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PREDICTION OF SOIL/AIR CONCENTRATION RATIOS FOR CALCULATING CRITICAL CONCENTRATIONS IN AIR AIMED AT SOIL PROTECTION

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SUMMARY

Using the multimedia model SimpleBox, Steady-State soil/air Concentration Ratios (SSCR) have been computed for 21 chemicals. With the SSCRs, critical concentrations of the chemicals in air were computed, starting from the Maximum Permissible Concentrations of the chemicals in soil. The uncertainties in computed SSCRs were assessed by means of Monte Carlo simulations, starting from uncertainties and variabilities in input parameters. For the chemicals studied, the uncertainty in the SSCRs was approximately a factor of 5. The time necessary for establishing 95% of the steady-state ($t_{95\%}$) was also computed. For the chemicals studied, the response times varied from 0.2 to 40 years.

SAMENVATTING

Voor 21 stoffen zijn met het multimedia model SimpleBox de verhoudingen van de stationaire concentraties in bodem en lucht berekend. Met deze Stationaire Concentratie Verhoudingen (SCV-waarden) zijn, uitgaande van de bekende Maximaal Toelaatbaar Risiconiveau's (MTR-waarden) voor grond, critische concentraties in lucht afgeleid. De onzekerheden in de berekende SCV-waarden zijn bepaald door Monte Carlo simulaties te doen met als uitgangspunt de onzekerheid en variabiliteit in de invoergegevens voor het model. Voor de beschouwde stoffen was de onzekerheid in de berekende SCV-waarden ruwweg een factor 5. De tijd die nodig is voor het bereiken van 95% van het stationaire eindniveau ($t_{95\%}$) is eveneens berekend. Voor de beschouwde stoffen varieerden deze tijden van 0,2 tot 40 jaar.

1 INTRODUCTION

Steady-State Concentration Ratio Concept

In The Netherlands and elsewhere, long-term environmental quality objectives are being derived for individual chemicals and for different environmental compartments separately and independently. In response to growing awareness that in real-world situations concentrations of chemicals in air, water and soil are interdependent, attempts are being made to harmonize the quality objectives. Van de Meent and De Bruijn [1] have suggested a modeling procedure to test the coherence of specific sets of independently derived environmental quality objectives for air, water and soil. In The Netherlands this procedure, the Steady-State Concentration Ratio (SSCR) concept, is presently being used as one of the tools in the process of deriving harmonized sets of environmental quality objectives [2]. In essence, the SSCR concept uses a "Mackay-type" multimedia box model in which environmental compartments (air, water, sediment, soil) are modeled as homogeneous boxes. In the model used here [3], the input parameters that characterize the environment are set to represent a typical regional environment that resembles The Netherlands. Using compound-specific data for partition coefficients and rate constants, the model is used to compute the ratios of concentrations in pairs of environmental media at steady state ("level 3", according to the Mackay-nomenclature).

Derivation of Critical Air Concentrations

In this study the SSCR concept is applied to a number of chemicals for which it was felt that atmospheric deposition to natural soil systems could pose a risk on terrestrial ecosystems. Since from a human health point of view no immediate concerns appeared to exist, no air quality objectives have been set for these chemicals so far. It has been suggested, however, that development of air quality objectives aimed at soil protection should be considered. It was envisaged that even at low concentration levels in air atmospheric deposition could result in such high concentrations in soil that possibly the Maximum Permissible Concentration (MPC) could be exceeded. The purpose of the present study was to determine soil/air concentration ratios, from which critical air concentrations could then be be computed, starting from the MPC_{soil} values.

$$CritCONC_{air} = \frac{MPC_{soil}}{SSCR_{soil/air}} \qquad (1)$$

with

$CritCONC_{air}$:	Critical Concentration in air [g/m^3]
MPC_{soil}:	Maximum Permissible Concentration in soil [g/kg(dry weight)]
$SSCR_{soil/air}$:	Steady-State Concentration Ratio soil/air [m^3/kg(dry weight)]

The chemicals and their MPC_{soil} values are listed in Table 1.

Time to steady state

As a reasonable approximation, concentrations in the environment are expected to become constant in time (steady state) if emissions and imports remain constant. It takes time to approach the steady state. For a number of the chemicals of table 1 long response times are anticipated: the results of the present emission levels may not have become fully visible yet and the results of possible emission reductions may not be observed until after a considerable period of time. Since, in the case of long response times, one may want to base environmental management decisions not on the expected steady-state but on the state after a given period of time, response times were computed by means of a quasi-dynamic ("level 4") model. The time necessary to reach 95% of the predicted steady-state concentration level in soil, t_{95}, is reported.

Table 1: Chemicals of this study and their Maximum Permissible Concentrations in soil [4].

