

# **Special Report No. 8**

## **HAZCHEM**

### **A Mathematical Model for Use in Risk Assessment**

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## **ECETOC Special Report No. 8**

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# **HAZCHEM**

## **A MATHEMATICAL MODEL FOR USE IN RISK ASSESSMENT OF SUBSTANCES**

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## **Part 1**

### **The HAZCHEM Model**

#### **Description of the Mathematical Equations**

## SECTION 1. INTRODUCTION

Substances which are released to the environment may pose a risk to man and/or environmental organisms. The magnitude of the risk depends on the intrinsic toxicological properties of the substance on the one hand and on level, duration and route of exposure of organisms to the substance on the other.

EU legislation requires that an assessment of the risk to the environment be carried out on the principle of a comparison of a "Predicted Environmental Concentration" (PEC) and a "Predicted No-Effect Concentration" (PNEC) (EEC, 1992; 1993a, 1993b, 1994).

ECETOC (1993a) described a scientifically-based risk assessment strategy as an iterative process allowing, where necessary, a step-wise refinement of the data used for an estimation of PEC and PNEC. The use of mathematical exposure models on a regional and on a local scale is essential in the process of risk assessment. Therefore, a model called HAZCHEM, based on a "Mackay Level III model" was programmed by an ECETOC Task Force Member (see p. 107). It was developed and used by ECETOC (1993a) and was compared to another model called PRISEC (USES, 1992).

In ECETOC (1993a) a number of steps in the overall process could at the time not be described in detail and are further elaborated in ECETOC (1994a). In addition, a strategy for the assessment of non-occupational exposure of man to chemicals was published (ECETOC, 1994b) which includes indirect human exposure via the food chain. In the frame of the elaboration of these reports, the HAZCHEM model was developed further, adapted to European conditions and subjected to sensitivity analyses. HAZCHEM calculations were more widely used in these reports.

Recently, USES became publicly available (RIVM, VROM, WVC, 1994). It appears that major parts of the two models are identical but that a number of differences exist, mainly concerning the following subjects:

- modelling of wastewater treatment plants;
- modelling of the steady-state concentration in soil;
- application factors used to derive NOEC or TDI values.



It is the intention of ECETOC to collaborate with the Commission of the European Communities and competent authorities, including those of The Netherlands who developed USES, with the aim of developing one program fully compatible with the EEC Technical Guidance documents on risk assessment of substances and adapted to European conditions.

The reasons for publishing HAZCHEM in the present state are:

- to provide a building block for the European program mentioned above;
- to ensure transparency of the scientific contents of ECETOC reports (ECETOC, 1993a; 1994a; 1994b) in which HAZCHEM was used as a tool to achieve results and to draw conclusions from these results;
- to make a computerised version of the model available to ECETOC member companies as an instrument suitable within the overall process of risk assessment;
- to stimulate scientific discussions on such models.

It must be emphasized that the report as presented here reflects the state of knowledge of the time at which the ECETOC reports mentioned above were elaborated. The improvement of such models is a continuous process. Discussions and developments within the various ECETOC Task Forces revealed the necessity for a number of changes and amendments which led to **HAZCHEM Version 2.0** which is presented here. Discussions are ongoing, especially on the topics of modelling sludge application and concentrations in soil. The contents of the EEC Technical Guidance documents on environmental risk assessment of existing substances, which presently are being evaluated, will also have to be taken into account. It is expected that these developments will require an update of such models in the future.

The purpose of this program is to provide the user with:

- an insight into environmental fate processes of chemical substances;
- an estimation of the concentration of substances in the environmental compartments at steady-state;
- a preliminary estimate of the tolerable daily intake for man;

- a preliminary estimate of quality criteria for the environmental compartments water and soil;
- a ratio between estimated daily human exposure and the tolerable daily intake;
- a ratio between estimated steady-state concentrations and quality criteria for the compartments water and soil.

The HAZCHEM program consists of a number of models which can be used independently from each other or consecutively for effects assessment, exposure assessment and/or risk characterisation. Moreover, it provides flexibility by displaying results of intermediate calculations and allows that these results be overwritten whenever more reliably estimated or measured data are available.

HAZCHEM consists of the following models:

- extrapolation of NOECs or TDIs from toxicological data;
- estimation of release to the environment;
- wastewater treatment model;
- environmental exposure on a regional scale;
- environmental exposure of water/air/soil on a local scale;
- characterisation of the risk by means of the PEC/PNEC-ratio.

In Part 1 of this report the mathematical equations are described. Part 2 is a user manual describing the individual screens and giving advice on how to run the model.

The symbols used in an equation are usually explained on the same or previous page, mostly below the equations. The symbols listed in Table 1, however, are widely used in physico-chemistry and are not repeated each time. An alphabetical list of all symbols used in HAZCHEM is given in Appendix A.

**Table 1**      **Symbols Frequently Used in Equations**

Symbol	Identification	Dimension	Numerical value (where relevant)
T	temperature	Kelvin	
T <sub>k</sub>	ambient temperature	Kelvin	293
R	gas constant	J/(°K -Mol)	8.314
Mw	molecular mass	g/Mol	
P	vapour pressure	Pascal	
S	water solubility	Mol/m <sup>3</sup>	
Sg	water solubility	mg/l	
H	Henry constant (= P/S)	Pascal -m <sup>3</sup> /Mol	
K <sub>ow</sub>	octanol/water partition coefficient		
BCF (sometimes BF)	bioconcentration factor		

## SECTION 2.                    EXTRAPOLATION    OF    TOXICOLOGICAL DATA

In this section a Predicted No Effective Concentration (PNEC) or a Tolerable Daily Intake (TDI) are extrapolated from the toxicological data. These values are derived in the same way as described in the EC Technical Guidance documents accompanying the risk assessment directive for new substances (EEC, 1993c). The assessment factors used in HAZCHEM therefore are not necessarily identical to the assessment factors proposed by ECETOC (see, for instance, ECETOC, 1993a; 1993b).

### 2.1 AQUATIC ENVIRONMENT

#### 2.1.1 Surface Water

The PNEC is estimated by one of the following options, depending on data availability:

- the  $PNEC_{aq}$  is estimated by dividing the lowest value of 3 long-term NOECs by a factor of 10;
- the  $PNEC_{aq}$  is estimated by dividing the lower value of 2 long-term NOECs (one of which is the algae NOEC of the base set) by a factor of 50;
- the  $PNEC_{aq}$  is estimated by dividing the lowest value of short-term  $LC_{50}$  or  $EC_{50}$  by a factor of 1,000.

#### 2.1.2 Sediment

In the absence of data it is recommended to estimate the  $PNEC_{sediment}$  from the  $PNEC_{aq}$  by multiplication with the sediment/water partition coefficient.

### 2.2 SOIL

The  $PNEC_{soil}$  is estimated by one of the following options, depending on data availability:

- the  $PNEC_{soil}$  is estimated by dividing the lower value of 2 long-term NOECs (e.g. the  $NOEC_{earthworm}$  and the  $NOEC_{plant}$ ) by a factor of 50;

- the  $PNEC_{soil}$  is estimated by dividing the only long-term NOEC by a factor of 100;
- the  $PNEC_{soil}$  is estimated by dividing the lowest value of short-term  $LC_{50}$  or  $EC_{50}$  by a factor of 1,000.

## 2.3 PNEC AND BIOMAGNIFICATION IN THE FOODCHAIN

For predatory aquatic and terrestrial organisms the Tolerable Daily Intake ( $TDI_{non-human}$ ) is derived by one of the following options, depending on data availability:

- the observed no effective daily oral dose over life time divided by 10;
- the observed no effective daily oral dose in a 90-day study divided by 30;
- the observed no effective daily oral dose in a 28-day study divided by 100;
- the oral  $LD_{50}$  divided by 1,000.

The  $PNEC_{pr}$  for predatory organisms is derived from:

- Predicted No-Effect Dose (PNED);
- bioconcentration factor ( $BCF_{terr}$  or  $BCF_{aq}$ );
- feeding rate (FR).

The  $PNEC_{praq}$  for predatory organisms in the aquatic environment is calculated according to the following equation (USES 1992):

$$PNEC_{praq} = \frac{PNED}{BCF_{aq} \cdot FR} \quad (1)$$

PNED = Predicted No-Effect Dose [mg/(kgbw -d)]

$BCF_{aq} = 0.05 \cdot K_{ow}$

FR = feeding rate [kg feed/(kgbw -d)]

The PNEC for predatory organisms in the terrestrial environment is calculated according to the following equation (USES 1992):

$$PNEC_{pterr} = \frac{PNED}{BCF_{terr} \cdot K_{ow}} \quad (2)$$

where  $BCF_{terr}$  is given by:

$$BCF_{terr} = 1.52 \cdot \frac{0.01 \cdot K_{ow}^{1.07}}{0.41 \cdot F_{oc} \cdot K_{ow}} \quad (3)$$

$F_{oc}$  = fraction organic carbon in soil [kg/kg]

In Equation 3 the numerator may be considered as the partitioning ratio earthworm/water and the denominator as the partitioning ratio soil-solids/water.

## 2.4 THE DAILY TOLERABLE INTAKE (TI) FOR MAN

The daily human daily TI [(mg/(kgbw -day))] is derived from feeding studies in the rat by one of the following options, depending on data availability:

- NOED lifetime divided by 100;
- NOED 90-day divided by 1,000;
- NOED 28-day divided by 3,000;
- $LD_{50}$  oral divided by 100,000.

The NOED is the No-Observed Effect Dose and is expressed in mg/(kgbw -d).

### SECTION 3. ESTIMATION OF RELEASE TO THE ENVIRONMENT

If no data on releases are available, a first estimate may be gained by applying this model which, for reasons of consistency, was taken from USES (RIVM, VROM, WVC, 1994). It calculates releases of a substance on the basis of tonnage produced, the use category and a number of physico-chemical parameters.

It should be noted that this model is a non-validated approach which in most cases will lead to a significant overestimate of releases. Furthermore, it could be demonstrated in a number of cases that the releases of substances were determined by the processes (including treatment) involved in production and/or use (ECETOC, 1994a) rather than by their physico-chemical properties. This model may be used **in the Screening Phase only**, and the user should be aware of its limitations.

As soon as realistic release estimates can be gained, these should be used and should overwrite the values predicted by means of the USES model.

Measured release data, where available, will always replace predicted releases.

## SECTION 4. MODELLING WASTE WATER TREATMENT

The modelled waste water treatment plant consists of only two compartments:

- a primary settler;
- a secondary treatment.

The model presented in this report was derived from models discussed by Pirt (1975), Namkung and Rittmann (1987), Clark *et al* (1991), Struijs *et al* (1991), and Cowan *et al* (1993).

### 4.1 PRIMARY SETTLER

In the primary settler partitioning of the chemical is assumed between water and solids. Two thirds of the solids are assumed to be removed by sedimentation. One third of the solids and the water phase will flow into the secondary treatment tank.

The individual parameters are calculated as follows:

#### *Influent flow*

$$Q_{sf} = \frac{V_{win} \cdot N_{ieq}}{24,000} \quad (4)$$

$Q_f$  = influent flow to WWTP [m<sup>3</sup>/h]

$V_{win}$  = volume of waste water per inhabitant equivalent [l/d]

$N_{ieq}$  = number of inhabitant equivalents discharging to the WWTP

#### *Partitioning of the substance between sludge and water*

$$F_{pw} = \left( 1 + \frac{C_{ps} \cdot P_{sf}}{1,000} \right)^{-1} \quad (5)$$

$F_{pw}$  = fraction of substance in primary settler dissolved

$F_{ps}$  = fraction of substance in primary settler adsorbed  
 $= 1 - F_{pw}$

$C_{ps}$  = concentration of primary sludge [g/l]



- $P_{sf}$  = partition coefficient primary sludge/water [l/kg]  
 If  $P_{sf} = 0$  (no input value), then  $P_{sf} = 0.411 - F_{C1} - 10^{\log K_{ow}}$   
 $F_{C1}$  = organic carbon content of primary sludge [kg/kg]

**Removal via primary sludge and primary sludge concentration**

$$S_{lp} = \frac{2Q_f \cdot C_{ps}}{3} \quad (6)$$

$$R_{ps} = \frac{2F_{ps} \cdot D_c}{3} \quad (7)$$

$$S_{lpc} = \frac{10^6 \cdot R_{ps}}{S_{lp}} \quad (8)$$

- $S_{lp}$  = primary sludge production per hour [kg/h]  
 $S_{lpc}$  = substance concentration in primary sludge [mg/kg]  
 $R_{ps}$  = removal rate of substance via primary sludge [kg/h]  
 $Q_f$  = influent flow to WWTP [m<sup>3</sup>/h]  
 $F_{ps}$  = fraction of substance in primary settler adsorbed  
 $C_{ps}$  = concentration of primary sludge [g/l]  
 $D_c$  = discharge of substance to waste water treatment plant [kg/h]

## 4.2 SECONDARY TREATMENT

**Volume of the aeration tank**

$$V_{as} = H_{rt} \cdot Q_f \quad (9)$$

- $V_{as}$  = Volume aeration tank [m<sup>3</sup>]  
 $H_{rt}$  = hydraulic retention time [h]  
 $Q_f$  = influent flow to WWTP [m<sup>3</sup>/h]

**Partitioning of the substance between sludge and water**

$$F_{sw} = \left( 1 + \frac{C_{sf} \cdot S_{ca}}{1,000} \right)^{-1} \quad (10)$$

- $F_{sw}$  = fraction of substance in aeration tank dissolved  
 $F_{ss}$  = fraction of substance in aeration tank suspended  
 $\quad = 1 - F_{sw}$   
 $C_{sf}$  = partition coefficient secondary sludge/water [l/kg]  
 If  $C_{sf} = 0$  (no input value), then  $C_{sf} = 0.411 - F_{c2} - 10^{\log Kow}$   
 $S_{ca}$  = sludge concentration in aeration tank [g/l]  
 $F_{c2}$  = organic carbon content of secondary sludge [kg/kg]

**Removal by volatilization**

$$R_a = 5.5 \cdot Q_f \cdot F_{sw} \cdot F_a \quad (11)$$

- $R_a$  = removal rate via volatilization [m<sup>3</sup>/h]  
 $Q_f$  = influent flow to WWTP [m<sup>3</sup>/h]  
 $F_{sw}$  = fraction of substance in aeration tank dissolved  
 $F_a$  = partitioning coefficient air/water  
 $\quad = H/(R - T_k)$

**Removal rate via effluent in the dissolved state**

$$R_{di} = Q_f \cdot F_{sw} \quad (12)$$

- $R_{di}$  = removal rate in dissolved state via effluent [m<sup>3</sup>/h]  
 $Q_f$  = influent flow to WWTP [m<sup>3</sup>/h]  
 $F_{sw}$  = fraction of substance in aeration tank dissolved

**Removal rate via effluent in the adsorbed state**

$$R_{su} = R_{di} \cdot C_{sf} \cdot E_{fp} \cdot 10^{-6} \quad (13)$$

- $R_{su}$  = removal rate in adsorbed state via effluent [m<sup>3</sup>/h]  
 $C_{sf}$  = partition coefficient secondary sludge/water [l/kg]  
 $E_{fp}$  = sludge concentration effluent [mg/l]

The conversion factor of  $10^{-6}$  is needed for converting the sludge concentration in the effluent into kg/litre.

**Removal rate via the secondary sludge removal**

$$R_{so} = \frac{V_{as} \cdot F_{ss}}{S_{rt}} \quad (14)$$

- $R_{so}$  = removal rate via secondary sludge [ $m^3/h$ ]
- $V_{as}$  = volume aeration tank [ $m^3$ ]
- $F_{ss}$  = fraction of substance in aeration tank suspended
- $S_{rt}$  = sludge retention time [h]

**Removal rate without biodegradation**

$$R_{bw} = R_a + R_{di} + R_{su} + R_{so} \quad (15)$$

- $R_a$  = removal rate via volatilization [ $m^3/h$ ]
- $R_{di}$  = removal rate in dissolved state via effluent [ $m^3/h$ ]
- $R_{su}$  = removal rate in adsorbed state via effluent [ $m^3/h$ ]
- $R_{so}$  = removal rate via secondary sludge [ $m^3/h$ ]

**Removal rate by biodegradation according to Namkung and Rittmann (1987) and Clark et al (1991)**

$$R_b = K_d \cdot V_{as} \quad (16)$$

- $R_b$  = removal rate by biodegradation [ $m^3/h$ ]
- $K_d$  = biodegradation rate [1/h]
- $V_{as}$  = volume aeration tank [ $m^3$ ]

If biodegradation takes place only in the dissolved state, then:

$$R_b = F_{sw} \cdot K_d \cdot V_{as} \quad (17)$$

- $F_{sw}$  = fraction of substance in aeration tank dissolved

**Removal rate by biodegradation according to Cowan et al (1993)**

$$R_{b1} = K_d \cdot H_{rt} \cdot F_{sw} \cdot V_{as} \quad (18)$$

$R_{b1}$  = removal rate by biodegradation in the dissolved state [ $m^3/h$ ]

$$R_{b2} = K_d \cdot S_{rt} \cdot F_{ss} \cdot V_{as} \quad (19)$$

$R_{b2}$  = removal rate by biodegradation in the adsorbed state [ $m^3/h$ ]

If biodegradation takes place only in the dissolved state then:

$$R_{b2} = 0$$

$R_b$  = total removal rate by biodegradation [ $m^3/h$ ]

$$= R_{b1} + R_{b2}$$

$H_{rt}$  = hydraulic retention time [h]

$S_{rt}$  = sludge retention time [h]

$F_{ss}$  = fraction of substance in aeration tank suspended

**Removal rate by biodegradation according to Pirt (1975) following a simplified approach**

$$C_{tr1} = \frac{1,000 \cdot D_{cs}}{R_{bw}} \quad (20)$$

$C_{tr1}$  = Estimated hypothetical concentration in aeration tank considering all removal processes except biodegradation [ $g/m^3$ ]

$D_{cs}$  = amount of chemical substance entering the aeration tank [kg/h]

$R_{wb}$  = removal rate without biodegradation [ $m^3/h$ ]

$$C_{tr2} = \frac{\frac{K_m}{S_{rt}}}{\left( V_{max} - \frac{1}{S_{rt}} \right)} \quad (21)$$

$C_{tr2}$  = Estimated final concentration in aeration tank considering all removal processes

$K_m$  = Michaelis-Menten constant [ $g/m^3$ ]

$V_{max}$  = Maximum degradation rate [1/h]

$S_{rt}$  = Sludge retention time [h]

If  $C_{tr1} - C_{tr2} < 0$ , then  $C_{tr2} = C_{tr1}$ ; if  $C_{tr2} < 0$ , then  $C_{tr2} = C_{tr1}$ .

