Appendix B - Modelling Assessment Based On 2002 TA Luft Guideline values

Appendix B – Modelling Assessment Based on TA Luft 2002 Limits

This report is a revision of an assessment completed as part of a request for further information from the EPA in relation to the IPPC licence application submitted by Schwarz to the EPA in September 2004. This report has been prepared on the basis of a number of issues as follows:

- The EPA has indicated that ethanol and methanol should be considered as TA Luft Class I organic compounds under the requirements of the TA Luft 2002 guidelines;
- A number of main emission points at the Schwarz Pharma plant are now no longer in operation. These are BVE-002, BVE-003, BVE022 and VE-135. These points have therefore no been included in the current assessment.

This report therefore reassess the organics emissions based on the points noted above.

B.1 TA Luft 2002 Emission Limits

The latest TA Luft emission limits were published in 2002, 'First General Administrative Regulation Pertaining the Federal Immission Control Act (Technical Instructions on Air Quality Control – TA Luft)'. In relation to the emissions from the Schwarz site, the guidance document contains revised guideline values for organics, inorganics and particulates. These are summarised briefly below.

B.1.1 Organic Substances

The classification system for organics in TA Luft 2002 has changed from that specified in TA Luft 1986. Section 5.2.5 of the guidelines states that with regard to organic substances contained in waste gas, except organic particulate matter:

A total mass flow of	0.50 kg/hour
Or	
A total mass concentration of	50 mg/m^3

Each of which to be indicated as total carbon, may not be exceeded.

There are also specific limits for Class I and Class II organic substances as defined in TA Luft 2002. Class I and Class II concentrations may not exceed the following mass concentrations or mass flows in waste gases, each of which to be indicated as mass of organic substances:

Class I

Mass flow	0.10 kg/hour
Or	
Mass concentration	20 mg/m^3.

Class II

Mass flow	0.50 kg/hour
Or	
Mass concentration	0.10 g/m^3.

TA Luft 2002 provides a partial list of compounds categorised in Class I, with a complete list (10 compounds) for Class II compounds. Criteria for classification of Class I compounds is also provided. It is assumed that any compound not categorised in Class I or Class II need only comply with the total organic substances emission limit as detailed above.

Classification of the compounds emitted from the Schwarz site was carried out based on the criteria in the TA Luft 2002 guidelines. No Class II compounds were identified in the Schwarz organics emissions, with the following classified as Class I:

- Dichloromethane (emitted from VE-079);
- Toluene (emitted from VE-079 and NVE-001);
- Methanol (emitted from VE-079);
- Ethanol (emitted from VE-079);
- IMS (emitted from VE-079 and NVE-001).

The remainder of the organic compounds (see Table 3.1 in main report) therefore need to comply with the 50 mgC/m^3 limit if the mass flow is above 0.50 kgC/hour.

B.2 Modelling Methodology

The modelling methodology for each emission point is discussed below. In the modelling assessment the flow rate, stack diameter, stack height and temperature characteristics are as detailed in Table 2.3, i.e. identical to the modelling assessment in the main report. The buildings included in the assessment are as reported in Table 2.2. The terrain data employed in the modelling assessment detailed in the main report is also employed in this assessment.

Therefore, the only variation between the modelling assessment detailed in the main report and the current assessment is the mass emission rates as described below (and summarised in the following table). The data in this table is based on the TA Luft mass emission limit or the concentration limit, based on whichever results in the highest mass flow from the stack as explained in the following sections.

Table B.1: Summary of mass emission data employed in modelling exercise

Parameter	VE-079	NVE-001
General Organics (kgC/hour)	0.5	0.5
Class I Organics (kg/hour)	0.14	0.10

B.2.1 VE-079

Organic compounds emitted from this emission point are DCM, toluene, methanol, ethanol and IMS (all Class I), and tetrahydrofuran, xylene, acetone, IPA, hexane and ethyl acetate (general organics limit applies).

The maximum flow rate from this stack is reported at 7,000Nm^3/hr. The maximum Class I mass emission from this stack would occur at the Class I concentration limit of 20 mg/m^3, giving a mass flow of 0.14 kg/hour. This value is therefore employed in the modelling assessment as a worst case emission scenario.

In terms of the general organics emissions limit of 50 mgC/m^3, this would result in a mass flow of 0.35 kgC/hour at 7,000 Nm^3/hour. This is below the maximum allowed mass flow of 0.5 kgC/hour, hence the value of 0.5 kgC/hour is employed in the modelling scenario as a worst case emission scenario.

B.2.2 NVE-001

Reported organic emissions from this stack are toluene and IMS (Class I) and acetic acid and MIBK (general organics limit applies).