	MPCsoil [μg/kg(dry)]
Aldrin	50
Carbofuran	4.7
Chlordane	4.3
Chlorpyrifos	1.1
p,p'-DDD	10
p,p'-DDE	10
p,p'-DDT	10
Dieldrin	50
Endosulfan	50
Endrin	2.9
Fenthion	0.35
α-HCH	220
β-HCH	92
γ-HCH (Lindane)	5
Heptachlor	0.7
Heptachlor epoxide	0.7
Hexachlorobenzene	28
Pentachlorobenzene	120
Pentachlorophenol	170
Quintozene	330
Thiram	38

Uncertainty

The validity of the SSCR concept as a predictor of real-world concentration ratios and the uncertainty associated with the predicted values have only marginally been addressed. The SimpleBox model that was used for computing the SSCRs is deterministic: single values are assumed for the model parameters that characterize the environment and the process rates, and the model produces single values as output. Obviously, the input values can only represent "typical" situations. In reality, however, environmental characteristics (areas, heights and depths, residence times of air and water, soil run-off rates, etc.) show natural variation in time and space. Rate constants for transport and degradation are not only variable, but the exact values of these parameters are usually uncertain and sometimes not known at all. This is particularly true for degradation rates in soil, for which wide ranges of half lives were reported for each of the chemicals. There is reason to believe that, in general, soil/air concentration ratios are dependent on this input. In view of this it was decided that uncertainty and variability in input was to be taken into account in this study. In addition to the computed "typical" or "most likely" SSCRs, ranges of uncertainty that resulted from variability and uncertainty in input parameters were computed by means of Monte Carlo simulations.

2 METHODS

Quality

The study has been carried out according to the quality assurance system of the Laboratory of Ecotoxicology [5]. The study plan is reproduced in Appendix 1. Specification of uncertainties in the computed SSCRs was not part of the plan; this was added as an extra.

At the time of this study, no detailed instructions for carrying out model computations were available in the quality assurance system. A check was performed on what is regarded as the most important aspect of quality in this type of work: the reproducibility of the results. After completion of the work, an independent scientist selected three of the chemicals and repeated the calculation of SSCRs.

Scenario

The SSCRs were computed according to the procedure described by Van de Meent and De Bruijn [1] and Bockting and Van de Plassche [2], using the SimpleBox model. A standard emission scenario was used, in which continuous emission of equal amounts to air, water and agricultural soil simultaneously was assumed. The absolute values of the emission rates were chosen arbitrarily since the SSCRs were not expected to be influenced by the absolute emissions. For all other general (not compound-specific) input data, the default values of SimpleBox were used for all chemicals. This is illustrated in Appendix 2, for the case of Thiram.

Compound-specific input

Compound-specific data as input into the model were obtained from the literature by the Toxicology Advisory Centre (TAC), according to the quality assurance procedures of the Center at that time (Sept-Dec, 1993). No major check was performed on the data. The data are given in Appendix 3. Since K_{ow} data were not reviewed, the data reported in a critical review of Henry's Law constants by Suntio *et al.* [12], that was used by TAC as one of the sources for data, were taken. Additional search was done in the IRPTC database [7], the MEDCHEM database [8], and the ASTER database [20]; the results are printed in Appendix 4. LogPstar-data reported for some of the chemicals appeared to be considerably higher than the data reported by Suntio. In these cases, the logPstar data were given preference. In addition, ClogP-calculated values from the MEDCHEM database were inserted for the missing K_{ow} data. For DDD, DDE, and endrin, no degradation rates in soil were available. The rate constant for DDT was used for DDE and DDD; the rate constant of dieldrin was used for endrin. The data reported for pentachlorophenol are to be considered with special care, since the pH of measurement for the solubility was not available. According to the solubility estimation by ASTER, the solubilty is most likely related to the (partly) dissociated form; it was assumed that the reported value of the solubility applies to the pH of natural water. Because the model is likely to be sensitive to these properties, the results should be considered with care. The input data used are given in Table 2. The ranges of uncertainty mentioned there reflect subjective assessment of the differences in reported data and the reliabilities of these data.

Computation of Steady-State Concentration Ratios

SSCRs were computed with the SimpleBox version 1.1 (950101) spreadsheet for Excel version 5.0. The version used here was an update of the original SimpleBox version 1.0 (930801) [3]. The following modifications were made:

- The original Lotus 123 spreadsheet was converted into an Excel spreadsheet.
- The lay-out of the spreadsheet was updated and some output tables were added/modified. One addition was the computation of steady-state concentration- and fugacity ratios for the compartments water and air, and natural soil and air, respectively. These results were not available in the 1.0 version of SimpleBox.
- The numerical integration routine that is used to compute the quasi-dynamic ("level 4") output was replaced by a faster procedure. This is described elsewhere [6].