The estimated total removal assuming a steady-state continuous culture of waste degrading bacteria, not influenced by other removal processes ( $R_{tot}$  in  $m^3/h$ ) is calculated as follows:

$$R_{tot} = \frac{1,000 \cdot D_{cs}}{C_{r2}} \quad (22)$$

$$\begin{aligned} R_b &= \text{estimated contribution of removal by biodegradation [m}^3/\text{h]} \\ &= R_{tot} - R_{wb} \end{aligned}$$

### ***Secondary sludge production or secondary sludge removal***

The total mass of suspended solids in the aeration tank ( $T_{ss}$  in kg) and the sludge removal ( $S_{ir}$  in kg/h) are given by:

$$T_{ss} = V_{as} \cdot S_{ca} \quad (23)$$

$$S_{ir} = \frac{T_{ss}}{S_{rt}} \quad (24)$$

$$\begin{aligned} S_{rt} &= \text{sludge retention time [h]} \\ V_{as} &= \text{volume aeration tank [m}^3\text{]} \\ S_{ca} &= \text{concentration of suspended solids in the aeration tank [g/l or kg/m}^3\text{]} \end{aligned}$$

### ***Total removal rate in the aeration tank***

$$R_{tot} = R_a + R_b + R_{di} + R_{su} + R_{so} \quad (25)$$

$$\begin{aligned} R_{tot} &= \text{total removal rate [m}^3/\text{h]} \\ R_a &= \text{removal rate via volatilization [m}^3/\text{h]} \\ R_b &= \text{total removal rate by biodegradation rate [m}^3/\text{h]} \\ R_{di} &= \text{removal rate in dissolved state via effluent [m}^3/\text{h]} \\ R_{su} &= \text{removal rate in adsorbed state via effluent m}^3/\text{h]} \\ R_{so} &= \text{removal rate via secondary sludge [m}^3/\text{h]} \end{aligned}$$

The transport rate of substance to the aeration tank ( $D_{cs}$  in kg/h) is given by:

$$D_{cs} = D_c - R_{ps} \quad (26)$$

$D_c$  = discharge of substance to waste water treatment plant [kg/h]

$R_{ps}$  = removal rate of substance via primary sludge [kg/h]

The total concentration of substance in the aeration tank ( $C_{tw}$  in kg/m<sup>3</sup> or g/l) is given by:

$$C_{tw} = \frac{D_{cs}}{R_{tot}} \quad (27)$$

#### ***Substance concentration in secondary sludge***

$$S_{lc} = \frac{10^6 \cdot F_{ss} \cdot C_{tw}}{S_{ca}} \quad (28)$$

$S_{lc}$  = substance concentration in secondary sludge [mg/kg]

$10^6$  = factor needed for conversion from g/g into mg/kg

$F_{ss}$  = fraction of substance in aeration tank suspended

$S_{ca}$  = concentration suspended solids in the aeration tank [g/l or kg/m<sup>3</sup>]

#### ***Dissolved and suspended effluent concentration***

$$C_{di} = 1,000 \cdot F_{sw} \cdot C_{tw} \quad (29)$$

$$C_{su} = 10^{-6} \cdot C_{di} \cdot C_{sf} \cdot E_{fp} \quad (30)$$

$C_{di}$  = effluent concentration in dissolved state [mg/l]

1,000 = factor needed for conversion from g/l into mg/l

$F_{sw}$  = fraction of substance in aeration tank dissolved

$C_{su}$  = effluent concentration in suspended state [mg/l]

$C_{sf}$  = partition coefficient secondary sludge/water [l/kg]

$E_{fp}$  = sludge concentration effluent [mg/l]

$10^{-6}$  = factor needed for conversion of sludge concentration in the effluent into kg/l

**Specific removal of substance (kg/hour)**

Removal can be calculated separately for specific pathways, i.e. for biodegradation ( $=R_b - C_{tw}$ ), for volatilization ( $=R_a - C_{tw}$ ), with primary sludge ( $=R_{ps} - C_{tw}$ ) and with secondary sludge ( $=R_{so} - C_{tw}$ ), where:

$C_{tw}$  = total concentration of substance in the aeration tank [kg/m<sup>3</sup> or g/l]

$R_b$  = total removal rate for biodegradation [m<sup>3</sup>/h]

$R_a$  = removal rate via volatilisation [m<sup>3</sup>/h]

$R_{ps}$  = removal rate of substance via primary sludge [kg/h]

$R_{so}$  = removal rate via secondary sludge [m<sup>3</sup>/h]

$$\% \text{ removal by primary sludge} = \frac{100 \cdot R_{ps}}{D_c} \quad (31)$$

$$\% \text{ removal by biodegradation} = \frac{100 \cdot R_b \cdot C_{tw}}{D_c} \quad (32)$$

$$\% \text{ total removal} = \frac{100 \cdot [D_c - (R_{di} + R_{su}) \cdot C_{tw}]}{D_c} \quad (33)$$

$D_c$  = discharge of substance to waste water treatment plant [kg/h]

$R_{di}$  = removal rate in dissolved state via effluent [m<sup>3</sup>/h]

$R_{su}$  = removal rate in adsorbed state via effluent m<sup>3</sup>/h]

## **SECTION 5. ESTIMATION OF THE HUMAN AND ENVIRONMENTAL EXPOSURE FROM A LOCAL POINT SOURCE**

### **5.1 LOCAL CONDITIONS**

In order to estimate the concentration in environmental compartments in the neighbourhood of local point sources the following settings are applied:

- the emissions to air, waste water, surface water or soil are estimated (Section 3);
- purification of industrial waste water is calculated employing a wastewater treatment plant of 10,000 inhabitant equivalents (Section 4);
- concentrations in surface water and sediment are calculated (Section 8);
- the yearly average concentration in air at a distance of 1,000 m from a local industrial plant and the wastewater treatment plant (Section 5.2);
- arable soil is exposed by means of:
  - application of activated sludge from the sewage treatment plant;
  - deposition from the air (Section 5.3);
- natural soil is exposed by deposition from the air only;
- the removal from soil is assumed to occur by evaporation, leaching and biodegradation (Section 5.4).

### **5.2 YEARLY AVERAGE CONCENTRATION IN THE AIR**

In order to estimate this concentration it is assumed, that:

- all emissions are at a stack height of 10 meters;



- an emission of 1 g/s will result in an annual average immission concentration of 1 µg/m<sup>3</sup>. This has been derived from calculations on the basis of the Dutch National Air Dispersion Model (RIVM, VROM, WVC, 1994).

### 5.3 DEPOSITION FROM AIR TO SOIL

The deposition velocity in m/h is dependent on the physical state of the substance in the air, i.e. as an aerosol or as a gas. The deposition velocity is dependent on the Henry coefficient for gaseous substances.

The fraction of the compound bound to an aerosol is estimated from:

$$F_{ab} = \frac{0.00017}{(0.00017 + P)} \quad (34)$$

$F_{ab}$  = aerosol-bound fraction

The deposition velocity of the aerosol-bound fraction ( $Dpv_{part}$ ) is assumed to be 36 m/h. The deposition velocity of the vapour fraction is assumed to be related to the Henry coefficient according to Table 1 below (USES, 1992).

**Table 1          Deposition Velocity of Gaseous Substances**

log H	deposition velocity ( $Dpv_{gas}$ ) in m/h
≤ -2	1.8
> -2 < 2	1.44
≥ 2	1.08

The deposition rate  $Dpr$  in  $\mu\text{g}/(\text{m}^2 \cdot \text{h})$  can be estimated from:

$$Dpr = Dpv \cdot E_a \cdot \frac{1,000}{3,600} \quad (35)$$

$E_a$  = Emission to air [kg/h]

$1,000/3,600$  = Conversion factor

The total deposition velocity  $Dpv$  in m/h is given by:

$$Dpv = Dpv_{part} \cdot F_{ab} + (1 - F_{ab}) \cdot Dpv_{gas} \quad (36)$$

$F_{ab}$  = aerosol-bound fraction

## 5.4 ESTIMATION OF THE STEADY-STATE CONCENTRATION IN SOIL

For this process a module different from USES (1992) was developed. It aims at describing a steady-state concentration after many years of exposure via aerial deposition and sludge application.

The local model as preferred in this report estimates a steady-state concentration in soil. It should be noted that such a steady-state concentration will be achieved only after many years of aerial deposition and/or sludge application.

The steady-state concentration in soil is controlled by:

- the deposition rate from air which can be estimated on the basis of the above equations;
- the application of sludge at a rate of about 2 t/(ha · y) resulting in an annual soil load of the substance ( $Sl_{Appl}$  in  $\mu\text{g}/(\text{m}^2 \cdot \text{h})$ ) of:

$$Sl_{Appl} = \frac{2 \cdot 10^6 \cdot Sl_{co}}{10^4 \cdot 365 \cdot 24} \quad (37)$$

$Sl_{co}$  = substance concentration in sludge in ppm;

- the removal by evaporation, leaching and degradation.

### 5.4.1 Removal by evaporation

Mass transfer by evaporation takes place at the following sites:

- from soil surface to air via an air boundary layer. The mass transfer coefficient for this process  $MTC_a$  is 5 m/h;
- from soil air to the soil surface via diffusion. The mass transfer coefficient for this process  $MTC_{sa}$  is 0.02 m/h;
- from soil water to the soil surface via diffusion. The mass transfer coefficient for this process  $MTC_{sw}$  is 0.01 mm/h.

The removal rate by evaporation  $K_{evap}$  in 1/h for arable and natural soil can be formulated by means of the fugacity modelling of Mackay *et al* (1992):

$$K_{evap} = \frac{1}{\left( \frac{1}{MTC_a \cdot Z_a} + \frac{1}{(MTC_{sa} \cdot Z_a + MTC_{sw} \cdot Z_w)} \right) \cdot Z_{soil} \cdot H_{soil}} \quad (38)$$

$H_{soil}$  = soil depth (= 0.2m for arable and 0.05m for natural soil)

$Z_{soil}$  =  $V_a \cdot Z_a + V_w \cdot Z_w + V_s \cdot Z_s$  [Mol/(m<sup>3</sup> · Pa)]

$Z_a$  =  $1/RT$  [Mol/(m<sup>3</sup> · Pa)]

$Z_w$  =  $1/H$  [Mol/(m<sup>3</sup> · Pa)]

$Z_s$  =  $K_{sol} \cdot \text{Dens}/H$  [Mol/m<sup>3</sup> · Pa]

$K_{sol}$  =  $0.41 \cdot F_{oc} \cdot K_{ow}$  [l/kg]

$F_{oc}$  = fraction organic carbon soil

$\text{Dens}_s$  = density solids in soil = 2.4 kg/l

$V_a$  = air volume in soil = 0.2 m<sup>3</sup>/m<sup>3</sup>

$V_w$  = water volume in soil = 0.3 m<sup>3</sup>/m<sup>3</sup>

$V_s$  = solids volume in soil = 0.5 m<sup>3</sup>/m<sup>3</sup>

### 5.4.2 Removal by leaching

It is assumed, that the annual rain excess is 0.3 meter per year. The removal rate by leaching is now formulated as:

$$K_{leach} = \frac{0.3 \cdot Z_w}{Z_{soil} \cdot H_{soil} \cdot 365 \cdot 24} \quad (39)$$

$K_{leach}$  = leaching rate arable or natural soil [1/h]

### 5.4.3 Removal by (bio)degradation

The (bio)degradation half life in soil ( $T_{1/2\text{soil}}$ ) is of decisive influence on the concentration of a substance in the soil. Assuming a first order degradation rate, the (bio)degradation rate constant  $K_{deg}$  expressed in 1/h can be derived as follows:

$$K_{deg} = \frac{\ln 2}{T_{1/2\text{soil}}} \quad (40)$$

### 5.4.4 The concentration in arable and natural soil

The concentration in arable soil ( $c_{\text{soil-ar}}$  in  $\mu\text{g/kg}$ ) is controlled by:

- deposition from the air;
- sludge application;
- removal by evaporation, leaching and biodegradation;
- the arable soil depth;

assuming uniform mixing. It is calculated as follows:

$$C_{\text{soil-ar}} = \frac{D_{pr} + SI_{\text{Appl}}}{(K_{deg} + K_{leach} + K_{evap}) \cdot H_{\text{soil-ar}} \cdot Den_{\text{soil}}} \quad (41)$$

The concentration in natural soil is controlled by:

- deposition from the air;
- removal by evaporation, leaching and biodegradation;
- the natural soil depth.

$$C_{\text{soil-nat}} = \frac{D_{\text{pr}}}{(K_{\text{deg}} + K_{\text{leach}} + K_{\text{evap}}) \cdot H_{\text{soil-nat}} \cdot \text{Den}_{\text{soil}}} \quad (42)$$

$D_{\text{pr}}$  = deposition rate [ $\mu\text{g}/(\text{m}^2 \cdot \text{h})$ ]

$SI_{\text{Appl}}$  = substance application rate via activated sludge [ $\mu\text{g}/(\text{m}^2 \cdot \text{h})$ ]

$H_{\text{soil-ar}}$  = arable soil depth [m]

$H_{\text{soil-nat}}$  = natural soil depth [m]

$\text{Den}_{\text{soil}}$  = density of soil [ $\text{kg}/\text{m}^3$ ]

$$= V_{\text{a}} \cdot \text{Den}_{\text{a}} + V_{\text{w}} \cdot \text{Den}_{\text{w}} + V_{\text{s}} \cdot \text{Den}_{\text{s}}$$

$\text{Den}_{\text{a}}$  = density of air in soil =  $1.2 \text{ kg}/\text{m}^3$

$\text{Den}_{\text{w}}$  = density of water in soil =  $1,000 \text{ kg}/\text{m}^3$

$\text{Den}_{\text{s}}$  = density of solids in soil =  $2,400 \text{ kg}/\text{m}^3$

$V_{\text{a}}$  = fraction of air volume in soil =  $0.2 \text{ m}^3/\text{m}^3$

$V_{\text{w}}$  = fraction of water volume in soil =  $0.3 \text{ m}^3/\text{m}^3$

$V_{\text{s}}$  = fraction of solids volume in soil =  $0.5 \text{ m}^3/\text{m}^3$

## SECTION 6. THE REGIONAL MODEL

### 6.1 INTRODUCTION

The regional model described in this report is mainly based on the generic level III model of Mackay *et al* (1992) but the settings for surface areas, compartment volumes and organic carbon contents of soil and sediment were adapted to conditions more similar to those of the European Union member countries. In addition, a second soil compartment was introduced, a so-called natural soil compartment, on which no activated sludge of the sewage treatment plant is applied. Further deviations from the Mackay model are described below.

### 6.2 DEVIATIONS FROM THE MACKAY LEVEL III MODEL

The following elimination pathways were remodelled:

- sediment deposition and sediment resuspension;
- the advective air flow and air residence time;
- the advective water flow and water residence time.

These modules are described below.

#### 6.2.1 Sediment deposition, resuspension and burial rate

The density of solids in the suspended matter is assumed to be 2,400 kg/m<sup>3</sup>. This assumption is needed to achieve a closed mass balance of the sediment by deposition, resuspension and burial. The sediment deposition rate ( $Dv_{sed}$  in m/h) is assumed to be linearly related to the suspended matter content according to the equation:

$$Dv_{sed} = 6.67 \cdot 10^{-8} \cdot Spma \quad (43)$$

$Spma$  in [mg/l] but considered dimensionless in this specific equation.

The sediment burial rate is an input parameter in the modification of the Mackay level III model. The sediment burial rate can never exceed the sediment deposition rate. Therefore, if the sediment burial

rate is set to a figure exceeding the deposition rate, then the burial rate becomes equal to the deposition rate. The difference between the sediment deposition and burial rate is considered to be the sediment resuspension rate. If the sediment burial rate is set to zero, then the resuspension rate becomes equal to the deposition rate.

The residence time of the sediment ( $S_{ert}$  in h) is estimated from:

$$S_{ert} = \frac{V_{sed} \cdot D_{sed}}{B_{ur}} \quad (44)$$

$V_{sed}$  = fraction of solids in sediment

$D_{sed}$  = sediment depth [m]

$B_{ur}$  = burial rate [m/h]

### 6.2.2 The residence time of air in the regional model

The residence time of air is estimated from the square root of the area of the region ( $A_r$  in  $m^2$ ), divided by the wind velocity ( $W_{vi}$ ) in m/h. Wind velocity is an input parameter of the program, so the influence of the wind velocity on the air residence time can be demonstrated.

The residence time of air ( $A_{rt}$ ) is estimated to be:

$$A_{rt} = \frac{\sqrt{A_r}}{W_{vi}} \quad (45)$$

### 6.2.3 The residence time of water in the regional model

The residence time of water is estimated from the volume of the water compartment ( $V_w$  = water area - depth in  $m^3$ ) divided by the sum of the advective water flows VR1 and VR2 in  $m^3/sec$ .