The maximum flow rate from this stack is reported at approximately 549 Nm^3/hr (based on 2004 monitoring data). At the maximum Class I concentration limit, the Class I mass flow would be 0.011 kg/hour. This is below the mass flow limit of 0.1 kg/hour hence this higher mass flow rate is employed in the assessment as a worst case emission scenario.

In terms of the general organics emissions limit of 50 mgC/m^3, this would result in a mass flow of 0.027 kgC/hour at 549 Nm^3/hour. This is below the maximum allowed mass flow of 0.5 kgC/hour, hence the value of 0.5 kgC/hour is employed in the modelling scenario as a worst case emission scenario.

B.3 Results & Conclusions

B.3.1 Class I Organics

Class I organics emissions were modelled from emission Point VE-079 and NVE-001. The stack parameters employed were as detailed in Table 2.3 of the main report, while the Class I emission rates used were as detailed in Section B.2.

The worst-case short-term ground level concentrations are reported in Table B.2 below. As a worst-case assumption, ground level Class I concentrations are compared to the Class I compound with the lowest guideline limit value as detailed in Table 3.1. In this case the chosen compound is dichloromethane (DCM).

The assessment conservatively assumes emissions from the stack at the maximum TA Luft rate throughout the course of each year, thus the results are considered highly conservative. The maximum predicted concentration for each year of meteorological data is below the OEL derived limit value for DCM, while the predicted 99th percentile value is below the Danish C-value for DCM. No significant impact is therefore predicted.

Table B.2: Worst-case short-term ground level Class I organics concentrations, $\mu g/m^3$

Parameter	2001	2002	2003	OEL Limit	C-Value
100th percentile hourly concentration	10.5	10.0	11.5	4,350	
99th percentile hourly concentration	5.8	5.7	5.8		20

B.3.2 General Organics

General organics emissions were modelled from emission point VE-079 and NVE-001. The stack parameters employed were as detailed in Table 2.3 of the main report, while the general organics emission rates used were as detailed in Section B.2.

The worst-case short-term ground level concentrations are reported in Table B.3 below. As a worst-case assumption, ground level General Organics concentrations are compared to the organic compound (excluding Class I compounds) with the lowest guideline limit value as detailed in Table 3.1. In this case the chosen compound is acetic acid.

The assessment conservatively assumes emissions from all the stacks at the maximum TA Luft rate throughout the course of each year, thus the results are considered highly conservative. The maximum predicted concentration for each year of meteorological data is below the OEL derived limit value for acetic acid, while the predicted 99th percentile value is above the Danish C-value for acetic acid. In reality acetic acid is released only from the nitration plant (NVE-001) and will not form 100 % of the predicted ground level concentrations. Other compounds are likely to be more dominant, i.e. acetone. This compound has higher ground level concentration guideline values (see Table 3.1) hence in practice the guideline values are unlikely to be breached for the individual compounds. Review of actual emissions monitoring data for 2004 indicates the following relative organics release rates (% of maximum measured 2004 mass release to air):

- Acetone – 51.4 %;
- Acetic Acid – 1.3 %;
- MIBK – 10.5 %;
- Ethyl acetate – 10.4 %;
- THF – 1.9 %;
- Xylene – 0.8 %;
- IPA – 16.1 %;
- Hexane – 7.6 %.

Based on the figures above the assumption that 100 % of the emissions are acetic acid is overly conservative and cannot reasonably be assumed in this case. Assuming the predicted ground level concentrations are composed of the above compounds in the same relative proportions the air quality guideline values in Table 3.1 would not be breached.

Based on the conservative assumptions employed in the modelling exercise (including the assumption that all stacks release at the maximum TA Luft 2002 rate) no significant impact is therefore predicted.

Table B.3: Worst-case short-term ground level General Organics concentrations, $\mu g/m^3$ (assuming all general organics present as acetic acid)

Parameter	2001	2002	2003	OEL Limit	C-Value
100th percentile hourly concentration	310.5	344.8	396.5	625	
99th percentile hourly concentration	113.4	110.6	116.9		100

B.3.3 General Conclusions

Emissions modelling based on the TA Luft 2002 guidelines was carried out for NVE-001 and VE-079, the two main emission points currently operating at the Schwarz site. Modelling of Class I organics emissions indicated compliance with the relevant guideline values. Modelling of general organics indicated that the likely ground level concentration and organics composition would be within the OEL derived guideline values. If all general organics emissions were assumed to be acetic acid there is potential for exceedence of the Danish C-value for acetic acid, however in practice acetic acid emissions of this magnitude will not take place. No significant impact due to organics emissions is therefore likely.