Table 2: Input data used

	CAS no.	MP [C°]		$logK_{ow}$ [-]		range	Solubility [$mg.l^{-1}$]		range	Vap. Press. [Pa]		range	DT50(soil [d]		range
Aldrin	309-00-2	104	[7]	6.5	[8,9]	+/- 0.33	0.02	[12]	+/- factor 3.3	0.005	[12]	+/- factor 3.3	50	[18]	40-400
Carbofuran	1563-66-2	153	[7]	2.3	[8,10]	+/- 0.33	650	[12]	+/- factor 3.3	0.0015	[12]	+/- factor 3.3	50	[11]	16-160
Chlordane	57-74-9	104	[12]	5.8	*	+/- 0.33	0.05	[12]	+/- factor 3.3	0.0011	[12]	+/- factor 3.3	1200	[18]	400-3600
Chlorpyrifos	291-88-2	43	[7]	5.3	[8,9]	+/- 0.33	0.3	[12]	+/- factor 3.3	0.0015	[12]	+/- factor 3.3	30	[18]	7-140
p,p'-DDD	72-54-8	112	[12]	6.2	[8,9]	+/- 0.33	0.05	[12]	+/- factor 3.3	0.0001	[12]	+/- factor 3.3	2000	†	100-3600
p,p'-DDE	72-55-9	89	[12]	7.0	[8,9]	+/- 0.33	0.04	[12]	+/- factor 3.3	0.001	[12]	+/- factor 3.3	2000	†	100-3600
p,p'-DDT	50-29-3	109	[12]	6.9	[8,9]	+/- 0.33	0.003	[12]	+/- factor 3.3	0.00002	[12]	+/- factor 3.3	2000	[13]	100-3600
Dieldrin	60-57-1	177	[12]	5.2	[8,9]	+/- 0.33	0.17	[12]	+/- factor 3.3	0.0005	[12]	+/- factor 3.3	2000	[18]	400-3600
Endosulfan	115-29-7	85	[12]	3.6	[12]	+/- 0.33	0.15	[12]	+/- factor 3.3	0.0011	[12]	+/- factor 3.3	15	[18]	5-1000
Endrin	72-20-8	209	[7]	5.2	[8,9]	+/- 0.33	0.23	[12]	+/- factor 3.3	0.00002	[12]	+/- factor 3.3	3000	[18]	100-5000
Fenthion	55-38-9	liquid	[12]	4.1	[8,14]	+/- 0.33	50	[12]	+/- factor 3.3	0.004	[12]	+/- factor 3.3	100	‡	70-200
α-HCH	319-84-6	158	[12]	3.8	[8,15]	+/- 0.33	1	[12]	+/- factor 3.3	0.003	[12]	+/- factor 3.3	100	[16]	70-200
β-HCH	319-85-7	309	[12]	3.8	[8,15]	+/- 0.33	0.1	[12]	+/- factor 3.3	0.00004	[12]	+/- factor 3.3	100	[16]	70-300
γ-HCH	58-89-9	113	[12]	3.7	[8,17]	+/- 0.33	6.5	[12]	+/- factor 3.3	0.003	[12]	+/- factor 3.3	365	[16]	10-1000
Heptachlor	76-44-8	95	[12]	4.9	*	+/- 0.33	0.1	[12]	+/- factor 3.3	0.03	[12]	+/- factor 3.3	200	[18]	60-600
Heptachlor epoxide	1024-57-3	158	[7]	4.6	[7]	+/- 0.33	0.2	[18]	+/- factor 3.3	0.0026	[18]	+/- factor 3.3	500	§	150-1500
Hexachlorobenzene	118-74-1	231	[12]	5.7	[8,9]	+/- 0.33	0.005	[19]	+/- factor 3.3	0.001	[12]	+/- factor 3.3	1000	[18]	360-3600
Pentachlorobenzene	608-93-5	86	[20]	5.2	[8,9]	+/- 0.33	0.56	[19]	+/- factor 3.3	0.0015	[19]	+/- factor 3.3	200	[19]	60-600
Pentachlorophenol**	87-86-5	190	[12]	5.1	[8,21]	+/- 0.33	12	[12]	+/- factor 3.3	0.002	[12]	+/- factor 3.3	50	[18,19]	7-200
Quintozene	82-68-8	144	[7]	4.2	[8,22]	+/- 0.33	0.032	[18]	+/- factor 3.3	0.32	[18]	+/- factor 3.3	100	[23]	10-300
Thiram	137-26-8			1.8	*	+/- 0.33	30	[18]	+/- factor 3.3	0.008	[18]	+/- factor 3.3	20	[24]	7-70

* MEDCHEM-calculated (ClogP)
† No data available; value of DDT used
‡ No data available; data of α- and β-HCH used
§ Estimated on the basis of data in Howard [18]
** pH of measurement for solubility indicated (see text)

- Some minor improvements/corrections were made:
  - For computing default-values for the fraction associated with aerosol particles, FRass(aerosol), melting point dependence of the sub-cooled liquid vapor pressure is incorporated. For details, see [6]
  - Collection efficiency of aerosol particles by rain drops has been introduced as a variable that can be set by the user; the default value of 200,000 was maintained in this study.
  - Mass flow of chemical associated with biota was included in the mass balance (was neglected in SimpleBox 1.0).

Compatibility with the original version 1.0 was verified by checking the results obtained for the default settings of the model. When the input parameters of SimpleBox 1.1 (950101) were set equal to the default settings of SimpleBox 1.0 (930801), the two versions produced essentially the same results; the largest difference observed for steady-state concentrations, other than the concentration in biota was 0.5 % (for the water compartment).