The advective flow rates are:

VR1 = waste water flow, related to the number of inhabitant equivalents [ $m^3/h$ ];

VR2 = rain precipitation excess multiplied with the area of the region [ $m^3/h$ ]

VR3 = the advective flow of river water [ $m^3/h$ ]

The residence time of the water (Wrt) in the regional model is estimated to be:

$$Wrt = \frac{V_w}{(VR1 + VR2 + VR3)} \quad (46)$$



## SECTION 7. DESCRIPTION OF THE FOOD CHAIN

### 7.1 ESTIMATION OF PLANT UPTAKE OF CHEMICALS FROM SOIL

It is assumed that absorption from soil is controlled by the concentration of the substance in pore water. This is described by:

$$C_{pw} = F_w \cdot C_{tot} \quad (47)$$

$C_{pw}$  = concentration in pore water

$C_{tot}$  = total soil concentration

$F_w$  = ratio of concentrations in pore water and in total soil:

$$F_w = \frac{1}{V_a \cdot \frac{H}{RT} + V_w + V_s \cdot f_{oc} \cdot K_{oc}} \quad (48)$$

$V_a$  = air volume in soil (0.2 m<sup>3</sup>/m<sup>3</sup>)

$V_w$  = water volume in soil (0.3 m<sup>3</sup>/m<sup>3</sup>)

$V_s$  = solid volume in soil (0.5 m<sup>3</sup>/m<sup>3</sup>)

$f_{oc}$  = fraction organic carbon in soil

$K_{oc}$  = partition coefficient soil organic carbon/water [kg/l]

= 0.41  $\cdot K_{ow}$   $\cdot \text{Den}_s / 1,000$

$\text{Den}_s$  = density of soil (2,400 kg/m<sup>3</sup>)

Briggs *et al* (1982, 1983) described methods for the estimation of concentration factors for plants, based on barley shoots:

- from pore water into root tissue (RCF = Root Concentration Factor);
- from pore water into the xylem fluid (TSCF = Transportation Stream Concentration Factor);
- from the xylem fluid into stems and leaves (SCF = Stem Concentration Factor).

The RCF was described by:

$$RCF = 10^{(0.77 \cdot \log(K_{ow}) - 1.52)} + 0.82 \quad (49)$$

The RCF was based on roots with relatively much peel, containing lipids. In order to get a more realistic RCF for potatoes with relatively more pulp and less skin, containing lipids, this RCF was lowered with a factor of 10:

$$RCF_{potato} = 10^{(0.77 \cdot \log(K_{ow}) - 2.52)} + 0.82 \quad (50)$$

The concentration in potatoes in HAZCHEM is estimated as follows:

$$C_{potato} = RCF_{potato} \cdot F_w \cdot C_{tot} \quad (51)$$

The TSCF was described by:

$$TSCF = 0.784 \cdot 10^{\left(-\frac{(\log(K_{ow}) - 1.78)^2}{2.44}\right)} \quad (52)$$

and the SCF by:

$$SCF = 10^{(0.95 \cdot \log(K_{ow}) - 2.05)} + 0.82 \quad (53)$$

The concentration in stem and leaves is estimated by means of the TSCF and the SCF from the total concentration in soil as follows:

$$C_{slpw} = TSCF \cdot SCF \cdot F_w \cdot C_{tot} \quad (54)$$

$C_{slpw}$  = concentration in stem, leaves by absorption from pore water

TSCF = Transportation Stream Concentration Factor

SCF = Stem Concentration Factor

$F_w$  = ratio between pore water concentration and total soil concentration

$C_{tot}$  = total soil concentration

The  $C_{slpw}$  and the  $C_{potato}$  is used in HAZCHEM for estimation of the contribution to the level in vegetables and cereals or potatoes respectively by transfer of environmentally dispersed chemicals from soil to the human food chain.

## 7.2 ESTIMATION OF PLANT UPTAKE OF CHEMICALS FROM AIR

The plant may be contaminated by deposition from the air. The level of contamination is dependent on:

- the partitioning of the chemical between particulates and the gas phase in air;

- the deposition rate of the chemical;
- the interception factor of the crop ( $I_{cf} = 0.4$ );
- the crop weight per  $m^2$  ( $Crw = 1.4$  kg fresh weight);
- the elimination rate of the deposited chemical from the plant ( $Elr = 0.0014 \text{ h}^{-1}$ ).

The following assumptions were made about the deposition rates:

- $F_{part}$  = fraction of substance in air as particulate  
=  $0.00017 / (P + 0.00017)$
- deposition velocity of particles ( $V_{part}$ ) is 0.01 m/s
- deposition velocity of gases ( $V_{gas}$ ) is  
0.0005 m/s if  $H \leq 0.01$   
0.0004 m/s if  $0.1 < H < 100$   
0.0003 m/s if  $H \geq 100$

The deposition rate  $Dpr$  in  $\mu\text{g}/(\text{m}^2 \cdot \text{h})$  is estimated by:

$$Dpr = C_{air} \cdot (F_{part} \cdot V_{part} + (1 - F_{part}) \cdot V_{gas}) \cdot 3,600 \quad (55)$$

$C_{air}$  = concentration in air ( $\mu\text{g}/\text{m}^3$ )

The concentration in vegetables due to deposition from air is estimated by assuming equilibrium between deposition and elimination processes:

$$C_{sldp} = \frac{Dpr \cdot I_{cf}}{Elr \cdot Crw} \quad (56)$$

$C_{sldp}$  = Concentration in stem and leaves due to deposition [ $\mu\text{g}/\text{kg}$ ]

$Dpr$  = Deposition rate [ $\mu\text{g}/\text{m}^2/\text{h}$ ]

$I_{cf}$  = Interception factor for crops

$Elr$  = Elimination rate of deposited chemical [ $1/\text{h}$ ]

$Crw$  = Crop fresh weight per  $m^2$

Finally a check is made whether  $C_{sldp}$  exceeds the plant level, being assumed to be in equilibrium with the air level (equal fugacity in plant tissue and air):

$$Z_{plant} = \frac{F_{water} + F_{lipid} \cdot K_{ow}}{H} \quad (57)$$

$$Z_{air} = \frac{F_{air} + F_{prt} \cdot \frac{6 \cdot 10^6}{P}}{RT} \quad (58)$$

$Z_{plant}$  = fugacity capacity constant plant

$Z_{air}$  = fugacity capacity constant air

$F_{water}$  = water fraction ( $0.8 \text{ m}^3/\text{m}^3$ )

$F_{lipid}$  = lipid content ( $0.01 \text{ m}^3/\text{m}^3$ ) (Mackay, 1991)

$F_{air}$  = volume fraction gas phase ( $1 \text{ m}^3/\text{m}^3$ )

$F_{prt}$  = volume fraction aerosol ( $10^{-11} \text{ m}^3/\text{m}^3$ )

The concentration in plant in equilibrium with air based on fugacity considerations ( $C_{plfug}$ ) in  $\mu\text{g}/\text{kg}$  is given by:

$$C_{plfug} = \frac{Z_{plant}}{Z_{air}} \cdot \frac{C_{air}}{1,000} \quad (59)$$

If  $C_{sldp} > C_{plfug}$ , then  $C_{sldp} = C_{plfug}$

The  $C_{sldp}$  is used in HAZCHEM for an estimation of the contribution of chemicals dispersed in air being transferred from the air to vegetables and cereals as well as potatoes, i.e. to the human food chain.

### 7.3 ESTIMATION OF THE CONCENTRATION OF CHEMICALS IN THE PLANT AFTER UPTAKE FROM THE AIR AND FROM SOIL

The contributions of  $C_{slpw}$  and  $C_{sldp}$  are added in order to obtain the final concentration in stems and leaves ( $C_{sl}$ ).

$$C_{sl} = C_{slpw} + C_{sldp} \quad (60)$$

## 7.4 ESTIMATION OF THE LEVEL OF CHEMICALS IN MEAT AND DAIRY PRODUCTS

For the estimation of the level in meat and milkfat the regression equations derived by Travis and Arms (1988) were used. The bioconcentration factor was defined as the ratio of the concentration in milk or meat (in mg/kg) to the uptake (in mg/day). The authors have related the observed bioconcentration factors of chemicals in meat ( $BF_{meat}$ ) and milk ( $BF_{milk}$ ) to the octanol/water partition coefficient.

$$BF_{meat} = 10^{(\log K_{ow} - 7.6)} \quad (61)$$

$$BF_{milk} = 10^{(\log K_{ow} - 8.1)} \quad (62)$$

The dairy products derived from cow milk, eg butter and cheese, may contain variable amounts of milkfat. Therefore, the equation for the bioconcentration factor for dairy products was transformed to the bioconcentration factor for milkfat on the basis of a fat content of 4%. The combination of the of the data on milkfat content of butter (80 %), cheese (25 %), milk and yogurt (4 %) with the data on food consumption allows a more accurate estimation of the uptake of chemicals via milkfat:

$$BF_{milkfat} = 10^{(\log K_{ow} - 6.7)} \quad (63)$$

In order to estimate levels in meat and milkfat, the daily uptake of chemicals for cattle in mg/day is needed. This daily uptake is estimated in HAZCHEM from the following exposure routes:

- 86 kg fresh feed, consisting of grass with the level  $C_{sl}$  (90 %) and of fodder beets with the level of  $C_{potato}$  (10 %);
- 0.576 kg of wet soil;
- 55 l of drinking water;
- 122 m<sup>3</sup> air.

The Daily Uptake of Cattle (DUC) in µg/kg is estimated from:

$$DUC = 122C_{air} + 55C_{water} + 0.576C_{soil} + 86 \cdot (0.9C_{sl} + 0.1C_{potato}) \quad (64)$$

$C_{air}$  is expressed in µg/m<sup>3</sup>, the other concentrations in µg/kg.

The concentration in meat and dairy products is estimated according to the equations below:

$$C_{meat} = BF_{meat} \cdot DUC \quad (65)$$

$$C_{milkfat} = BF_{milkfat} \cdot DUC \quad (66)$$

$$C_{milk} = 0.04 \cdot BF_{milkfat} \cdot DUC \quad (67)$$

$$C_{butter} = 0.80 \cdot BF_{milkfat} \cdot DUC \quad (68)$$

$$C_{cheese} = 0.25 \cdot BF_{milkfat} \cdot DUC \quad (69)$$

## 7.5 ESTIMATION OF THE CONCENTRATION OF SUBSTANCES IN DRINKING WATER

Groundwater and surface water may be used as sources for drinking water.

The concentration in groundwater is set equal to the pore water concentration in steady-state. This means that equilibrium is assumed between the daily supply, averaged over many years, and the daily elimination from degradation, leaching and volatilisation. The level in groundwater for use as drinking water is estimated by averaging the pore water level in natural and arable soil. The groundwater is assumed not to be subject to any purification.

The concentration in surface water is set equal to the steady-state, i.e. equilibrium is assumed between the daily supply and elimination by degradation, sedimentation and volatilisation. Surface water may be purified by means of two purification systems (USES, 1992). The extent of removal is assumed to be dependent on the physico-chemical properties of the substance and of its biodegradation behaviour.

**Table 2** Purification Factors of Surface Waters as assumed by Hrubec and Toet (1992)

Physico-chemical properties and degradation behaviour	Purification System 1 purification factors	Purification System 2 purification factors
Henry coefficient $H \leq 100$ $> 100$	PF1= 1 0.5	PF1= 1 0.5
$\log(\text{octanol/water})$ $< 4$ $\geq 4$ and $\leq 5$ $> 5$	PF2= 1 0.25 0.0625	PF2= 1 0.5 0.25
Half-life days (bio)degradation $\geq 240$ $< 240$	PF3= 1 1	PF3= 1 0.25
Total purification	$PFT1 = PF1 \cdot PF2 \cdot PF3$	$PFT2 = PF1 \cdot PF2 \cdot PF3$

The level in drinking water is estimated by multiplying the surface water level with the greater factor of PFT1 or PFT2. If the drinking water level of purified surface water is lower than the level in ground water, then ground water is assumed to be used as drinking water.

## SECTION 8. THE RIVER MODEL

The river model consists of 2 parts, i.e. the river dilution model and the river fate model.

### 8.1 THE RIVER DILUTION MODEL

This model was derived from de Nijs and de Greef (1992) and further adapted after personal discussions with de Nijs (1993). Calculations are performed in the following sequence of steps:

***Stream velocity, transversal dispersion coefficient and distance downstream needed for complete mixing***

$$U_{avg} = \frac{Q_w + Q_e}{W_r \cdot H_r} \quad (70)$$

$U_{avg}$  = average longitudinal stream velocity [m/s]

$Q_w$  = river flow rate [m<sup>3</sup>/s]

$Q_e$  = effluent flow rate [m<sup>3</sup>/s]

$W_r$  = river width [m]

$H_r$  = river depth [m]

$$R_h = \frac{W_r \cdot H_r}{W_r + 2H_r} \quad (71)$$

$R_h$  = hydraulic radius of the river [m]

$C_z$  = Chezy coefficient =  $60 \cdot R_h^{(1/6)}$

$$U_{ss} = \frac{U_{avg} \cdot \sqrt{9.81}}{C_z} \quad (72)$$

$U_{ss}$  = shear stress velocity [m/s]

$$D_t = 0.6 \cdot H_r \cdot U_{ss} \quad (73)$$

$D_t$  = transversal dispersion coefficient [m<sup>2</sup>/s]



$$L_{mix} = \frac{0.4 \cdot U_{avg} \cdot W_r^2}{D_t} \quad (74)$$

$L_{mix}$  = maximum longitudinal distance downstream from the point of discharge needed for complete mixing

***Increase of concentration in water after discharge of effluent***

$$C_{wa} = \left\langle \sum_{n=-3}^3 \left[ \operatorname{erf} \left( \frac{Y_{acc} + \frac{R_{mix}}{W_r} + 2n}{\sqrt{4X_{acc}}} \right) - \operatorname{erf} \left( \frac{Y_{acc} - \frac{R_{mix}}{W_r} + 2n}{\sqrt{4X_{acc}}} \right) \right] \right\rangle \cdot \frac{C_e \cdot W_r}{2R_{mix}} \quad (75)$$

$C_{wa}$  = increase of concentration in riverwater after partial mixing with effluent, dependent on X and Y [mg/l]

erf = error function

$$C_{inf} = \frac{Q_e \cdot C_e}{Q_e + Q_w} \quad (76)$$

$C_{inf}$  = increase of concentration in river water after complete homogeneous mixing

$C_e$  = effluent concentration [mg/l]

$Q_w$  = river flow rate [m<sup>3</sup>/s]

$Q_e$  = effluent flow rate [m<sup>3</sup>/s]

X = distance downstream from point of discharge [m]

$X_{acc} = X - D_t / (U_{avg} - W_r^2)$  [dimensionless]

Y = cross-sectional distance from point of effluent discharge [m]

$Y_{acc} = Y / W_r$  [dimensionless]

$D_t$  = transversal dispersion coefficient [m<sup>2</sup>/s]

$U_{avg}$  = average longitudinal stream velocity [m/s]

$W_r$  = river width [m]

$R_{mix}$  = radius/width of the instantaneous mixing zone [m]

**Estimated concentration of the substance after dispersion of the effluent in river water without considering removal processes**

$$C_{wd} = C_{wa} + \left(1 - \frac{C_{wa}}{C_e}\right) \cdot C_{wr} \quad (77)$$

- $C_{wd}$  = concentration in the waste water plume in the river [mg/l]  
 $C_{wa}$  = increase of concentration in riverwater after partial mixing with effluent [mg/l]  
 $C_e$  = concentration effluent [mg/l]  
 $C_{wr}$  = background concentration of the substance in river water

In the above calculations it is assumed, that the substance does not disappear from the water by volatilization, sedimentation and biodegradation.

## 8.2 MODEL OF FINAL FATE CONSIDERING VOLATILIZATION, SEDIMENTATION AND (BIO)DEGRADATION

The modelling of the final fate of the chemical in a river is based upon the Quantitative Air Water Sediment Interaction model developed by Mackay *et al* (1983). The volatilization process was modelled according to Southworth (1979). The following equations describing the processes were developed.

### Volatilization

$$K_{dvap} = \frac{K_{gl} \cdot F_{rdi}}{H_r \cdot 3,600} \quad (78)$$

- $K_{dvap}$  = removal rate for volatilization from the river water [1/s]  
 $H_r$  = mean river depth [m]  
 $F_{rdi}$  = fraction of substance in dissolved state in river water  
 $= 1 / (1 + S_{pa} \cdot K_{spw} / 10^6)$   
 $S_{pa}$  = concentration suspended particulates [mg/l]  
 $K_{spw}$  = partition coefficient between suspended particulates and river water [l/kg]  
 $K_{gl}$  = overall mass transfer coefficient from water to air [m/h]  
 $= P_{aw} \cdot K_g \cdot K_l / (P_{aw} \cdot K_g + K_l)$   
 $P_{aw}$  = partitioning coefficient air/water  
 $= H / (R_g \cdot T_k)$

$$K_g = 11.375 \cdot (U_{fr} + U_{avg}) \cdot \sqrt{\frac{18}{Mw}} \quad (79)$$

$K_g$  = the gas phase exchange constant, a measure of the rate of transport of the material away from the interphase in the air [m/h]

$$K_l = \frac{0.2351 \cdot \sqrt{\frac{32}{Mw}} \cdot U_{avg}^{0.969}}{H_r^{0.673}} \quad (80)$$

$K_l$  = the liquid phase exchange constant, a measure of the rate of transport of the material to the interphase in the water [m/h]

If  $U_{fr} \geq 1.9$  m/s, then  $K_l = K_l - 10^{U_{fr}-1.9}$

$U_{avg}$  = longitudinal stream velocity [m/s]

$H_r$  = mean depth of the river [m]

$$U_{fr} = \frac{0.4 \cdot W_{vl}}{\log\left(\frac{10}{0.03}\right)} \quad (81)$$

$U_{fr}$  = friction velocity [m/s]

$W_{vl}$  = wind velocity at a height of 10 meter [m/s]

### **Sedimentation**

Mackay *et al* (1992) assumed that the top layer of the sediment contains 80% (v/v) of water and 20% (v/v) of solids. Therefore, deposition of the suspended particulates contributes only 20% to the total increase in thickness [m/h] of the bulk sediment. The density of the sediment solids is 2.4 kg/l. These assumptions results in a total sediment density of 1.28 kg/l. The density of the suspended particulates is assumed to be equal to the density of solids in the bulk sediment.

