **Table 17C**. The soil PAH concentrations used in the analysis cover the ranges that have been measured in the plume area, with the results of the analyses for the six target PAHs presented in **Figure 18**.

- **Figure 18 Relationship Between Soil and Source Vapour Concentrations for PAH Contamination in the Unsaturated Soils in the Shallow Plume Area**



The results of the shallow unsaturated soil analysis show similar trends to the groundwater analysis, namely:

- There is a linear relationship between volatile soil concentrations and the source vapour concentrations that would be measured in the shallow unsaturated soil layer above the water table; and
- There is a wide divergence in the vapour generating potential between the six target PAH compounds. **Figure 18** shows naphthalene to generate by far the highest vapours of all the PAH compounds, with benzo(b)fluorene and chrysene generating very little vapour.



9.4 Comparison between Field Measurements and Computer Analysis

The results of the computer analysis have been used to predict the range of soil vapour measurements that could have been expected to have been measured by the soil-gas monitoring wells that were installed at the Former Gasworks site. The analysis has used the range of volatile contaminant concentrations that have been measured in the shallow groundwater aquifer in the plume area, as previously presented in **Table 17B**. The results of the analysis are presented in **Table 18D**, where a comparison is also provided with the soil vapour results that were measured in the field, as previously presented in **Tables 18A** and **18B**.

■ **Table 18D Comparison between Measured and Predicted Soil Vapour Concentrations in the Area of the Volatile Contaminant Plume**

Target Chemical	Measured Groundwater Concentration (µg/L)	Measured Soil Concentration (mg/kg)	Measured Soil Vapour Concentration (µg/m ³)	Predicted Soil Vapour Concentration (µg/m ³)
Benzene	nd – 704	nd	nd – 16.7	nd - 1.03E+05
Toluene	nd	nd	nd – 28,000	Nd
Ethylbenzene	nd – 213	nd	nd	nd – 3.92E+04
m-Xylene	nd – 417	nd	nd	nd - 6.49E+04 (1)
o-Xylene				
p-Xylene				
Naphthalene	nd - 1460	nd - 280	nd – 5.41	nd – 6.61E+05
Acenaphthene	nd – 14	nd - 33	nd	nd – 3.04E+03
Fluorene	nd – 15	nd - 120	nd	nd – 2.48E+03
Pyrene	nd – 2	nd - 600	nd	395
Chrysene	nd	nd - 200	nd	12.1
Benzo(b)fluoranthene	nd	nd - 310	nd	4.90

Notes:

- (1) Predicted total xylene concentration based on average concentrations given by computer model for m-, o- and p-Xylene.

Comparison of the results from the computer analysis and the field measurements shows that highly variable field results are to be expected given the highly variable volatile concentrations that have been measured in the shallow groundwater and unsaturated soils at the Former Gasworks site. The low soil gas levels measured in wells MW30-MW34 in March 2005 are consistent with the low groundwater concentrations that were measured in the last monitoring undertaken also in March 2005 and the low soil concentrations that have been measured in the plume area.



However, the computer analysis shows that much higher soil gas vapours may be present at the site than were measured by the investigation. This is because the results of the computer analyses show that much higher soil gas levels may occur if the higher volatile concentrations measured in the earlier groundwater monitoring rounds and/or higher soil concentrations measured in some shallow soil samples are more representative of site conditions. Due to this high degree of variability, there is potential for elevated levels of soil gas vapours to be emitted from the ground surface of the site and the exposure pathway from volatile soil vapours needs to be included in this risk assessment.

The analysis also shows that the primary source of BTEX in the soil vapour at the volatile plume area is likely to be from the shallow groundwater, since no significant BTEX levels have been measured in the shallow soils. On the other hand, the analyses show that the primary source of the six target PAHs in the soil vapour at the volatile plume area is likely to be from the unsaturated shallow soils, due to the relatively higher PAH concentrations in these soils compared to the shallow groundwater. For example, 98% of the naphthalene concentrations in the soil vapour are predicted by the computer analysis to come from the unsaturated shallow soils compared to the shallow groundwater based on the average concentrations measured in the plume area.