The reported $SSCR_{soil/air}$ were computed by taking the quotient of the steady-state concentration in natural soil, expressed in g/kg(dry), and the steady-state concentration in air (gas phase + aerosol phase), expressed in g/m3, from output table 1 (Analysis report) in SimpleBox version 1.1 (950101).

Uncertainty analysis

Monte Carlo simulations were done by means of Crystal Ball version 3.02 (Decisioneering, Inc., Bolder, CO, USA). Crystal Ball is an add-in for Excel. The parameter ranges given in Table 1 for the chemical-specific parameters were used. For the general (non chemical-specific) parameters, the ranges of uncertainty/variability were estimated by the author. For the purpose of this study, these uncertainties were represented as triangular distributions, with the base set equal to the estimated range of uncertainty/variability (Appendix 5).

Computation of Critical Air Concentrations

Critical Air Concentrations were computed according to Equation 1. The MPC_{soil} values were provided by the Toxicology Advisory Centre [4]. The values were taken without further questioning; the MPCs are listed in Table 2.

3 RESULTS

Identification of most important uncertainties

Monte Carlo simulations of uncertainty were done for three hypothetical chemicals with properties chosen to stand as example for the chemicals of study. With these three chemicals the uncertainties of a number of possible model-outputs were generated:

- steady-state concentration in air
- steady-state concentration in water
- steady-state concentration in sediment
- steady-state concentration in agricultural soil
- steady-state concentration in natural soil
- steady-state fugacity ratio soil/air
- steady-state concentration ratio soil/air
- steady-state fugacity ratio water/air
- steady-state concentration ratio water/air

The results (not shown here) indicated that single concentrations had broader ranges of uncertainty than had the concentration and fugacity ratios. The $SSCR_{soil/air}$ appeared sensitive to only a few parameters, notably the rate constant for degradation in natural soil, k_{deg}(soil1), the soil depth, DEPT(soil1), the soil-water partition coefficient, as influenced by the soil organic matter content, CORG(soil1), and the vapor pressure of the chemical. This result was expected. For this specific model result (quotient of the steady-state concentration in natural soil and the steady-state concentration in air) the secondary compartment (soil) is loaded only indirectly, via the primary compartment (air). Therefore, the soil-air concentration ratio depends only on the factors that control the rate of disappearance of the chemical from the soil compartment. Of course, the concentrations in absolute terms, also for natural soil, show much more variance, as do the water-air concentration ratios.

On the basis of this systematic analysis it was concluded that, for the purpose of predicting $SSCR_{soil/air}$, no major effort to characterize uncertainties other than those mentioned above was needed.

Computation of soil/air concentration ratios

For all of the chemicals listed in Table 1, the standard SimpleBox computation was carried out and the output printed. A typical result is shown in Appendix 6, where the analysis report for Thiram is reproduced. Only the result on the second last row, marked "SOIL-AIR concentration ratio", the $SSCR_{soil/air}$, was used. The computed SSCRs are listed in Table 3.

Associated uncertainties

In addition, a standard Crystal Ball simulation was carried out for all the chemicals. Analysis reports of all the chemicals are given in Appendix 7. Of this output, the 5- and 50-percentiles of the distribution of $SSCR_{soil/air}$, and the names of the parameters of which the uncertainty/variability contributed more than 5% to the uncertainty in SSCR are listed in Table 3, in addition to the most likely values. The 5-percentile of the $SSCR_{soil/water}$ can be used to compute upper limits of the Critical Air Concentrations. Exceedance of MPC_{soil} is unlikely if air concentrations stay below Critical Air Concentrations that are based on the 5-percentile of $SSCR_{soil/water}$. It should be emphasized that assessment of the uncertainty in SSCR is only a first step in assessment of the overall uncertainty in ecosystem protection. In addition to this, the uncertainty in MPC_{soil} as a measure for ecosystem "safety" should be taken into account.

Time to steady state

Standard quasi-dynamic runs were done with SimpleBox "level 4"-routine. This yielded concentration-time series of predicted concentrations (development towards steady state). The output obtained for Thiram is given in Appendix 8 as an illustration. From this output, the time at which 95% of the steady-state concentration in the soil compartment was reached, t_{95}, was read. The t_{95}-values for the chemicals are listed in Table 3.