Burial in the sediment is next to (bio)degradation a route of removal. The resuspension rate of the sediment  $R_{se}$  is assumed to be equal to the deposition rate  $H_{dse}$  minus the burial rate  $B_{rs}$ .

$$K_{dsp} = \frac{(B_{rs} + \log 2 \cdot \frac{H_s}{H_{ls}}) \cdot F_{rse}}{3600 \cdot H_r} \quad (82)$$

- $K_{dsp}$  = removal rate from the river due to sedimentation [1/s]  
 $B_{rs}$  = burial rate of sediment [m/h]  
 $H_s$  = depth of sediment layer [m]  
 $H_{ls}$  = half life time in sediment for biodegradation [h]  
 $F_{rse}$  = ratio between the concentration [mg/l] in sediment and in river water.  
 $H_r$  = mean river depth [m]

$$F_{rse} = \frac{\left( \frac{K_{tse} + H_{dse} \cdot K_{spw} \cdot F_{pr} \cdot D_{pr}}{1 + S_{pa} \cdot K_{spw} \cdot 10^{-6}} \right)}{\left( B_{rs} + R_{se} + \frac{\log 2 \cdot H_s}{H_{ls}} + \frac{K_{tse}}{(1 - F_{pr} + F_{pr} \cdot D_{pr} \cdot K_{sed})} \right)} \quad (83)$$

- $K_{tse}$  = mass transfer coefficient for diffusion between sediment and water  
 = 0.0001 m/h (Mackay *et al*, 1992)  
 $H_{dse}$  = sediment deposition thickness rate [m/h]  
 =  $3.33 \cdot 10^{-7} - S_{pa}$  m/h.

Mackay *et al* (1992) proposed  $6.67 \cdot 10^{-8}$  (m/h)/(mg/l susp. part) for the solids. Because the sediment contains only 20% solids, this figure was multiplied by 5 in order to adapt it to bulk sediment.

- $S_{pa}$  = concentration of suspended particulates [mg/l]  
 $K_{spw}$  = partition coefficient between suspended particulates and river water [l/kg]  
 $F_{pr}$  = volume fraction 0.2 of suspended particulates in bulk sediment  
 $D_{pr}$  = density of solids of suspended particulates and sediment  
 = 2.4 kg/l  
 $B_{rs}$  = sediment burial rate [m/h]  
 =  $1.141 \cdot 10^{-7} - R_{sx}$   
 $R_{sx}$  = sediment burial rate [mm/y] (via input screen)  
 $R_{se}$  = sediment resuspension rate [m/h]  
 =  $H_{dse} - B_{rs}$   
 $H_s$  = depth of sediment layer [m]  
 $H_{ls}$  = half life time in sediment for biodegradation [h]  
 $K_{sed}$  = partition coefficient between sediment solids and river water [l/kg]

**Biodegradation**

$$K_{deg} = \frac{\log 2}{H_{lw} \cdot 3,600} \quad (84)$$

$K_{deg}$  = removal rate from the river water due to biodegradation [(1/s)]

$H_{lw}$  = half life time in water for biodegradation [h]

**Total removal rate from the river water at steady-state**

$$K_{elt} = K_{deg} \cdot K_{dsp} \cdot K_{dvap} \quad (85)$$

$K_{elt}$  = sum of all removal rates in river water [1/s]

$K_{deg}$  = removal rate from the river water due to biodegradation [1/s]

$K_{dsp}$  = removal rate from the river water due to sedimentation [(1/s)]

$K_{dvap}$  = removal rate from the river water due to volatilization [1/s]

**The final concentration in river water taking into account dispersion and removal processes**

$$C_{wf} = F_{rel} \cdot C_{wd} \quad (86)$$

$C_{wf}$  = final concentration in river water, taking into account removal processes and dispersion [mg/l]

$C_{wd}$  = expected concentration at distance X downstream and distance Y from the border of discharge on the basis of sole dilution modelling

$$F_{rel} = 10^{-\frac{K_{elt} \cdot X}{U_{avg}}} \quad (87)$$

$F_{rel}$  = residual fraction of substance in river water, considering all removal processes

$K_{elt}$  = sum of all removal rates in river water [1/s]

$X$  = longitudinal distance downstream from point of discharge [m]

$U_{avg}$  = average longitudinal stream velocity

$$C_{wdi} = F_{rdi} \cdot C_{wf} \quad (88)$$

$C_{wdi}$  = concentration of substance in river water in dissolved state [mg/l]

$F_{rdi}$  = fraction of substance in dissolved state in river water

$$F_{rdi} = \frac{10^6}{1 + S_{pa} \cdot K_{spw}} \quad (89)$$

- $C_{wsu}$  = concentration of substance in river water, adsorbed to suspended particulates [mg/l]  
 $= F_{rsu} \cdot C_{wf}$   
 $F_{rsu}$  = fraction of substance in river water, adsorbed to suspended particulates  
 $= 1 - F_{rdi}$

***Final concentration of substance in sediment influenced by dispersion and removal process***

In the steady-state of a continuous discharge it is assumed, that a fixed ratio exists between the concentration in sediment and the total concentration in river water.

$$C_{sed} = \frac{F_{rse} \cdot C_{wf}}{Dens_{Sed}} \quad (90)$$

- $C_{sed}$  = Concentration in sediment (w/w on the basis of wet weight)  
 $F_{rse}$  = ratio between concentration in sediment [mg/l] and riverwater [mg/l]  
 $Dens_{Sed}$  = density of sediment containing 80% water (with density 1 kg/dm<sup>3</sup>) and 20% solids (with density 2.4 kg/dm<sup>3</sup>) resulting in a wet weight density of 1.28 kg/dm<sup>3</sup>  
 $C_{wf}$  = final concentration in river water, taking into account removal processes and dispersion [mg/l]

***Distance downstream from point of discharge required for 50% removal of the substance from river water by all elimination processes considered***

$$Lr_{50} = \frac{\ln 2 \cdot U_{avg}}{K_{elt}} \quad (91)$$

- $Lr_{50}$  = distance downstream corresponding with 50% removal [m]  
 $U_{avg}$  = longitudinal stream velocity [m/s]  
 $K_{elt}$  = sum of all removal rates in river water [1/s]

## SECTION 9. RISK CHARACTERISATION

### 9.1 INTRODUCTION

Risk assessment for man and for the environment follows different pathways and is presented separately in the model.

### 9.2 HUMAN HEALTH RISK CHARACTERISATION

The daily intake (DI) for adults and children is estimated from:

- the intake of the various food constituents [g/(kgbw -day)] as:
  - meat
  - fish
  - milk/yoghurt
  - butter
  - cheese
  - vegetables
  - cereals
  - potatoes
- the concentration of the chemical in these food constituents, an estimation of which is presented in Section 7.

The ratio DI/TDI indicates whether or not there is a reason for concern.

DI = Daily Intake [mg/(kgbw -day)]

TDI = Tolerable Daily Intake [mg/(kgbw -day)]

### 9.3 ENVIRONMENTAL RISK CHARACTERISATION

The following predicted no effective concentrations (PNEC) are considered:

- $PNEC_{aq}$  in the water compartment for aquatic organisms
- $PNEC_{praq}$  in the water compartment for aquatic predatory organisms
- $PNEC_{terr}$  in the soil compartment for soil organisms (earth worms)
- $PNEC_{prterr}$  in the soil compartment for terrestrial predatory organisms

The ratios between the different PNECs and the estimated concentrations in the water and soil compartments indicate whether or not there is a reason for concern.



## **Part 2**

### **The HAZCHEM Model**

#### **Manual to the PC-Program**

Part 2 gives advice on how the program is operated and describes the individual screens of HAZCHEM in detail.

Select the drive and directory where HAZCHEM is stored in your computer, type 'HAZCHEM' and press <ENTER>. The following screen will appear:

### Screen 1

```
Welcome to the program HAZCHEM.EXE!

Name of logfile (default = HAZCHEM.TXT)    ?

The logfile will contain a print of the screen after
pressing Ctrl <W>
```

Each time HAZCHEM is started, it opens and overwrites a file HAZCHEM.TXT. Therefore it is recommended to give the logfile a specific name related to your study object. The logfile is meant to store the text screens of the PC-program HAZCHEM, containing the results of the estimations or calculations. Pressing '<Ctrl>w' copies the screen displayed to the logfile.

### Screen 2

```
Program HAZCHEM  Version 2.00
15 July 1994

W.F. ten Berge,
DSM, Corporate Department for
Safety, Health, Environment & Technology,
P.O. Box 6500,
6401 JH Heerlen,
Het Overloon 1,
6411 TE Heerlen,
The Netherlands.
Telephone : 31 45 787 128
Telefax   : 31 45 787 112
```

If this manual is not sufficiently clear, you may ask for help via the fax while sending a print-out of the specific part of the program.

**Screen 3****Main menu**

Environmental effect assessment of chemicals  
-----

Data on compound

Data on production and use

Data on human food constituents

Discharge to sewage treatment plant

Discharge into river

Discharge into local environment

Discharge into regional environment

End of program

up & down cursor and enter keys for selection of menu!

up & down cursor keys for input data selection,  
type data and press enter!

This is the main menu of the program. By pressing the up and down cursor keys the different menu options are presented in reverse video. By pressing the <ENTER> key the option in reverse video is selected. Each menu option has its own data handling routine for retrieval from and saving data to the hard disk or single diskette.

The PC-program HAZCHEM.EXE contains seven submenus:

- Data on compound. This submenu provides input and estimation routines on physico-chemical and toxicological data of the compound of interest. These data are used in the remaining modules;
- Data on production and use. This submenu provides input and estimation routines for the release of the compound to the environmental compartments and to sewage treatment plants in relation to the production or use volume per geographic area;
- Data on human food constituents. This submenu allows you to use the characteristic feeding habits of EU member countries. It is used to provide an estimation of the indirect exposure of humans via the food chain;

- Discharge to sewage treatment plant. This submenu provides input and estimation routines for estimation of the release to the environment via sewage treatment. Without any other information the releases should be estimated by means of the Namkung-Rittman method. Further it is assumed that the installed capacity of sewage treatment in inhabitant equivalents is equal to the number of inhabitants of the EC-member states. If this is not the case, the real data should be used as input in the submenu on sewage treatment and on production and use (display of.....);
- Discharge into river. This submenu is identical to the RIVMODEL (ten Berge, 1992). It considers the impact of releases to channels and rivers and estimates the mixing length, the length for 50% elimination of the discharged compound, the dissolved and suspended concentration in water and in sediment dependent on the distance of the point of discharge;
- Discharge into local environment. This submenu allows you to make both an exposure and hazard assessment of a compound released from a point source. It provides input and estimation routines for evaluation of the impact of point discharges to the air, the water and the soil environment in the surroundings of the point of discharge. It is similar to the program DRANC (Toet *et al*, 1991);
- Discharge into regional environment. This submenu allows you to make both an exposure and hazard assessment of a compound released into a regional environment, e.g. into a member country of the European Union. Via data retrieval from the hard disk the different characteristics of the EU member countries can be taken into account in the hazard assessment of compounds.

**Screen 4**

```
Input of data on chemicals
-----
Input environmentally relevant properties of compound
Input data on toxicity
No effective concentrations or dose levels
Data retrieval/saving
Return to main menu
```

This is the submenu 'Input of data on chemicals'. If you have already saved data on the compound of interest, you will go to 'Data retrieval/saving' and press <ENTER>.

**Screen 5**

```
Data handling on properties of compound
-----
Data retrieval
Data saving
Return to menu
```

By selecting 'Data retrieval' and pressing <ENTER> you will arrive at the next menu.

**Screen 6**

Data retrieval on properties of compound

C:\ECETOC\HAZCHEM

TRCHLBZ .CMP            LAS            .CMP            DICHLMET.CMP            DEHP            .CMP

DECABRBP.CMP

52852736 Bytes free

file name without extension    ?LAS

All the datafiles on compounds have the extension <.CMP>. Type the name of the datafile to be retrieved and press <ENTER>. This will bring you automatically in the next screen. If you type the name of a file, which does not exist, no data will be retrieved.

**Screen 7**

LAS.CMP

Data handling on properties of compound

Data retrieval

Data saving

Return to menu

You will notice that the name of the file retrieved is printed in the upper right corner of the screen. If you put in the name of a file which does not exist, the name of the file will not be printed. In that case you try again the option 'Data retrieval', otherwise select the option 'Return to menu' and press <ENTER>.

If you have entered new data on properties of chemicals, it is recommended to save them. Select the option saving data and you will arrive at the next screen.

**Screen 8**

Saving data on properties of compound

-----

file name <= 8 characters ?

Type the name of the file the data of which you want to save. If you type more than 8 letters, this screen returns immediately without the file name. If you put in a valid file name, the name of the file is printed in the screenmenu 'Data handling on properties of compound' in the right upper corner of the screen.

**Screen 9**

Environmentally relevant input data on compound

-----

LAS.CMP

name of substance		?LAS
CAS number		
vapour pressure	(Pascal)	1E-10
boiling point	°C	400
water solubility	(mg/l)	350
log(octanol/water) part. coeff.		2.5
molecular weight		347
melting point	°C	10
environmental temperature	°C	20
degradation half life air	(hours)	20
degradation half life water	(hours)	35
degradation half life soil	(hours)	350
degradation half life sedim.	(hours)	17
Henry coefficient	(Pa*m <sup>3</sup> /Mol)	9.914286E-11
part. coeff. prim. sludge STP	(l/kg)	2800
part. coeff. sec. sludge STP	(l/kg)	2800
part. coeff. susp. part./w	(l/kg)	1000
part. coeff. sediment/water	(l/kg)	1000
part. coeff. soil/water	(l/kg)	1000
part. coeff. fish/water	(l/kg)	30
part. coeff. earthworm/water	(l/kg)	10

Press <ESC> to return to menu!

Everywhere a question mark in reverse video is presented, you may change the data displayed by overtyping and pressing <ENTER>. If you have retrieved a file from the disk, the file name in the upper right corner of the screen will disappear as soon as one of the data has been overwritten.

The Henry-coefficient and partition coefficients require special attention. If you fill in the Henry coefficient and the partition coefficients, they will be used in all modules and submenus. If you like

these coefficients to be estimated dependent on the vapour pressure, solubility, octanol/water partition coefficient and/or the organic carbon content, you have to assign the value zero to these coefficients. During the execution of the program the value of the partition coefficients will change depending on the organic carbon content. You can read the estimated values on this screen. However, the estimated figures can not be saved in the submenu 'Data handling on properties of compound - Data saving' unless these data are entered (as values > 0) via the submenu 'Environmentally relevant input data on compound'.

You can only leave this submenu by pressing <ESC>. You will arrive then at the next screen.

#### Screen 10

Will you estimate solubility from oct/wat-part    y/n    ?

If you have assigned the value 0 to the partition coefficients and you want to know the influence of the octanol/water partition coefficients on the former partition coefficients, this question should be answered with y(es). The program then estimates the water solubility from the octanol/water partition coefficient and the melting point according to Mackay *et al* (1992).

The reason for adapting the water solubility is that it is not allowed to change the octanol/water partition coefficient deliberately without changing the water solubility in relation to it.



**Screen 11**

Input data on toxicological effects of LAS			LAS.CMP
-----			
LC50 fish 96 h	mg/l	? 5	
LC50 daphnia 48 h	mg/l	8	
EC50 algae	mg/l	10	
IC50 bacteria	mg/l	500	
LC50 earthworm	mg/kg soil	1000	
EC50 plant	mg/kg soil	0	
NOEC fish	mg/l	.22	
NOEC daphnia	mg/l	.43	
NOEC algae	mg/l	.28	
NOEC bacteria	mg/l	1	
NOEC earthworm	mg/kg soil	1000	
NOEC plant	mg/kg soil	0	
LD50 rat	mg/kg	2000	
NOED 28 day rat	mg/kg/day	0	
NOED 90 day rat	mg/kg/day	250	
NOED lifetime rat	mg/kg/day	0	
Feed consumption rate	kg/kg/day	.1	

This submenu can only be left by pressing <ESC>. This will prompt the next question.

**Screen 12**

LAS.CMP	
Do you want to calculate No Effect Levels y/n ?y	

Answer this question with y(es) if you want to have an estimate of NOEL from the available data. Concerning aquatic toxicology the lowest acute value will be divided by a factor of 1000. The lowest chronic value will be divided by a factor of 100, unless there are three chronic values available. In this case the lowest chronic value is divided by 10. The estimated values may be overwritten in the next screen.

For bacteria there is a fixed ratio of 100 between the IC50 bacteria and the PNEC bacteria.

For extrapolation of mammalian studies it is assumed, that the NOED is equal to:

- LD<sub>50</sub> rat / 1000
- NOED 28 day rat / 30
- NOED 90 day rat / 10
- NOED lifetime rat

In order to derive the TI for man the NOED is divided by 100.

In order to derive the TI for non-human mammals the NOED is divided by 3, unless the NOED is estimated from the LD<sub>50</sub>.

### Screen 13

LAS.CMP		
No effective concentrations or dose levels for LAS		
-----		
Pred. tol.int. humans (TDI)	mg/kg/day	? .25
PNED mammals/birds	mg/kg/day	8.333333
PNEC water, aquatic organisms	mg/l	.022
PNEC soil, earthworms/plants	mg/kg	10
PNEC water, bacteria STP	mg/l	1
PNEC sediment (extrapolated)	mg/kg	22
Press <ESC> to return to menu!		

In this screen the estimated values of TI (Tolerable Intake) for man and for non-human mammals and the PNECs may be overwritten by better and validated data.

**Screen 14**

```
Estimation of environmental release of LAS
-----

Data input on production and use category

Calc. of release fractions (excl. compounding)
Calc. of release fractions (incl. compounding)

Display / input of release fractions

Data retrieval / saving

Return to main menu
```

This is the submenu of the release estimation. If data on production and release are already available on disk, you can retrieve them by going to "Data retrieval / saving". <ENTER> will you bring to the next screen.