Table 3: Results

	$SSCR_{soil\text{-}air}$ [m3/kg(dry)]			UF*	Sources of	MPC_{soil}	$CritCONC_{air}$	t 95 †
	likeliest	median	5-perc.		uncertainty ‡	[g/kg(dry)]	[g/m3]	[yr]
Aldrin	2.4E+00	4.5E+00	1.5E+00	1.6	1, 3, 5, 10	5.0E-05	2.1E-05	0.6
Carbofuran	9.6E+03	8.3E+03	2.3E+03	4.2	5, 3, 6, 1, 4	4.7E-06	4.9E-10	0.54
Chlordane	9.0E+01	1.8E+02	5.0E+01	1.8	3, 5, 1, 10, 7	4.3E-06	4.8E-08	14.5
Chlorpyrifos	1.6E+01	1.3E+01	3.2E+00	5.1	3, 5, 1, 10, 7	1.1E-06	6.9E-08	0.36
p,p'-DDD	2.8E+03	7.1E+02	1.3E+02	21	3, 1, 5	1.0E-05	3.6E-09	24
p,p'-DDE	5.1E+02	1.3E+02	2.4E+01	21	3, 5, 1, 10	1.0E-05	2.0E-08	24
p,p'-DDT	9.6E+03	2.5E+03	5.2E+02	18	3, 1, 5, 7	1.0E-05	1.0E-09	24
Dieldrin	3.9E+02	2.8E+02	7.5E+01	5.2	3, 5, 1, 10, 6	5.0E-05	1.3E-07	24
Endosulfan	4.3E+00	4.6E+00	9.6E-01	4.5	3, 5, 1, 10	5.0E-05	1.2E-05	0.18
Endrin	1.4E+04	2.3E+03	4.5E+02	31	3, 5, 6, 1, 4, 10	2.9E-06	2.1E-10	36
Fenthion	6.7E+02	5.0E+02	1.3E+02	5.2	5, 3, 6, 1, 4, 10	3.5E-07	5.2E-10	1.2
α-HCH	6.2E+01	8.3E+01	2.7E+01	2.3	5, 1, 3, 10, 8, 7	2.2E-04	3.5E-06	1.2
β-HCH	1.2E+02	1.4E+02	3.6E+01	3.3	5, 6, 1, 4, 3, 10	9.2E-05	7.7E-07	1.2
γ-HCH	3.7E+02	4.3E+01	6.4E+00	58	3, 6, 1, 5, 4	5.0E-06	1.4E-08	4.2
Heptachlor	1.2E+01	1.2E+01	3.6E+00	3.3	3, 5, 1, 10, 7	7.0E-07	5.8E-08	2.3
Heptachlor epoxide	2.9E+01	2.7E+01	8.5E+00	3.4	3, 1, 5, 10, 11	7.0E-07	2.4E-08	5.8
Hexachlorobenzene	2.4E+01	3.0E+01	9.7E+00	2.5	3, 1, 12, 10, 5, 11	2.8E-05	1.2E-06	12
Pentachlorobenzene	7.8E+01	7.0E+01	1.9E+01	4.1	3, 5, 1, 10, 6	1.2E-04	1.5E-06	2.4
Pentachlorophenol	1.6E+02	8.3E+01	1.6E+01	9.8	3, 6, 5, 1, 4, 10	1.7E-04	1.1E-06	0.58
Quintozene	4.5E-01	3.6E-01	1.3E-01	3.4	3, 12, 1, 5, 2	3.3E-04	7.3E-04	0.78
Thiram	2.8E+01	2.6E+01	7.1E+00	3.9	5, 3, 1, 6	3.8E-05	1.4E-06	0.21

* Uncertainty factor = likeliest value / 5-percentile value

† Time necessary to reach 95% of the steady state in soil

‡ In order of contribution to variance (only sources > 5%): 1 = DEPTH(soil), 2 = CORG(soil), 3 = kdeg(soil), 4 = Kow, 5 = VAPOR PRESSURE, 6 = SOLUBILITY, 7 = COLLECTeff, 8 = AEROSOLdepreate, 9 = Frwater(soil), 10 = Frair(soil), 11 = Frwater(soil), 12 = kasl(soilair)

Critical concentrations in air

Critical Air Concentrations were obtained by dividing the MPC_{soil} value (Table 1) by the computed $SSCR_{soil/air}$, as in equation (1). The results are listed in Table 3.

4 FINAL REMARKS

- Critical Air Concentrations, computed from Maximum Permissible Concentrations in soil using the Steady-State Concentration Ratio concept, are given in this report without further comment. No attempt is made to discuss the possible application of the Critical Air Concentrations as a starting point for setting Air Quality Objectives.
- No attempt is made to further use the uncertainties associated with the SSCRs to quantify confidence limits of the computed Critical Air concentrations. It is noted that the ranges of uncertainty in SSCRs indicate that, in this specific set of computations, the difference between the 5th percentiles and the most likely values of the SSCRs was typically smaller than a factor of 5.
- Uncertainties in SSCRs can be further narrowed down if some key parameters, notably the rate constants for degradation in soil, the vapor pressures, the soil depths, and the solubilities can be given with more certainty. Of these, the degradation rates in soil are most important.

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APPENDIX 1: Project plan

DEELPROJECTBESCHRIJVING "INS-luchtbox"

Projectgegevens:

Project:	Ecorouting
Projectnummer:	719101
Deelproject:	Berekening van de doorwerking van concentraties in lucht naar concentraties in bodem voor geselecteerde stoffen ("INS-luchtbox")
Opdrachtgever:	DGM/SVS; contactpersoon J.H.M. de Bruijn.
Laboratorium:	Laboratorium voor Ecotoxicologie.
Deelprojectleider:	D. van de Meent
Deelprojectteam:	Van de Meent, Van de Plassche
Startdatum:	1-1-1993
Einddatum:	31-12-1994

Samenvatting projectinhoud:

Ten behoeve van de Integrale Normstelling voor Stoffen wordt voor een aantal geselecteerde stoffen onderzocht of, en op welke manier kwaliteitsdoelstellingen voor lucht kunnen worden afgestemd met die voor bodem en water. Het projekt bestaat uit drie onderdelen:

i Verkenning. Hierin wordt de probleemstelling nader geanalyseerd. Er wordt een modelmatige rekenmethode ontwikkeld waarmee de vraag kan worden beantwoord;

ii Testen van coherentie van kwaliteitsdoelstellingen voor een selectie van"vluchtige organische stoffen"; berekend wordt of de verhouding van onafhankelijk afgeleide doelstellingen voor water en bodem enerzijds, en lucht anderzijds afwijkt van de concentratieverhoudingen zoals die op termijn mogen worden verwacht bij sectoraal beleid;

iii Berekening van kritische luchtconcentraties voor een selectie van "atmosferisch deponerende stoffen"; berekend wordt bij welke concentratie in lucht naar verwachting juist de kwaliteitsdoelstelling in bodem wordt bereikt.

Akkoord betrokkenen:

Opdrachtgever (J. de Bruijn):

Labhoofd ECO (H.de Kruijf):

Projectleider ECOROUTING (W. Peijnenburg):

ProjektleiderINS (E. van de Plassche):

Deelprojektleider (D. van de Meent):

1. Inleiding, beschrijving van de opdracht.

In het kader van het projekt "Integrale Normstelling Stoffen" (ACT, Van de Plassche) is de vraag aan de orde of de intercompartimentale doorwerking van concentraties voor de Nederlandse situatie zodanig kan worden gekwantificeerd dat het kan worden gebruikt als basis voor afstemming van kwaliteitsdoelstellingen voor de verschillende milieucompartimenten. Eerder is voor afstemming van doelstellingen voor water, sediment en bodem het evenwichtspartitiebeginsel als uitgangspunt gebruikt.

Nu wordt nagegaan hoe afstemming van de kwaliteitsdoelstellingen voor water en bodem met die voor lucht kan worden gerealiseerd. Toepassing van het evenwichtspartitiebeginsel naar analogie met de werkwijze voor water en bodem lijkt niet vanzelfsprekend, want voor de gewone Nederlandse situatie wordt verwacht dat het compartiment lucht niet in een toestand van thermodynamisch evenwicht verkeert met de compartimenten water en bodem. Als alternatief is daarom als mogelijk uitgangspunt genomen om de modelmatig berekende intercompartimentale concentratieverhoudingen in de stationaire (mogelijk niet-evenwichts) toestand te gebruiken als afstemmingsbasis. Berekeningen met het model SimpleBox zouden daarbij in de plaats kunnen treden van het gebruik van evenwichtspartitiecoëfficiënten. Hierbij wordt vervolg gegeven aan eerdere besprekingen die over dit onderwerp hebben plaatsgevonden in en buiten de INS onderzoekbegeleidingsgroep.

Er is een lijst van stoffen waarvoor integrale normen worden afgeleid, en waarvoor afstemming van kwaliteitsdoelstellingen voor lucht met die voor water en bodem aan de orde is. In dit projekt gaat het om de "vluchtige organische stoffen" en de "atmosferisch deponerende stoffen".

2. Doel van het onderzoek.

Doel van het onderzoek is om

(i) nader te onderzoeken of de berekening van stationaire concentratieverhoudingen een praktisch uitvoerbare optie is voor afstemming van kwaliteitsdoelstellingen en, op basis hiervan, een berekeningsprocedure voor te stellen;

(ii) voor de "vluchtige organische stoffen" te becijferen of de sets (onafhankelijk van elkaar) afgeleide maximaal toelaatbaar risico-niveaus voor lucht en water/bodem coherent zijn;

(iii) voor de "atmosferisch deponerende stoffen" te berekenen bij welke concentraties in lucht de maximaal toelaatbare concentraties in bodem worden bereikt en hoe lang het duurt voordat de stationaire toestand is bereikt; de lijst van "atmosferische stoffen" is opgenomen als appendix.

3. Aanpak.

Onderdeel (i), de uitwerking van de rekenmethode, is afgerond. De resultaten zijn beschreven in publikaties (De Bruijn *et al.*., 1992; Van de Meent en De Bruijn, 1993).

Onderdeel (ii), de berekeningen voor de "vluchtige stoffen", is uitgevoerd. De resultaten zijn beschreven in een RIVM-rapport (Bockting en Van de Plassche, 1993).