**Screen 15**

```
Data retrieval / saving on production and use
-----

Data retrieval

Data saving

Return to menu
```

By selecting 'Data retrieval' and pressing <ENTER> you will arrive at the next menu.

**Screen 16**

Data retrieval on production and use

-----

C:\ECETOC\HAZCHEM

LAS .PRU DEHP .PRU DECABRBP.PRU

52832256 Bytes free

File name (without extension) ?LAS

All the datafiles on compounds have the extension <.PRU>. Type the name of the datafile to be retrieved and press <ENTER>. This will bring you to the submenu as displayed in Screen 15. If you type the name of a file which does not exist, no data will be retrieved. Choose the option 'Return to menu' and you will arrive at the submenu "Estimation of environmental release of ... "

**Screen 17**

LAS.PRU

Data on prod. volume and use pattern of LAS

-----

Production/Use in kg/hour	? 1000	type of main	
	fraction	use	prod -
Agricultural chemicals	0	0	0
Basic chemicals in chemical ind.	0	0	0
Chemicals for electric equipment	0	0	0
Chemicals personal & household use	0	0	0
Chemicals public areas -general-	0	0	0
Chemicals public areas -pesticides-	0	0	0
Chemicals public areas -detergents-	1	7	4
Chemicals leather processing	0	0	0
Chemicals for metal extr. & proc.	0	0	0
Fuel and fuel additives	0	0	0
Chemicals photographic industry	0	0	0
Chemicals used in polymers	0	0	0
Chemicals pulp, paper, board	0	0	0
Chemicals as intermediates	0	0	0
Chemicals for textile processing	0	0	0
Chemicals paint, lacquer, varnish	0	0	0
Others	0	0	0

This screen appears on selection of the option "Data input on production and use category" of the submenu "Estimation of environmental release of ....".

Here it is possible to enter:

- the fraction of the product applied in an industrial category. The sum of the fractions must be equal to 1. If this is not the case, the next screen will show the 'sum of fractions = ..' and you cannot continue in the program until the necessary correction is made;
- the production type (see next screen <F1>);
- the main use type (see next screen <F1>).

### Screen 18

LAS.PRU

\* = Choice of main prod. and use type affects release!  
Inappropriate choice may yield worst case!

Information on main production and use type

0 = Not applied  
1 = Closed systems non-isolated  
2 = Isolated on site or continuous production  
3 = Isolated off site or batch prod. dedicated equipment  
4 = Batch production multipurpose equipment

Information on main use type

5 = Inclusion into matrix  
6 = Non-dispersive use  
7 = Wide dispersive use

This screen appears after pressing <F1> in the previous screen. It offers an explanation of the options for the production process and of the main use type both of which determine the amount assumed to be released to the environment.

**Screen 19**

Environmental release pattern of LAS		LAS.PRU
-----		
Production volume kg/hr		1000
Release by production		27.01
Release by compounding		8
Release by commercial use		991.9999
Release by private use		0
Release by recovery		0
Release to air	?	25.81
Release to waste water		922.8
Release to surface water		24.8
Release to soil		53.6
Release to waste		0
Total release		1027.01
Press <ESC> to return to menu!		

This screen appears after selection of the submenu options:

- Calc. of release fractions (excl. compounding);
- Calc. of release fractions (incl. compounding);
- Display / input of release fractions.

The estimation of the release to air, waste water, surface water, soil and waste is performed, if one of the first two options is selected from the submenu "Estimation of environmental release of .....". It is possible to substitute the estimated data on release with actual data. If the third option is selected, the release data stored on disk will be retrieved and presented. However, as soon as one of the former two options is selected, these release data will be replaced by estimated release data.

**Screen 20**

```
Data on human food constituents
-----

Input of data on human food constituents

Data retrieval/saving

Return to main menu
```

This is the submenu on human food constituents and enables to enter food habits of the population of the different EU member countries from the keyboard or from disk. The choice of the option "Data retrieval/saving" will bring you into the next screen.

**Screen 21**

```
Data handling on human food constituents
-----

Data retrieval

Data saving

Return to menu
```

Choosing the option "Data retrieval" will bring you into the next screen for entering data from disk.

**Screen 22**

```
Data retrieval on human food constituents
-----

C:\ECETOC\HAZCHEM
EEC      .HFC      BELGIUM .HFC      DANMARK .HFC      FRANCE  .HFC
GERMANY  .HFC      GREECE  .HFC      IRELAND .HFC      ITALY   .HFC
NL       .HFC      PORTUGAL.HFC      SPAIN   .HFC      UK      .HFC

52807680 Bytes free

file name without extension  ?NL
```

All files with data on food constituents consumption in the EC member states have the extension ".HFC". By typing the name of the file without extension and pressing <ENTER> the specific food constituents consumption for the selected EC member state is entered. These data are of interest for the estimation of human exposure via the food chain. In addition you will arrive into the next screen.

**Screen 23**

```

NL.HFC

Data handling on human food constituents
-----

Data retrieval

Data saving

Return to menu
```

By choosing the option return to menu you will enter the submenu "Data on human food constituents". In the last submenu the selection of the option "Input of data on human food constituents" will bring you into the next screen.



**Screen 24**

NL.HFC	
Input of data on human food constituents in g/kg/day	
adult intake of meat	? 4.2
adult intake of fish	.5
adult intake of milk/yoghurt	3.7
adult intake of butter	.2
adult intake of cheese	.7
adult intake of vegetables	11.5
adult intake of cereals	3.5
adult intake of potatoes	4.1
child intake of meat	6.6
child intake of fish	.6
child intake of milk/yoghurt	15.7
child intake of butter	.8
child intake of cheese	3
child intake of vegetables	20.5
child intake of cereals	8.6
child intake of potatoes	7.3
Press <ESC> to return to menu!	

This screen displays the food constituents consumption in g/kg/day for the population of the EC-member state selected. In addition, the data can be overtyped and re-entered from this screen. By pressing <ESC> you arrive in the submenu "Data on human food constituents" and you are able to save the retyped data by selection of the option "Data retrieval/saving" etc.

**Screen 25**

```
Discharge into sewage treatment plant
-----

Input parameters on sewage treatment plant

Calculation according to Namkung-Rittmann
Calculation according to Cowan et al.
Calculation according to Monod kinetics

Data retrieval/saving

Return to main menu
```

This is the submenu of the sewage treatment plant. The specific characteristics of the sewage treatment plant for the different scenarios (river, local or regional) may be entered from the keyboard or from disk. The choice of the option "Data retrieval/saving" will bring you into the next screen.

**Screen 26**

```
Data handling of sewage treatment plant
-----

Data retrieval

Data saving

Return to menu
```

The option 'Data retrieval' will bring you in the next screen.

**Screen 27**

Data retrieval for sewage treatment plant

C:\ECETOC\HAZCHEM

RIVER .STP	EEC .STP	NL .STP	LOC .STP
BELGLUXB.STP	DANMARK .STP	FRANCE .STP	GERMANY .STP
GREECE .STP	IRELAND .STP	ITALY .STP	PORTUGAL.STP
SPAIN .STP	UK .STP	EPEMMEN .STP	

52795392 Bytes free

file name without extension ?NL

You have to select one of the file names displayed by typing the name without the extension '.STP' and pressing <ENTER>. The name of the selected file will appear in the upper right corner of the next screen.

**Screen 28**

NL.STP

Data handling of sewage treatment plant

Data retrieval

Data saving

Return to menu

By selecting the option 'Return to menu' you will re-enter the submenu 'Discharge to sewage treatment plant'. By selecting the option 'input data on sewage treatment plant' you will arrive in the next screen.

## Screen 29

input data on sewage treatment plant		NL.STP
-----		
discharged compound is LAS		
number of inhabitant equivalents	? 1.5E+07	
waste water/inhabitant/day (l/day)	200	
concentration of primary sludge (g/l)	.22	
O.C.-content of primary sludge (w/w)	.3	
hydraulic retention time (hours)	7	
sludge retention time (hours)	216	
sludge conc. aeration tank (g/l)	2.5	
O.C.-content of secondary sludge (w/w)	.37	
sludge conc. effluent (mg/l)	40	
discharge of compound in kg/hour	922.8	A)
biodegradation rate (1/h)	3	A)
$\mu_{\max}$ Monod-kinetics (1/hr)	.05	A)
Michaelis-Menten constant (mg/l)	2	A)
biodegr. in adsorbed state (y/n)	n	A)
Press <ESC> to return to menu!		

Via this screen it is possible to enter characteristics of the sewage treatment plant and characteristics of the compound of interest related to the behaviour in the sewage treatment plant, marked with <sup>A)</sup>. Change of the input value of the first 9 parameters will remove the file name from the upper right corner of the screen, change of the input value of the parameter marked with <sup>A)</sup> does not.

The input file NL.STP is used in connection with the scenario for the regional model of the Netherlands. In order to get an idea on the Dutch domestic sewage load, it is assumed that the waste water of 15 million of inhabitants is treated in one huge sewage treatment plant and subsequently homogeneously dispersed to surface water and arable soil, whereas in reality this domestic sewage load is divided over more than 100 sewage treatment plants.

The discharge of the compound in kg/hour is estimated from the submenu 'Data on production and use'. The user may overwrite this figure. This figure, however, will not be saved to disk via this submenu, but via the submenu 'Data on production and use'. If the discharge is set to 0, calculations will not be carried out.

There are three ways for estimation of the removal by biodegradation. Two ways assume first order kinetics, that of Namkung-Rittmann (1987) and that of Cowan *et al* (1992), requiring an input value for the biodegradation rate. The Monod kinetics requires  $\mu_{\max}$  Monod and the Michaelis Menten

Constant. Without any additional information, the estimation according to Namkung-Rittmann should be preferred. In this option a biodegradation rate of 3/hour should be selected for a well biodegradable substance.

The sludge concentration in the effluent has a great impact on the removal percentage of the compound in case of non-biodegradable substances which are sparingly soluble in water and strongly adsorb to activated sludge. The value of 40 mg/l is adopted by the Dutch Ministry of the Environment, but may be too high for many sewage treatment plants.

### Screen 30

NL.STP	
Fate of compound LAS in STP (Namkung & Rittmann 1987)	
-----	
total influent concentration (mg/l)	7.3824
effluent concentration (dissolved mg/l)	.2464918
effluent concentration (suspended mg/l)	2.760709E-02
amount biodegraded per hour (kg)	647.0411
amount volatilized per hour (kg)	6.896981E-12
removed via primary sludge per hour (kg)	234.5069
removed via second. sludge per hour (kg)	6.989641
removed via effl./hour (dissolved kg)	30.81148
removed via effl./hour (suspended kg)	3.450886
primary sludge production per hour (kg)	18333.33
second. sludge production per hour (kg)	10127.31
comp. conc. in primary sludge (mg/kg)	12791.29
comp. conc. in second. sludge (mg/kg)	690.1771
percentage removal by primary sludge	25.41254
percentage removal by biodegradation	70.11715
percentage total removal	96.28713

This screen is produced if the option "Calculation according to Namkung-Rittmann" is selected. It provides detailed information on the fate of the compound in the sewage treatment plant.

**Screen 31**

NL.STP		
Hazard assessment for sewage treatment bacteria exposed to LAS		
-----		
total influent conc.	(mg/l)	7.3824
effluent conc. dissolved	(mg/l)	.2464918
NOEC water, bacteria STP	(mg/l)	1
PEC/PNEC bacteria influent		7.38E+00
PEC/PNEC bacteria effluent diss.		2.46E-01

This screen provides the comparison of the level in the influent and in the effluent with the NOEC of the bacteria in the sewage treatment plant. In addition, it shows the PEC/PNEC ratios.

**Screen 32**

Discharge into regional environment
-----
Characteristics of the regional environment
Input via sewage treatment and via direct discharge
Mackay level 3 calculation
Concentrations in environmental compartments and biota
No effective concentrations or dose levels
Hazard assessment
Data retrieval/saving
Return to main menu

This submenu allows you to make both an exposure and hazard/risk assessment of a substance released into a regional environment, e.g. into a Member State of the European Union.

The editing or keyboard input of the characteristics of the regional environment is provided by the option 'Characteristics of the regional environment'.

The release input to the regional environment may be provided from the results of the estimations according to the submenus 'Data on production and use' and 'Discharge to sewage treatment plant', but these results may be overwritten by selecting option 'Input via sewage treatment and via direct discharge'.

The option 'Mackay level III calculation' calculates the distribution of the compound over the compartments air, water, soil and sediment on the basis of the model for a generic environment according to Mackay *et al* (1992). The fugacity and transport equations used are according to Mackay *et al* (1992), but the estimation of the residence times of the compound in air, water and sediment was made dependent on the specific regional characteristics.

The option 'Concentrations in environmental compartments and biota' provides estimated concentrations in the regional environmental compartments and in the food chain. These data may be overwritten, while simultaneously the levels in the subsequent part of the food chain will change too. This enables the program user to get some feeling on the significance of levels in environmental compartments separately.

The option 'No effective concentrations or dose levels' reminds you to the estimated PNECs which will be used to calculate the PEC/PNEC ratios.

The option 'Hazard assessment' provides the ratios PEC/PNEC for humans and for aquatic and terrestrial organisms via the food chain.

The option 'Data retrieval/saving' enables you to retrieve the characteristics of the regional environment of interest. This option brings you to the next screen.

**Screen 33**

Data handling of discharge into regional environment  
-----

Data retrieval

Data saving

Return to menu

If the option 'Data retrieval' is chosen, you will arrive in the next submenu.

**Screen 34**

Data retrieval of discharge into regional environment  
-----

C:\ECETOC\HAZCHEM

BELGLUXB.RNV	EEC	.RNV	NL	.RNV	FRANCE	.RNV
--------------	-----	------	----	------	--------	------

GERMANY .RNV	GREECE	.RNV	IRELAND	.RNV	ITALY	.RNV
--------------	--------	------	---------	------	-------	------

PORTUGAL.RNV	SPAIN	.RNV	UK	.RNV		
--------------	-------	------	----	------	--	--

52781056 Bytes free

file name without extension ?NL

You have to select one of the file names displayed by typing the name without the extension '.RNV' and pressing <ENTER>. The name of the selected file will appear in the upper right corner of the next screen.

**Screen 35**

NL.RNV

Data handling of discharge into regional environment  
-----

Data retrieval

Data saving

Return to menu

By selecting the option 'Return to menu' you will re-enter the submenu 'Discharge into regional environment'. By selecting the option 'Characteristics of the regional environment' you will arrive in the next screen.



**Screen 36**

input data on environment		NL.RNV
-----		
total surface area (km2)	? 36850	
water surface fraction	.082	
arable land fraction	.57	
height of air compartment (m)	1000	
depth of water compartment (m)	3	
depth of arable soil compartment (m)	.2	
depth of natural soil compartment (m)	.05	
depth of sediment compartment (m)	.03	
conc. of susp. sed. in water (mg/l)	15	
fraction org. carbon soil	.05	
fraction org. carbon sediment	.05	
fraction org. carbon susp. sed.	.1	
wind velocity height 10 meter (m/sec)	5	
backgr. level in air (µg/m3)	0	
advective inflow river water (m3/sec)	1500	
backgr. level in water (mg/l)	0	
burial rate of sediment (mm/year)	.1	
rain precipitation excess (mm/year)	350	
Press <ESC> to return to menu!		

From this screen you may change the characteristics of the regional environment. Change of the first 12 characteristics will remove the file name from the upper right corner of the screen. The last 6 characteristics may be changed in order to get some feeling for the influence on distribution and or level in environmental compartments.

Leaving this screen by pressing <ESC> will prompt the question on the next screen.

**Screen 37**

Will you estimate advective residence time air and water y/n ?y		NL.RNV
---	--	--------

It is recommended to answer this question with y(es). The program HAZCHEM estimates the average residence time of air and surface water on the basis of the average wind velocity respectively the inflow of water via rain precipitation excess, sewage treatment effluents (only if the number of inhabitant equivalents and the waste water volume per inhabitant per day are put in) and advective

river flow rate considering the area in m<sup>2</sup> of the regional environment. If the answer is y(es), you will directly arrive in the next screen.

### Screen 38

NL.RNV		
Emission rates to regional environmental compartments of LAS		
-----		
Advective residence time air (h)	?	10.66464
Advective residence time water (h)		1295.511
Direct emission to air (kg/h)		25.81
Direct emission to water (kg/h)		24.8
Direct emiss. to arable soil (kg/h)		53.6
Direct emiss. to natural soil (kg/h)		0
STP emission to air (kg/h)		6.896981E-12
STP emission to water (kg/h)		34.26237
STP emission to arable soil (kg/h)		241.4966
Press <ESC> to return to menu!		

This screen provides the estimated advective residence time of air and of surface water for the regional environment. In addition, it provides the estimates of the direct discharge from the submenu 'Data on production and use' and of the indirect discharges via the submenu 'Discharge to sewage treatment plant'. These figures may be overwritten in order to allow for any form of sensitivity analysis. If the sum of the emissions is 0, HAZCHEM will not perform the Mackay level III calculation.

## Screen 39

Mackay level 3 calculation on LAS		NL.RNV
-----		
Steady state mass in area	(kg)	163211.2
Mass % in air		7.16527E-03
Mass % in water dissolved		1.72435
Mass % in water suspended		2.586524E-02
Mass % in arable soil		95.59119
Mass % in natural soil		2.616276
Mass % in sediment		.0351008
Mass % in fish		5.173049E-05
Overall residence time	h	429.5382
Degradation residence time	h	433.3033
Advection residence time	h	49432.45
Air conc	ug/m3	3.173547E-04
Dissolved water conc	mg/liter	3.104578E-04
Suspended water conc	mg/liter	4.656867E-06
Arable soil conc	ppm	2.475508E-02
Natural soil conc	ppm	4.439005E-03
Sediment conc	ppm	4.937241E-04
Susp.solids conc	ppm	.3104578
Fish conc	ppm	9.313733E-03

This is the output of the Mackay level III calculation. Most figures will also be displayed in the next submenu 'Concentrations in environmental compartments and biota' except the sediment and suspended solids concentration.