Onderdeel (iii), de berekeningen voor de "atmosferische stoffen", wordt in 1994 uitgevoerd; deze projectbeschrijving betreft dit laatste onderdeel. Anders dan bij de "vluchtige stoffen" is hier niet de vraag of de voor lucht op toxicologische gronden afgeleide MTR-waarden strijdig zijn met de MTR-waarden voor bodem: voor de "atmosferische stoffen" zijn geen toxicologische lucht-MTR's afgeleid. De vraag hier is of er kwaliteitsdoelstellingen voor lucht zouden moeten worden gesteld die zijn gericht op bescherming van het bodemsysteem. Daarom wordt voor deze stoffen de kritische concentratie in lucht berekend: die waarde van de concentratie in lucht, waarbij juist de kwaliteitsdoelstelling voor bodem wordt bereikt. De berekeningswijze is dezelfde als die voor onderdeel (ii): de SimpleBox-berekening voor "Nederland". Een aantal van de "atmosferische stoffen" behoort tot de groep van "persistente stoffen", waarvoor moet worden verwacht dat het

lang kan duren voordat de te berekenen stationaire concentratieverhouding zich zal hebben ingesteld. Daarom wordt, in aanvulling op berekening van de stationaire toestand, een quasi-dynamische berekening gedaan. Aan de hand hiervan wordt aangegeven hoe lang het duurt voordat de concentratie in de bodem 95% van de kwaliteitsdoelstelling heeft bereikt.

Voor de berekeningen zijn de volgende gegevens nodig als invoer:
- kritische concentratie in bodem (kwaliteitsdoelstelling)
- fractie geassocieerd met aerosol (kan eventueel geschat worden uit dampdruk)
- dampdruk
- wateroplosbaarheid
- Henry coëfficiënt (kan eventueel worden geschat uit dampdruk en wateroplosbaarheid)
- bodem-water partitiecoëfficiënt (kan eventueel worden geschat uit K_{ow} en f_{oc})
- degradatiesnelheidskonstante voor bodem (kan eventueel worden geschat uit degradatiesnelheidskonstante voor water en de bodem-water partitiecoëfficiënt)

De gegevens worden verzameld door ACT; de berekeningen worden uitgevoerd door ECO.

4. Te verwachten resultaat.

De berekeningsresultaten (per stof een kritische concentratie in lucht en de $t_{95\%}$ -waarde), worden gerapporteerd als RIVM-rapport.

5. Uitvoeringsplan.

De gegevens worden in het vierde kwartaal van 1993 verzameld door literatuuronderzoekers van ACT, in overleg met Van de Meent. De berekeningen worden in het eerste kwartaal van 1994 gedaan door Van de Meent.

Bij de werkzaamheden worden de voor het project relevante delen van paragraaf 5.3 van het Kwaliteitshandboek Laboratorium voor Ecotoxicologie: "De kwaliteitsbeheersing van Informatiserings- en Automatiseringswerkzaamheden" (verslaglegging, versiebeheer, functionaliteit, validatie), in acht genomen.

6. Verantwoordelijkheden.

Het werk maakt deel uit van het project ECOROUTING (projectleider: Peijnenburg, Laboratorium voor Ecotoxicologie).

Appendix

Lijst van stoffen waarvoor kritische concentraties in lucht worden berekend:

- aldrin
- carbofuran
- chlorpyrifos
- p,p'-DDD
- p.p'-DDE
- p,p'-DDT
- o,p'-DDT
- endosulfan
- endrin
- dieldrin
- fenthion
- α-HCH
- β-HCH
- γ-HCH
- heptachlor
- heptachlor epoxide
- hexachloorbenzeen
- pentachloorbenzeen
- pentachloorfenol
- quintozene
- thiram

APPENDIX 2: Chosen input data.

Example: Thiram (for chemical-specific data on other chemicals, see Table 2)