The data on residence times are important. The advection residence time provides information on the mobility of the compound in the regional environment and on the contribution of advection to the overall residence time. The degradation residence time provides information on the real disappearance from the regional environment and on the contribution of degradation to the overall residence time.

The user should be aware, that the provided concentrations are related to a steady-state condition that may have been achieved after a period of about 3 times the overall residence times.

**Screen 40**

Do you want to see intercompartmental transport      y/n      ?y

If this question is answered with yes, the next 5 screens provide information on the amount of substance which is transported by physico-chemical processes between the environmental compartments or which is removed by (bio)degradation or advection (inflow and outflow and sediment burial).

**Screen 41**

		NL.RNV
intercompartmental transport		
-----		
from air to water kg/hr	=	1.993274
from air to arable soil kg/hr	=	13.85568
from air to sediment kg/hr	=	0
from air to natural soil kg/hr	=	8.459259
degradation rate air kg/hr	=	.4052152

**Screen 42**

		NL.RNV
intercompartmental transport		
-----		
from water to air kg/hr	=	1.908031E-10
from water to arable soil kg/hr	=	0
from water to sediment kg/hr	=	2.345276
from water to natural soil kg/hr	=	0
degradation rate water kg/hr	=	56.56128

## Screen 43

NL.RNV

intercompartmental transport

-----

from arable soil to air kg/hr = 1.321842E-10

from arable soil to water kg/hr = 4.156406E-02

from arable soil to sediment kg/hr = 0

from arable soil to natural soil kg/hr = 0

degradation rate arable soil kg/hr = 308.9107

## Screen 44

NL.RNV

intercompartmental transport

-----

from sediment to air kg/hr = 0

from sediment to water kg/hr = 9.820543E-03

from sediment to arable soil kg/hr = 0

from sediment to natural soil kg/hr = 0

degradation rate sediment kg/hr = 2.335346

advection rate sediment kg/hr = 1.089962E-04

**Screen 45**

NL.RNV

intercompartmental transport

from natural soil to air kg/hr = 1.447122E-11

from natural soil to water kg/hr = 4.550337E-03

from natural soil to arable soil kg/hr = 0

from natural soil to sediment kg/hr = 0

degradation rate natural soil kg/hr = 8.454708

**Screen 46**

NL.RNV

Concentration in regional environmental compartments  
and in biota of LAS

concentration in air	µg/m3	? 3.173547E-04
diss.conc. surface water	µg/l	.3104578
conc. in arable soil	µg/kg	24.75508
conc. in natural soil	µg/kg	4.439005
diss.conc. groundwater	µg/l	1.824468E-02
diss.conc. drinking water	µg/l	.3104578
conc. in vegetables	µg/kg	2.389124
conc. in root crop	µg/kg	3.323374E-02
concentration in meat	µg/kg	1.694279E-03
conc. in milk fat	µg/kg	1.345814E-02
concentration in fish	µg/kg	9.313733
conc. earthworm ar.so.	µg/kg	.3094109
conc. earthworm nat.so.	µg/kg	5.548261E-02

In addition to the levels in the environmental compartments, this submenu provides the estimated levels in drinking water and in biota according to the algorithms provided by van de Meent and Toet (1992). The user may overwrite these data. The program then adapts simultaneously the levels in the subsequent part of the food chain. This enables the program user to get some feeling on the significance of the level in a separate environmental compartment for the levels in biota.

## Screen 47

LAS.CMP		
No effective concentrations or dose levels for LAS		
-----		
Pred. tol.int. humans (TDI)	mg/kg/day	? .25
PNED mammals/birds	mg/kg/day	8.333333
PNEC water, aquatic organisms	mg/l	.022
PNEC soil, earthworms/plants	mg/kg	10
PNEC water, bacteria STP	mg/l	1
PNEC sediment (extrapolated)	mg/kg	22

This screen provides the Tolerable Intakes (TI) for humans and non-human mammals and the PNECs, estimated from the mammalian and aquatic toxicity data on the compound of interest.

## Screen 48

NL.RNV		
PEC/PNEC-calculations for LAS		
-----		
Human hazard assessment for adults		
intake by vegetables	2.75E-05	mg/kg/day
intake by drinking water	9.31E-06	mg/kg/day
intake by cereals	8.36E-06	mg/kg/day
intake by fish	4.66E-06	mg/kg/day
intake by inhalation	9.52E-08	mg/kg/day
intake by potatoes	1.36E-07	mg/kg/day
intake by meat	7.12E-09	mg/kg/day
intake by cheese	2.36E-09	mg/kg/day
intake by butter	2.15E-09	mg/kg/day
intake by milk/yoghurt	1.99E-09	mg/kg/day
Predicted intake	5.01E-05	mg/kg/day
Tolerable intake	2.50E-01	mg/kg/day
Ratio PI/TI	2.00E-04	

This submenu provides intake values for adults for indirect exposure routes via the food chain in a regional environment. In addition, it presents the ratio between the predicted and tolerable intake.

**Screen 49**

NL.RNV

PEC/PNEC-calculations for LAS  
-----

## Human hazard assessment for children

intake by vegetables	4.90E-05	mg/kg/day
intake by cereals	2.05E-05	mg/kg/day
intake by drinking water	1.86E-05	mg/kg/day
intake by fish	5.59E-06	mg/kg/day
intake by inhalation	1.90E-07	mg/kg/day
intake by milk/yoghurt	8.45E-09	mg/kg/day
intake by potatoes	2.43E-07	mg/kg/day
intake by butter	8.61E-09	mg/kg/day
intake by cheese	1.01E-08	mg/kg/day
intake by meat	1.12E-08	mg/kg/day
Predicted intake	9.42E-05	mg/kg/day
Tolerable intake	2.50E-01	mg/kg/day
Ratio PI/TI	3.77E-04	

This submenu provides intake values for children for indirect exposure routes via the food chain in a regional environment. In addition, it presents the ratio between the predicted and tolerable intake. Children have a higher food intake per kg body weight than adults and therefore they may be at higher risk.



**Screen 50**

NL.RNV		
PEC/PNEC-calculations of LAS		
-----		
PEC/PNEC aquatic organisms		1.41E-02
PEC/PNEC sediment organisms		2.24E-05
PEC/PNEC ar.so. earthworms/plants		2.48E-03
PEC/PNEC na.so. earthworms/plants		4.44E-04
PED/PNED-calculations of LAS		
-----		
PED aq. mammals/birds	mg/kg/day	9.313733E-04
PNED aq. mammals/birds	mg/kg/day	8.333333
Ratio PED/PNED		1.117648E-04
PED mammals/birds ar.so.	mg/kg/day	3.094109E-05
PED mammals/birds na.so.	mg/kg/day	5.548261E-06
PNED mammals/birds	mg/kg/day	8.333333
Ratio PED/PNED arable soil		3.712931E-06
Ratio PED/PNED natural soil		6.657914E-07

This screen provides the PEC/PNEC ratios for several aquatic and terrestrial organisms in a regional environment.

**Screen 51**

Discharge into local environment
-----
Characteristics of the local environment
Input via sewage treatment and via direct discharge
Concentrations in environmental compartments and biota
No effective concentrations or dose levels
Hazard assessment
Data retrieval/saving
Return to main menu

This submenu may be entered from the main menu. It allows you to make both an exposure and hazard/risk assessment of a compound released from a point source. It provides input and estimation

routines for the evaluation of the impact of point discharges to the air, the water and the soil environment in the surroundings of the point of discharge. It is more or less identical to the program DRANC (Dutch Risk Assessment of New Chemicals) (Toet *et al*, 1991) with few exceptions. For instance, the concentration inhaled by inhabitants is the concentration on a distance of 1,000 meters from the source instead of 100 meters. Furthermore, there are differences in the estimation of the soil concentration after discharge of activated sludge of the sewage treatment plant.

#### Screen 52

```
Data handling of discharge into local environment
-----
```

```
Data retrieval
```

```
Data saving
```

```
Return to menu
```

If the option 'Data retrieval' is chosen, you will arrive in the next submenu.

#### Screen 53

```
Data retrieval of discharge into local environment
-----
```

```
C:\ECETOC\HAZCHEM
```

```
DRANC .LNV
```

```
52647936 Bytes free
```

```
file name without extension    ?DRANC
```

You have to select one of the file names displayed by typing the name without the extension '.LNV' and pressing <ENTER>. The name of the selected file will appear in the upper right corner of the next screen.

**Screen 54**

DRANC.LNV
Data handling of discharge into local environment
-----
Data retrieval
Data saving
Return to menu

By selecting the option 'Return to menu' you will re-enter the submenu 'Discharge into local environment'. By selecting the option 'Characteristics of the local environment' you will arrive in the next screen.

**Screen 55**

DRANC.LNV
Characteristics of the local environment
-----
Depth of arable soil compartment (m) ? .2
Depth of natural soil compartment (m) .05
Fraction org. carbon soil .029
Conc. of susp. sed. in water (mg/l) 30
Fraction org. carbon susp. part. .05
Dilution factor of effluent 32
Press <ESC> to return to menu!

This submenu shows the characteristics of the local environment as adopted in the PC-program DRANC (Toet *et al*, 1991). You may overwrite these settings. Change of these settings will remove the file name of the upper right corner in order to alert you to assign a file name to the revised characteristics via the submenu 'Data retrieval/saving'.

**Screen 56**

```

NL.STP

Discharge into sewage treatment plant
-----

Input parameters on sewage treatment plant

Calculation according to Namkung-Rittmann
Calculation according to Cowan et al.
Calculation according to Monod kinetics

Data retrieval/saving

Return to main menu

```

The input parameters of the sewage treatment plant are still in conformity with the regional environment of The Netherlands. The user should return to this submenu to adapt the setting of the sewage treatment plant to the local environment by selecting 'Data retrieval/saving'. This will bring you to the next screen.

**Screen 57**

```

NL.STP

Data retrieval for sewage treatment plant
-----

C:\ECETOC\HAZCHEM
RIVER .STP      EEC      .STP      NL      .STP      LOC      .STP
BELGLUXB.STP    DANMARK .STP      FRANCE .STP      GERMANY .STP
GREECE .STP     IRELAND .STP    ITALY  .STP      PORTUGAL.STP
SPAIN  .STP     UK        .STP    EPEMMEN .STP
52754432 Bytes free

file name without extension  ?LOC

```

You have to select the file name LOC by typing the name without the extension '.STP' and pressing <ENTER>. The name of the selected file 'LOC.STP' will appear in the upper right corner of the next screen.

**Screen 58**

LOC.STP
Data handling of sewage treatment plant -----
Data retrieval
Data saving
Return to menu

You may leave this submenu by selecting the option 'Return to menu'. By selection of the option 'Input parameters of the sewage treatment plant' you will arrive in the next screen.

**Screen 59**

LOC.STP
input data on sewage treatment plant -----
discharged compound is LAS
number of inhabitant equivalents           ? 10000
waste water/inhabitant/day (l/day)       200
concentration of primary sludge (g/l)     .22
O.C.-content of primary sludge (w/w)     .3
hydraulic retention time (hours)         7
sludge retention time (hours)           216
sludge conc. aeration tank (g/l)         2.5
O.C.-content of secondary sludge (w/w)   .37
discharge of compound in kg/hour         1           A)
biodegradation rate (1/h)                3           A)
$\mu_{\max}$ Monod-kinetics (1/hr)           1.5       A)
Michaelis-Menten constant (mg/l)       .5        A)
biodegr. in adsorbed state (y/n)         n        A)
Press <ESC> to return to menu!

Via this screen it is possible to enter characteristics of the sewage treatment plant and characteristics of the compound of interest related to the behaviour in the sewage treatment plant, marked with <sup>A)</sup>. Change of the input value of the first 8 parameters will remove the file name from the upper right corner of the screen, change of the input value of the parameter marked with <sup>A)</sup> does not.

The discharge of the compound in kg/h is estimated from the submenu 'Data on production and use'. The user may overwrite this figure. This figure, however, will not be saved to disk via this submenu, but via the submenu 'Data on production and use'. If the discharge is set to 0, calculations will not be carried out.

There are three ways for estimation of the removal by biodegradation. Two ways assume first order kinetics, that of Namkung-Rittmann (1987) and that of Cowan *et al* (1992), requiring an input value for the biodegradation rate. The Monod kinetics requires  $\mu_{\max}$  Monod and the Michaelis Menten Constant. Without any additional information, the estimation according to Namkung-Rittmann should be preferred. In this option a biodegradation rate of 3/hour should be selected for a well biodegradable substance.

If, for example, the input file NL.STP is used in connection with the scenario for the regional model of the Netherlands it is assumed that the waste water of 15 million of inhabitants is treated in one huge sewage treatment plant and subsequently homogeneously dispersed to surface water and arable soil, whereas in reality this domestic sewage load is divided over more than 100 sewage treatment plants.

The sludge concentration in the effluent has a great impact on the removal percentage of the compound in case of non-biodegradable substances which are sparingly soluble in water and strongly adsorb to activated sludge. The value of 40 mg/l is adopted by the Dutch Ministry of the Environment, but may be too high for many sewage treatment plants.

## Screen 60

LOC.STP

Fate of compound LAS in STP (Namkung &amp; Rittmann 1987)

total influent concentration (mg/l)	12
effluent concentration (dissolved mg/l)	.4006694
effluent concentration (suspended mg/l)	4.487498E-02
amount biodegraded per hour (kg)	.7011716
amount volatilized per hour (kg)	7.473971E-15
removed via primary sludge per hour (kg)	.2541254
removed via second. sludge per hour (kg)	7.574384E-03
removed via effl./hour (dissolved kg)	3.338912E-02
removed via effl./hour (suspended kg)	3.739582E-03
primary sludge production per hour (kg)	12.22222
second. sludge production per hour (kg)	6.751544
comp. conc. in primary sludge (mg/kg)	20792.08
comp. conc. in second. sludge (mg/kg)	1121.874
percentage removal by primary sludge	25.41254
percentage removal by biodegradation	70.11716
percentage total removal	96.28713

This screen is produced if the option "Calculation according to Namkung-Rittmann" is selected. It provides detailed information on the fate of the compound in the sewage treatment plant for the scenario of the local environment.

**Screen 61**

LOC.STP		
Hazard assessment for sewage treatment bacteria exposed to LAS		
-----		
total influent conc.	(mg/l)	12
effluent conc. dissolved	(mg/l)	.4006694
NOEC water, bacteria STP	(mg/l)	1
PEC/PNEC bacteria influent		1.20E-01
PEC/PNEC bacteria effluent diss.		4.01E-01

This screen provides the comparison of the level in the influent and in the effluent with the NOEC of the bacteria in the sewage treatment plant for the local environment. In addition, it shows the PEC/PNEC ratios.

**Screen 62**

DRANC.LNV		
Emission rates to local environmental compartments of LAS		
-----		
Direct emission to air (kg/h)	1	
Direct emission to water (kg/h)	0	
Volume of direct effluent (m3/sec)	0	
Direct emission to soil (g/m2/hr)	9.999995E-06	D)
STP emission to air (kg/h)	7.473971E-15	B)
STP emission to water (kg/h)	.0371287	
Volume of STP effluent (m3/sec)	2.314815E-02	B)
STP emission to arable soil (g/m2/hr)	3.144739E-04	B)
Press <ESC> to return to menu!		

The emission to the environmental compartments of the local environment may originate from the submenu 'Data on production and use' or may be overwritten in this screen by the user. The direct emission to soil is estimated from the aerosol deposition rate, dependent on the concentration in air <sup>D)</sup>. The concentration in air is controlled by the direct emission and the emission of the sewage treatment plant to air.



The estimation of the emissions of the sewage treatment plant originate from the submenu 'Discharge to sewage treatment plant' <sup>B)</sup>.

### Screen 63

```

DRANC.LNV

do you want to calculate levels in the environmental
compartments and in biota  y/n      ?y

```

It is recommended to answer this question with y(es). The results of these calculations will appear in the next screen.

### Screen 64

```

DRANC.LNV

Concentration in local environmental compartments
and in biota of LAS
-----

concentration in air      µg/m3      ? .2777778
diss.conc. surface water µg/l        13.51773
conc. in arable soil      µg/kg        546.0097
conc. in natural soil     µg/kg        67.29557
diss.conc. groundwater   µg/l        .3832813
diss.conc. drinking water µg/l        13.51773
conc. in vegetables       µg/kg        2042.085
conc. in root crops       µg/kg        .7330185
concentration in meat     µg/kg        1.24231
conc. in milk fat         µg/kg        9.86802
concentration in fish     µg/kg        405.5319
conc. earthworm ar.so.    µg/kg        6.824507
conc. earthworm nat.so.   µg/kg        .841119

Press <ESC> to return to menu!

```

This screen provides intermediate results which will be used for the estimation of the environmental hazard via the food chain. You may overwrite all the data, starting at the top. Changing the air level will only result in a change of the level in food crop. If one desires to estimate the influence of the air concentration on the soil concentration one has to go back to the submenu 'Emission rates to local environmental compartments of LAS'. Substitution of a figure for release to air in the latter will result into an estimate for direct emission to soil and in the screen above into an estimate of the level in air and into soil. This approach enables you to make a distinction between plant contamination from air deposition and that from soil uptake.

**Screen 65**

LAS.CMP		
No effective concentrations or dose levels for LAS		
-----		
Pred. tol.int. humans (TDI)	mg/kg/day	? .25
PNED mammals/birds	mg/kg/day	8.333333
PNEC water, aquatic organisms	mg/l	.022
PNEC soil, earthworms/plants	mg/kg	10
PNEC water, bacteria STP	mg/l	1
PNEC sediment (extrapolated)	mg/kg	22
Press <ESC> to return to menu!		

This screen is a repetition of Screen 13. It is provided in this submenu because of convenience for the user: if not all of these figures were entered, it is impossible to calculate the PEC/PNEC ratios.

**Screen 66**

DRANC.LNV		
PEC/PNEC-calculations for LAS		
-----		
Human hazard assessment for adults		
intake by vegetables	2.35E-02	mg/kg/day
intake by cereals	7.15E-03	mg/kg/day
intake by drinking water	4.06E-04	mg/kg/day
intake by inhalation	8.33E-05	mg/kg/day
intake by fish	2.03E-04	mg/kg/day
intake by meat	5.22E-06	mg/kg/day
intake by potatoes	3.01E-06	mg/kg/day
intake by cheese	1.73E-06	mg/kg/day
intake by butter	1.58E-06	mg/kg/day
intake by milk/yoghurt	1.46E-06	mg/kg/day
Predicted intake	3.13E-02	mg/kg/day
Tolerable intake	2.50E-01	mg/kg/day
Ratio PI/TI	1.25E-01	

This screen provides intake values for adults for indirect exposure routes via the food chain in a regional environment. In addition, it presents the ratio between the predicted and tolerable intake.

**Screen 67**

DRANC.LNV

PEC/PNEC-calculations for LAS  
-----

## Human hazard assessment for children

intake by drinking water	4.19E-02	mg/kg/day
intake by inhalation	1.76E-02	mg/kg/day
intake by cereals	8.73E-04	mg/kg/day
intake by vegetables	1.67E-04	mg/kg/day
intake by milk/yoghurt	8.73E-06	mg/kg/day
intake by meat	8.20E-06	mg/kg/day
intake by butter	7.40E-06	mg/kg/day
intake by cheese	6.32E-06	mg/kg/day
intake by potatoes	6.20E-06	mg/kg/day
intake by fish	5.36E-06	mg/kg/day
Predicted intake	6.05E-02	mg/kg/day
Tolerable intake	1.00E-01	mg/kg/day
Ratio PI/TI	6.05E-01	

This screen provides intake values for children in the same way as Screen 66. Children have a higher food intake per kg body weight than adults and therefore they may be at higher risk.

**Screen 68**

DRANC.LNV		
PEC/PNEC-calculations of LAS		
-----		
PEC/PNEC aquatic organisms		6.14E-01
PEC/PNEC ar.so. earthworms/plants		5.46E-02
PEC/PNEC na.so. earthworms/plants		6.73E-03
PED/PNED calculations of LAS		
-----		
PED aq. mammals/birds	mg/kg/day	4.055319E-02
PNED aq. mammals/birds	mg/kg/day	8.333333
Ratio PED/PNED		4.866384E-03
PED mammals/birds ar.so.	mg/kg/day	6.824507E-04
PED mammals/birds na.so.	mg/kg/day	8.41119E-05
PNED mammals/birds	mg/kg/day	8.333333
Ratio PED/PNED arable soil		8.189409E-05
Ratio PED/PNED natural soil		1.009343E-05

This screen provides the PEC/PNEC ratios for several aquatic and terrestrial organisms in the local environment as a first indication of a possible hazard.

**Screen 69**

Discharge into river
-----
Input parameters on receiving water
Input via sewage treatment and via direct discharge
Concentration in receiving water
Concentration in sediment
Data retrieval/saving
Return to main menu

This is the submenu of the RIVMODEL. The option 'Data retrieval/saving' brings the user in the next submenu.

**Screen 70**

```
Data handling of discharge into river
-----

Data retrieval

Data saving

Return to menu
```

Selection of 'Data retrieval' will bring you in the next screen.

**Screen 71**

```
Data retrieval of discharge into river
-----

C:\ECETOC\HAZCHEM
MEUSE .RVM      EPEMMEN .RVM
 52725760 Bytes free

file name without extension  ?MEUSE
```

This screen will provide the user with the names of files, containing parameter values describing the characteristics of a specific local river or channel. These files will always get the extension ".RVM". By typing one of the filenames on the screen and pressing <ENTER> the corresponding characteristics of the local surface water will be entered into the program.

**Screen 72**

```
MEUSE.RVM

Data handling of discharge into river
-----

Data retrieval

Data saving

Return to menu
```

By selection of the option 'Return to menu' and pressing <ENTER> you will arrive again in the submenu of the RIVMODEL.

## Screen 73

MEUSE.RVM	
input data on receiving water	
-----	
river water flow (m3/sec.)	? 100
concentration in river (µg/l)	0
concentration susp. matter (mg/l)	30
O.C. content susp.matter (w/w)	.1
depth of sediment layer (meter)	.03
O.C. content of sediment (w/w)	.04
burial rate of sediment (mm/year)	.1
wind velocity at 10 m height (m/sec)	5
river width (meter)	25
river depth (meter)	4
Y-distance from river bank (meter)	12.5
mixing diameter in river (meter)	1
1st X-distance downstream (meter)	100
2nd X-distance downstream (meter)	3000
X-distance step (meter)	100
Press <ESC> to return to menu!	

Most of the characteristics and parameters above are self-explaining. The wind velocity is needed, because it contributes to the evaporation of volatile substances from water. The burial rate is set to 0.1 mm/year in this example. The sediment deposition rate is dependent on the concentration of suspended particulates, and the resuspension rate is equal to the deposition rate minus the burial rate.

With the 'Y-distance from river bank' is meant the cross-sectional distance from the riverside, from which the waste water is discharged. The program estimates the concentration at certain X-distances downstream and at a certain Y-distance from the riverside, from which the discharge takes place. This makes it possible to estimate the different concentrations in the mixing plume of the waste water in the river. The mixing diameter indicates the radius/width of the instantaneous mixing zone. The mixing procedure in the RIVMODEL is derived from the confluence of two rivers. The diameter of the instantaneous mixing zone is then more or less the width of the smallest river. For the RIVMODEL this means that the mixing diameter may not be smaller than the ratio between the effluent and the riverflow, multiplied with the river width. If you choose a smaller value, you do not follow the normal physical mixing processes and the program will correct the input figure. If the X-distances downstream are set to numbers smaller than the mixing diameter, the program will treat this numbers as equal to the mixing diameter. By means of this screen each characteristic or parameter may be changed by typing the desired setting behind the question mark and pressing <ENTER>.

**Screen 74**

```
LOC.STP

Discharge into sewage treatment plant
-----

Input parameters on sewage treatment plant

Calculation according to Namkung-Rittmann

Calculation according to Cowan et al.

Calculation according to Monod kinetics

Data retrieval/saving

Return to main menu
```

It is possible to estimate the discharge in the river from a predefined sewage treatment plant. Return to the main menu and select the option 'Discharge to sewage treatment plant'. So you will arrive at the screen above. Subsequently the user is advised to select the option 'Data retrieval/saving' and after that the option 'Data retrieval'. This will bring the user to the screen below.

**Screen 75**

```
LOC.STP

Data retrieval for sewage treatment plant
-----

C:\ECETOC\HAZCHEM
RIVER .STP      EEC .STP      NL .STP      LOC .STP
BELGLUXB.STP   DANMARK .STP   FRANCE .STP  GERMANY .STP
GREECE .STP    IRELAND .STP   ITALY .STP   PORTUGAL.STP
SPAIN .STP     UK .STP       EPEMMEN .STP
52717568 Bytes free

file name without extension ?RIVER
```

This screen will provide the user with the names of files, containing parameter values describing the characteristics of specific sewage treatment plants. These files will always get the extension ".STP". By typing one of the filenames on the screen and pressing <ENTER> the corresponding characteristics of the local sewage treatment plant will be entered into the program. In this example the file 'RIVER' is selected. After pressing <ENTER> you will arrive in the next screen.

**Screen 76**

```

RIVER.STP

Data handling of sewage treatment plant
-----

Data retrieval

Data saving

Return to menu

```

Selection of the option 'Return to menu' will bring you back in the submenu of the sewage treatment plant. Selection of 'Input parameters on sewage treatment plant' will bring you to the next screen.

**Screen 77**

```

RIVER.STP

input data on sewage treatment plant
-----

discharged compound is LAS

number of inhabitant equivalents      ? 432000
waste water/inhabitant/day (l/day)    200
concentration of primary sludge (g/l) .22
O.C.-content of primary sludge (w/w)  .3
hydraulic retention time (hours)      7
sludge retention time (hours)         216
sludge conc. aeration tank (g/l)      2.5
O.C.-content of secondary sludge (w/w) .37
discharge of compound in kg/hour      100  A)
biodegradation rate (1/h)             3    A)
μmax Monod-kinetics (1/hr)            1.5  A)
Michaelis-Menten constant (mg/l)      .5   A)
biodegr. in adsorbed state (y/n)      n    A)

Press <ESC> to return to menu!

```

Via this screen it is possible to enter characteristics of the sewage treatment plant and characteristics of the compound of interest related to the behaviour in the sewage treatment plant, marked with <sup>A)</sup>. Change of the input value of the first 8 parameters will remove the file name from the upper right corner of the screen, change of the input value of the parameter marked with <sup>A)</sup> does not.



The discharge of the compound in kg/h is estimated from the submenu 'Data on production and use'. The user may overwrite this figure. This figure, however, will not be saved to disk via this submenu, but via the submenu 'Data on production and use'. If the discharge is set to 0, calculations will not be carried out.

There are three ways for estimation of the removal by biodegradation. Two ways assume first order kinetics, that of Namkung-Rittmann (1987) and that of Cowan *et al* (1992), requiring an input value for the biodegradation rate. The Monod kinetics requires  $\mu_{\max}$  Monod and the Michaelis Menten Constant. Without any additional information, the estimation according to Namkung-Rittmann should be preferred. In this option a biodegradation rate of 3/hour should be selected for a well biodegradable substance.

The sludge concentration in the effluent has a great impact on the removal percentage of the compound in case of non-biodegradable substances which are sparingly soluble in water and strongly adsorb to activated sludge. The value of 40 mg/l is adopted by the Dutch Ministry of the Environment, but may be too high for many sewage treatment plants.

## Screen 78

Fate of compound LAS in STP (Namkung & Rittmann 1987)		RIVER.STP
-----		
total influent concentration (mg/l)		27.77778
effluent concentration (dissolved mg/l)		.9274756
effluent concentration (suspended mg/l)		.1038773
amount biodegraded per hour (kg)		70.11716
amount volatilized per hour (kg)		7.473972E-13
removed via primary sludge per hour (kg)		25.41254
removed via second. sludge per hour (kg)		.7574384
removed via effl./hour (dissolved kg)		3.338912
removed via effl./hour (suspended kg)		.3739582
primary sludge production per hour (kg)		528
second. sludge production per hour (kg)		291.6667
comp. conc. in primary sludge (mg/kg)		48129.81
comp. conc. in second. sludge (mg/kg)		2596.932
percentage removal by primary sludge		25.41254
percentage removal by biodegradation		70.11716
percentage total removal		96.28713

This screen is produced by selection of the option "Calculation according to Namkung-Rittmann". It provides detailed information on the fate of the compound in the sewage treatment plant.

**Screen 79**

RIVER.STP		
Hazard assessment for sewage treatment bacteria exposed to LAS		
-----		
total influent conc.	(mg/l)	27.77778
effluent conc. dissolved	(mg/l)	.9274756
NOEC water, bacteria STP	(mg/l)	1
PEC/PNEC bacteria influent		2.78E+01
PEC/PNEC bacteria effluent diss.		9.27E-01

This screen provides the comparison of the level in the influent and in the effluent with the NOEC of the bacteria in the sewage treatment plant. In addition, it shows the PEC/PNEC ratios.

**Screen 80**

MEUSE.RVM		
Emission rates to environmental compartments of LAS		
-----		
Direct emission to water (kg/h)		? 0
Volume of direct effluent (m3/sec)		0
STP emission to water (kg/h)		3.71287
Volume of STP effluent (m3/sec)		1
Press <ESC> to return to menu!		

This screen provides information on the discharge of the compound into the surface water after sewage treatment.

It is possible to change the WWTP-emission to water and the effluent volume per time unit by means of this screen. This is desirable in case of estimating the final river water levels after a direct discharge. If the WWTP-unit of the program is not activated, the effluent volume remains zero (the effluent volume is also controlled by the number of inhabitant equivalents).

**Screen 81**

MEUSE.RVM		
fraction of elimination contributed by		
(bio)degradation	=	0.944
volatilization	=	0.000
sedimentation	=	0.056
total elimination rate per second	=	5.83E-06
length for complete mixing (meters)	=	2.40E+03
length for 50% elimination (meters)	=	1.20E+05

This screen provides information on the controlling processes for the removal of the compound from the river water after discharge.

It also provides the total elimination rate per second as well as the distance from the point of discharge needed for complete mixing of the effluent with the river water and the distance needed for 50% of elimination of the substance by all removal processes.

Press <ENTER> to arrive at the next screen.

## Screen 82

Concentration in the water compartment				MEUSE.RVM
X-distance	Y-distance	Conc. µg/l dissolved	Conc. µg/l suspended	
100.0	12.5	1.07E+00	3.22E-02	
200.0	12.5	4.74E+00	1.42E-01	
300.0	12.5	7.18E+00	2.15E-01	
400.0	12.5	8.48E+00	2.54E-01	
500.0	12.5	9.16E+00	2.75E-01	
600.0	12.5	9.50E+00	2.85E-01	
700.0	12.5	9.68E+00	2.90E-01	
800.0	12.5	9.77E+00	2.93E-01	
900.0	12.5	9.81E+00	2.94E-01	
1000.0	12.5	9.83E+00	2.95E-01	
1100.0	12.5	9.84E+00	2.95E-01	
1200.0	12.5	9.84E+00	2.95E-01	
1300.0	12.5	9.84E+00	2.95E-01	
1400.0	12.5	9.83E+00	2.95E-01	
1500.0	12.5	9.83E+00	2.95E-01	
1600.0	12.5	9.82E+00	2.95E-01	
1700.0	12.5	9.82E+00	2.95E-01	
1800.0	12.5	9.81E+00	2.94E-01	
1900.0	12.5	9.81E+00	2.94E-01	
2000.0	12.5	9.80E+00	2.94E-01	
2100.0	12.5	9.79E+00	2.94E-01	
2200.0	12.5	9.79E+00	2.94E-01	
2300.0	12.5	9.78E+00	2.93E-01	
2400.0	12.5	9.78E+00	2.93E-01	
2500.0	12.5	9.77E+00	2.93E-01	
2600.0	12.5	9.77E+00	2.93E-01	
2700.0	12.5	9.76E+00	2.93E-01	
2800.0	12.5	9.75E+00	2.93E-01	
2900.0	12.5	9.75E+00	2.92E-01	
3000.0	12.5	9.74E+00	2.92E-01	

X = distance downstream from the point of discharge;

Y = distance from the riverside, where the discharge of waste water occurs.

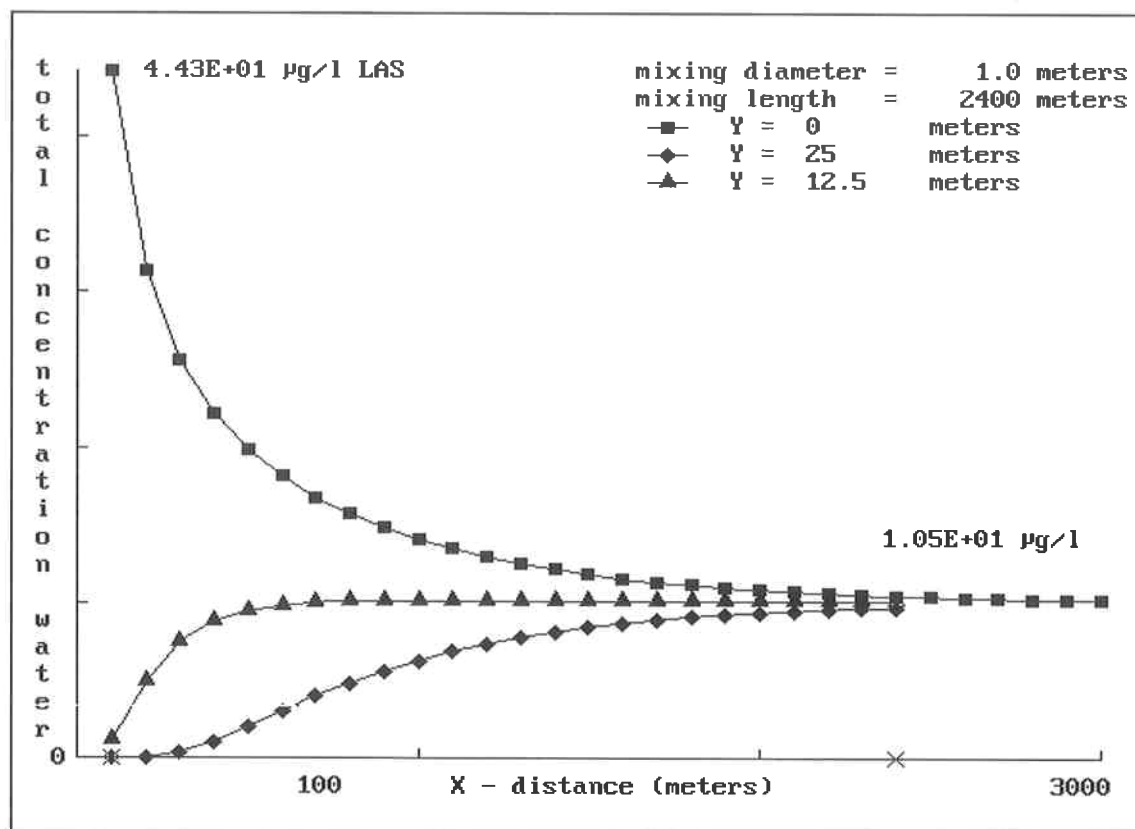
The settings for Y are entered in Screen 73 according to the local situation ('river width' and 'Y-distance from river bank' where the waste water is discharged). The settings for X can be varied. This screen provides the concentrations in the waste water plume at distances downstream of the point of discharge at intervals determined by the last three entries in Screen 73. Continue by pressing <ENTER> until Screen 83 appears.

## Screen 83

do you want a graphic picture? y/n ?y

If the answer to the question is 'yes', then the concentrations in the river water are plotted against the distances X and Y from the point of discharge, provided that a VGA-adaptor is installed in the PC.

## Screen 84



The concentrations at the first sampling point and after complete mixing are presented in numbers.

Screens 85 to 87 present the analogous data for the sediment compartment.

## Screen 85

Concentration in the sediment compartment			MEUSE.RVM
X-distance	Y-distance	ppb w/w	
100.0	12.5	3.32E+00	
200.0	12.5	1.47E+01	
300.0	12.5	2.23E+01	
400.0	12.5	2.63E+01	
500.0	12.5	2.84E+01	
600.0	12.5	2.95E+01	
700.0	12.5	3.00E+01	
800.0	12.5	3.03E+01	
900.0	12.5	3.04E+01	
1000.0	12.5	3.05E+01	
1100.0	12.5	3.05E+01	
1200.0	12.5	3.05E+01	
1300.0	12.5	3.05E+01	
1400.0	12.5	3.05E+01	
1500.0	12.5	3.05E+01	
1600.0	12.5	3.05E+01	
1700.0	12.5	3.04E+01	
1800.0	12.5	3.04E+01	
1900.0	12.5	3.04E+01	
2000.0	12.5	3.04E+01	
2100.0	12.5	3.04E+01	
2200.0	12.5	3.04E+01	
2300.0	12.5	3.03E+01	
2400.0	12.5	3.03E+01	
2500.0	12.5	3.03E+01	
2600.0	12.5	3.03E+01	
2700.0	12.5	3.03E+01	
2800.0	12.5	3.02E+01	
2900.0	12.5	3.02E+01	
3000.0	12.5	3.02E+01	

X = distance downstream from the point of discharge;

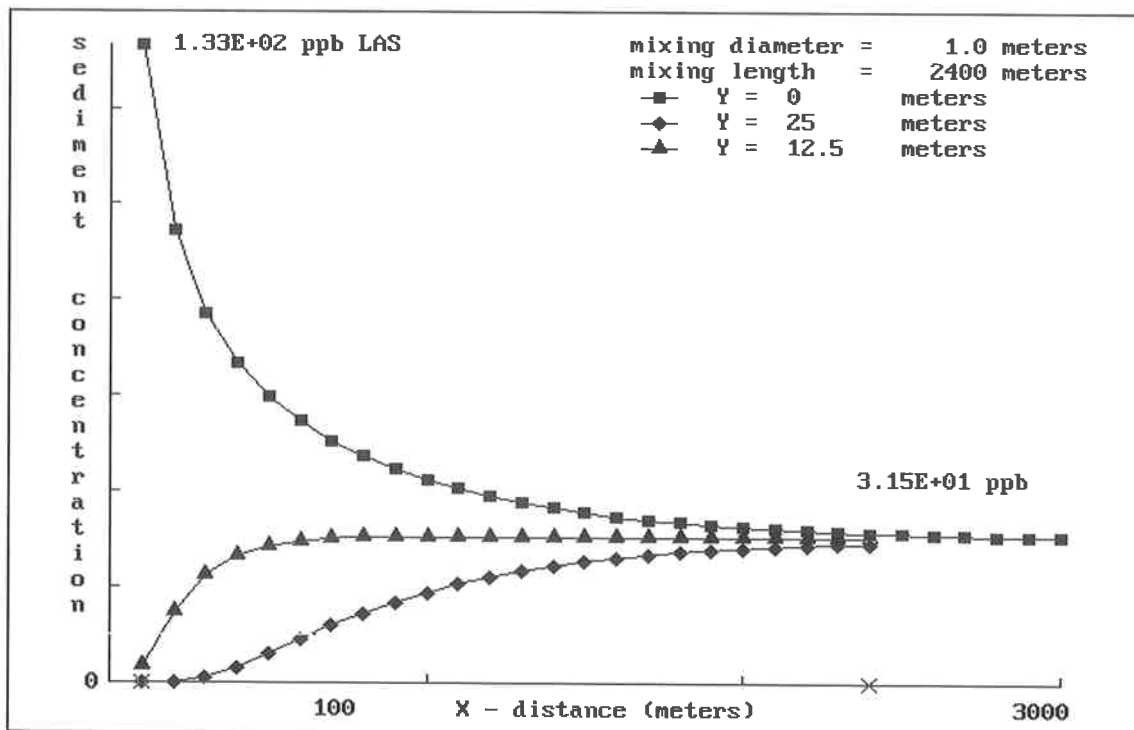
Y = distance from the riverside, where the discharge of waste water occurs.

The settings for Y are entered in Screen 73 according to the local situation ('river width' and 'Y-distance from river bank' where the waste water is discharged). The settings for X can be varied. This screen provides the concentrations in the waste water plume at distances downstream of the point of discharge at intervals determined by the last three entries in Screen 73. Continue by pressing <ENTER> until Screen 86 appears.

**Screen 86**

do you want a graphic picture? y/n ?

If the answer on the question on the top of the page is yes, then the level in the sediment is plotted against the distance from the point of discharge, provided that a VGA-adaptor is installed in the PC.

**Screen 87**

The concentrations at the first sampling point and after complete mixing are presented in numbers.

If you want to leave HAZCHEM, return to the main menu and select 'End of program'.



**APPENDIX A ALPHABETICAL LIST OF SYMBOLS USED IN HAZCHEM EQUATIONS**

$A_r$	=	area of a region [ $m^2$ ]
$A_t$	=	air residence time [h]
$BF$	=	bioconcentration factor
$B_{rs}$	=	sediment burial rate [m/h]
$B_{ur}$	=	burial rate [m/h]
$C_{air}$	=	concentration in air ( $\mu g/m^3$ )
$C_{di}$	=	effluent concentration in dissolved state [mg/l]
$C_e$	=	effluent concentration [mg/l]
$C_{inf}$	=	increase of concentration in river water after complete homogeneous mixing
$C_{ps}$	=	concentration of primary sludge [g/l]
$C_{pw}$	=	concentration in pore water
$Crw$	=	Crop fresh weight per $m^2$
$C_{sed}$	=	Concentration in sediment (w/w on the basis of wet weight)
$C_{sf}$	=	partition coefficient secondary sludge/water [l/kg]
$C_{sl}$	=	Concentration in stem and leaves [ $\mu g/kg$ ]
$C_{sl dp}$	=	Concentration in stem and leaves due to deposition [ $\mu g/kg$ ]
$C_{sl pw}$	=	concentration in stem, leaves by absorption from pore water
$C_{su}$	=	effluent concentration in suspended state [mg/l]
$C_{tot}$	=	total soil concentration
$C_{tr1}$	=	Estimated hypothetical concentration in aeration tank considering all removal processes except biodegradation [ $g/m^3$ ]
$C_{tr2}$	=	Estimated final concentration in aeration tank considering all removal processes
$C_{tw}$	=	total concentration of substance in the aeration tank [ $kg/m^3$ or g/l]
$C_{wa}$	=	increase of concentration in riverwater after partial mixing with effluent, dependent on X and Y [mg/l]
$C_{wd}$	=	concentration in the waste water plume in the river [mg/l]
$C_{wdi}$	=	concentration of substance in river water in dissolved state [mg/l]
$C_{wf}$	=	final concentration in river water, taking into account removal processes and dispersion [mg/l]
$C_{wr}$	=	background concentration of the substance in river water
$C_{wsu}$	=	concentration of substance in river water, adsorbed to suspended particulates [mg/l]

$C_z$	=	Chezy coefficient = $60 \cdot R_h^{(1/6)}$
$D_c$	=	discharge of substance to waste water treatment plant [kg/h]
$D_{cs}$	=	amount of chemical substance entering the aeration tank [kg/h]
$Den_a$	=	density of air in soil = $1.2 \text{ kg/m}^3$
$Den_s$	=	density solids in soil = $2.4 \text{ kg/l}$
$Den_{soil}$	=	density of soil [ $\text{kg/m}^3$ ]
$Dens_{Sed}$	=	density of sediment containing 80% water (with density $1 \text{ kg/dm}^3$ ) and 20% solids (with density $2.4 \text{ kg/dm}^3$ ) resulting in a wet weight density of $1.28 \text{ kg/dm}^3$
$Den_w$	=	density of water in soil = $1000 \text{ kg/m}^3$
DI	=	daily intake
$D_{pr}$	=	density of solids in suspended particulates
Dpr	=	deposition rate [ $\mu\text{g}/(\text{m}^2 \cdot \text{h})$ ]
Dpv	=	deposition velocity [m/h]
DUC	=	daily uptake of cattle [ $\mu\text{g/kg}$ ]
$Dv_{sed}$	=	sediment deposition rate [m/h]
$D_{sed}$	=	sediment depth [m]
$D_t$	=	transversal dispersion coefficient [ $\text{m}^2/\text{s}$ ]
$E_a$	=	emission to air [kg/h]
$E_{fp}$	=	sludge concentration effluent [mg/l]
Elr	=	elimination rate of deposited chemical [1/h]
erf	=	error function
$F_a$	=	partitioning coefficient air/water
$F_{ab}$	=	aerosol-bound fraction
$F_{air}$	=	volume fraction gas phase ( $1 \text{ m}^3/\text{m}^3$ )
$F_{C1}$	=	organic carbon content of primary sludge [kg/kg]
$F_{C2}$	=	organic carbon content of secondary sludge [kg/kg]
$F_{lipid}$	=	lipid content ( $0.01 \text{ m}^3/\text{m}^3$ ) (Mackay, 1991)
$F_{OC}$	=	fraction organic carbon in soil [kg/kg]
$F_{part}$	=	fraction of substance in air as particulate
$F_{pr}$	=	volume fraction 0.2 of suspended particulates in bulk sediment
$F_{prt}$	=	volume fraction aerosol ( $10^{-11} \text{ m}^3/\text{m}^3$ )
$F_{ps}$	=	fraction of substance in primary settler adsorbed
$F_{pw}$	=	fraction of substance in primary settler dissolved
FR	=	feeding rate [ $\text{kg feed}/(\text{kgbw} \cdot \text{d})$ ]
$F_{rdi}$	=	fraction of substance in dissolved state in river water

$F_{rel}$	=	residual fraction of substance in river water, considering all removal processes
$F_{rse}$	=	ratio between concentration in sediment [mg/l] and riverwater [mg/l]
$F_{rsu}$	=	fraction of substance in river water, adsorbed to suspended particulates
$F_{ss}$	=	fraction of substance in aeration tank suspended
$F_{sw}$	=	fraction of substance in aeration tank dissolved
$F_w$	=	ratio between pore water concentration and total soil concentration
$F_{water}$	=	water fraction ( $0.8 \text{ m}^3/\text{m}^3$ )
$H_{dse}$	=	sediment deposition thickness rate [m/h]
$H_{ls}$	=	half life time in sediment for biodegradation [h]
$H_{lw}$	=	half life time in water for biodegradation [h]
$H_r$	=	mean river depth [m]
$H_{rt}$	=	hydraulic retention time [h]
$H_s$	=	depth of sediment layer [m]
$H_{soil}$	=	soil depth (= 0.2m for arable and 0.05m for natural soil)
$H_{soil-ar}$	=	arable soil depth [m]
$H_{soil-nat}$	=	natural soil depth [m]
$I_{cf}$	=	Interception factor for crops
$K_d$	=	biodegradation rate [1/h]
$K_{deg}$	=	removal rate from the river water due to biodegradation [(1/s)]
$K_{dsp}$	=	removal rate from the river water due to sedimentation [(1/s)]
$K_{evap}$	=	removal rate from soil due to volatilization [1/h]
$K_{dvap}$	=	removal rate from the river water due to volatilization [1/s]
$K_{elt}$	=	sum of all removal rates in river water [1/s]
$K_g$	=	the gas phase exchange constant, a measure of the rate of transport of the material away from the interphase in the air [m/h]
$K_{gl}$	=	overall mass transfer coefficient from water to air [m/h]
$K_l$	=	the liquid phase exchange constant, a measure of the rate of transport of the material to the interphase in the water [m/h]
$K_{leach}$	=	leaching rate arable or natural soil [1/h]
$K_m$	=	Michaelis-Menten constant [g/m <sup>3</sup> ]
$K_{oc}$	=	partition coefficient soil organic carbon/water [kg/l]
$K_{sed}$	=	partition coefficient between sediment solids and river water [l/kg]
$K_{sol}$	=	$0.41 \cdot F_{oc} \cdot K_{ow}$ [l/kg]
$K_{spw}$	=	partition coefficient between suspended particulates and river water [l/kg]
$K_{tse}$	=	mass transfer coefficient for diffusion between sediment and water

$L_{mix}$	=	maximum longitudinal distance downstream from the point of discharge needed for complete mixing
$L_{r50}$	=	distance downstream corresponding with 50% removal [m]
$N_{leq}$	=	number of inhabitant equivalents discharging to the WWTP
$P_{aw}$	=	partitioning coefficient air/water
PNEC	=	Predicted No-Effect Concentration [mg/kg] or [mg/l]
$PNEC_{aq}$	=	Predicted No-Effect Concentration for the aquatic compartment [mg/l]
PNED	=	Predicted No-Effect Dose [mg/(kgbw -d)]
$P_{sf}$	=	partition coefficient primary sludge/water [l/kg]
$Q_e$	=	effluent flow rate [m <sup>3</sup> /s]
$Q_f$	=	influent flow to WWTP [m <sup>3</sup> /h]
$Q_w$	=	river flow rate [m <sup>3</sup> /s]
$R_a$	=	removal rate via volatilization [m <sup>3</sup> /h]
$R_b$	=	total removal rate by biodegradation rate [m <sup>3</sup> /h]
$R_{b1}$	=	removal rate by biodegradation in the dissolved state [m <sup>3</sup> /h]
$R_{b2}$	=	removal rate by biodegradation in the adsorbed state [m <sup>3</sup> /h]
$R_{bw}$	=	removal rate without biodegradation [m <sup>3</sup> /h]
RCF	=	root concentration factor
$R_{di}$	=	removal rate in dissolved state via effluent [m <sup>3</sup> /h]
$R_h$	=	hydraulic radius of the river [m]
$R_{mix}$	=	radius/width of the instantaneous mixing zone [m]
$R_{ps}$	=	removal rate of substance via primary sludge [kg/h]
$R_{se}$	=	sediment resuspension rate [m/h]
$R_{so}$	=	removal rate via secondary sludge [m <sup>3</sup> /h]
$R_{su}$	=	removal rate in adsorbed state via effluent [m <sup>3</sup> /h]
$R_{sx}$	=	sediment burial rate [mm/y] (via input screen)
$R_{tot}$	=	total removal rate [m <sup>3</sup> /h]
$R_{wb}$	=	removal rate without biodegradation [m <sup>3</sup> /h]
$S_{ca}$	=	concentration of suspended solids in the aeration tank [g/l or kg/m <sup>3</sup> ]
SCF	=	stem concentration factor
Sert	=	sediment residence time [h]
$SI_{Appl}$	=	substance application rate via activated sludge [ $\mu$ g/(m <sup>2</sup> -h)]
$S_{lc}$	=	substance concentration in secondary sludge [mg/kg]
$SI_{co}$	=	substance concentration in sludge in ppm;
$S_{lp}$	=	primary sludge production per hour [kg/h]
$S_{lpc}$	=	substance concentration in primary sludge [mg/kg]

Spma	=	suspended matter content [mg/l]
S <sub>pa</sub>	=	concentration of suspended particulates [mg/l]
S <sub>rt</sub>	=	sludge retention time [h]
T <sub>ss</sub>	=	total mass of suspended solids in the aeration tank [kg]
TDI	=	tolerable daily intake [mg/(kg bw <sup>-1</sup> d)]
TSCF	=	transportation stream concentration factor
U <sub>avg</sub>	=	average longitudinal stream velocity [m/s]
U <sub>fr</sub>	=	friction velocity [m/s]
U <sub>ss</sub>	=	shear stress velocity [m/s]
V <sub>a</sub>	=	fraction of air volume in soil = 0.2 m <sup>3</sup> /m <sup>3</sup>
V <sub>as</sub>	=	Volume aeration tank [m <sup>3</sup> ]
V <sub>max</sub>	=	Maximum degradation rate [1/h]
V <sub>gas</sub>	=	deposition velocity of gases [m/s]
V <sub>part</sub>	=	deposition velocity of particles [m/s]
VR1	=	waste water flow, related to the number of inhabitant equivalents [m <sup>3</sup> /h];
VR2	=	rain precipitation excess multiplied with the area of the region [m <sup>3</sup> /h]
VR3	=	the advective flow of river water [m <sup>3</sup> /h]
V <sub>sed</sub>	=	fraction of solids in sediment
V <sub>s</sub>	=	fraction of solids volume in soil = 0.5 m <sup>3</sup> /m <sup>3</sup>
V <sub>w</sub>	=	fraction of water volume in soil = 0.3 m <sup>3</sup> /m <sup>3</sup>
V <sub>w</sub>	=	volume of the water compartment in area [m <sup>3</sup> ]
V <sub>win</sub>	=	volume of waste water per inhabitant equivalent [l/d]
W <sub>r</sub>	=	river width [m]
W <sub>rt</sub>	=	water residence time [h]
W <sub>vl</sub>	=	wind velocity at a height of 10 meter [m/s]
X	=	longitudinal distance downstream from point of discharge [m]
X <sub>acc</sub>	=	$X - Dt/(U_{avg} - Wr^2)$ [dimensionless]
Y	=	cross-sectional distance from point of effluent discharge [m]
Y <sub>acc</sub>	=	Y/Wr [dimensionless]
Z <sub>a</sub>	=	1/RT [Mol/(m <sup>3</sup> · Pa)]
Z <sub>air</sub>	=	fugacity capacity constant air
Z <sub>plant</sub>	=	fugacity capacity constant plant
Z <sub>s</sub>	=	K <sub>sol</sub> · Dens/H [Mol/m <sup>3</sup> · Pa]
Z <sub>soil</sub>	=	V <sub>a</sub> · Z <sub>a</sub> + V <sub>w</sub> · Z <sub>w</sub> + V <sub>s</sub> · Z <sub>s</sub> [Mol/(m <sup>3</sup> · Pa)]
Z <sub>w</sub>	=	1/H [Mol/(m <sup>3</sup> · Pa)]

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