SIMPLEBOX MODEL DEFINITION

COMPOUND PROPERTIES			Formula	Value	Used	
(A)	COMPOUND NAME	Thiram		HYPO	HYPO	
(A)	FORMULA			HyPo	HyPo	
(A)	MOL WEIGHT [g.mol-1]	250		250	2.50E-01	kg.mol-1
(A)	Kow [m(w)3.m(o)-3]	6.31E+01		1E+05	6.31E+01	-
(A)	VAPOR PRESSURE [Pa]	8.00E-03		1E-03	8.00E-03	Pa
(A)	SOLUBILITY [mg.l-1]	9.90E+01	1.16E+04		1.20E-01	mol.m-3
(A)	MELTING POINT [deg. C]			0	2.73E+02	K
(A)	PASSreadytest [y/n]			n	n	
(D)	STND(water) [g.l-1]		1.85E-01		7.41E-01	mol.m-3
(D)	STND(sed) [g.kg(d)-1]		5.85E-01		2.34E-03	mol.kg-1
(D)	STND(soil) [g.kg(d)-1]		5.85E-01		2.34E-03	mol.kg-1
(D)	STND(gmdwater) [g.l-1]		1.85E-01		7.41E-01	mol.m-3
(D)	STND(air) [g.m-3]		5.21E-03		2.09E-05	mol.m-3
(A)	K(air-water) [-]		2.81E-05		2.81E-05	-
(A)	TEMPERATURE [deg. C]	12		12	2.85E+02	K
(A)	K(susp-water) [-]		2.48E+00		2.48E+00	-
(A)	Kp(susp) [l.kg(d)-1]		6.31E+00		6.31E+00	l.kg-1
(A)	CORG(susp) [% C]	10		10	1.00E-01	-
(A)	K(bio-water) [-]		3.15E+00		3.15E+00	-
(A)	BCF(fish) [l.kg(w)-1]		2.93E+00		2.93E+00	l.kg-1
(A)	FAT(fish) [vol %]	5		5	5.00E-02	-
(A)	K(sed-water) [-]		2.38E+00		2.38E+00	-
(A)	Kp(sed) [l.kg(d)-1]		3.15E+00		3.15E+00	l.kg-1
(A)	CORG(sed) [% C]	5		5	5.00E-02	-
(A)	K(soil1-water) [-]		3.55E+00		3.55E+00	-
(A)	Kp(soil1) [l.kg(d)-1]		3.15E+00		3.15E+00	l.kg-1
(A)	CORG(soil1) [% C]	5		5	5.00E-02	-
(A)	K(soil2-water) [-]		3.55E+00		3.55E+00	-
(A)	Kp(soil2) [l.kg(d)-1]		3.15E+00		3.15E+00	l.kg-1
(A)	CORG(soil2) [% C]	5		5	5.00E-02	-
(A)	K(soil3-water) [-]		3.55E+00		3.55E+00	-
(A)	Kp(soil3) [l.kg(d)-1]		3.15E+00		3.15E+00	l.kg-1
(A)	CORG(soil3) [% C]			5	5.00E-02	-

ENVIRONMENT CHARACTERISTICS			Formula	Value	Used	
(A)	SYSTEM NAME	NETHERLANDS		NETH	NETH	
(D)	VOLUME(air) [m3]		3.80E+13		3.80E+13	m3
(D)	VOLUME(water) [m3]		1.42E+10		1.42E+10	m3
(D)	VOLUME(susp) [m3]		8.54E+05		8.54E+05	m3
(D)	VOLUME(bio) [m3]		1.14E+05		1.14E+05	m3
(D)	VOLUME(sed) [m3]		1.42E+08		1.42E+08	m3
(D)	VOLUME(soil1) [m3]		7.88E+08		7.88E+08	m3
(D)	VOLUME(soil2) [m3]		3.42E+09		3.42E+09	m3
(D)	VOLUME(soil3) [m3]		1.90E+07		1.90E+07	m3
(D)	SYSTEMAREA [km2]			37975	3.80E+10	m2
(D)	AREAFRAC(water) [%]	12.5		12.5	1.25E-01	-
(D)	AREAFRAC(soil1) [%]	41.5		41.5	4.15E-01	-
(D)	AREAFRAC(soil2) [%]	45		45	4.50E-01	-
(D)	AREAFRAC(soil3) [%]			1	1.00E-02	-
(A)	HEIGHT(air) [m]	1000		1000	1.00E+03	m
(A)	DEPTH(water) [m]	3		3	3.00E+00	m
(A)	SUSP(water) [mg.l-1]			15	1.50E-02	kg.m-3
(A)	FRwater(susp) [-]			0.9	9.00E-01	-
(A)	BIO(water) [mg.l-1]			1	1.00E-03	kg.m-3
(A)	FRwater(bio) [-]			0.95	9.50E-01	-
(A)	DEPTH(sed) [cm]	3		3	3.00E-02	m
(A)	FRwater(sed) [-]			0.8	8.00E-01	-
(A)	DEPTH(soil1) [cm]	5		5	5.00E-02	m
(A)	DEPTH(soil2) [cm]	20		20	2.00E-01	m
(A)	DEPTH(soil3) [cm]			5	5.00E-02	m
(A)	FRair(soil) [-]	0.2		0.2	2.00E-01	-
(A)	FRwater(soil) [-]	0.4		0.4	4.00E-01	-
(A)	FRsolid(soil) [-]			0.4	4.00E-01	-
(A)	RHOsolid [kg.m-3]			2500	2.50E+03	kg.m-3
(D)	TAU(air) [d]	0.3997699	4.00E-01		3.45E+04	s
(A)	WINDspeed [m.s-1]			5	5.00E+00	m.s-1
(D)	TAU(water) [d]	54.535100	5.49E+01		4.71E+06	s
(A)	STREAMS [m3.s-1]			2600	2.60E+03	m3.s-1
(A)	RUNOFF [m3.s-1]		4.00E+02		4.00E+02	m3.s-1

LOADING PARAMETERS			Formula	Value	Used	
DIRECT EMISSIONS		0.6				
(D) Edirect(air)	[t.y-1]		4.85E-03		6.15E-07	mol.s-1
(D) Edirect(water)	[t.y-1]		4.85E-03		6.15E-07	mol.s-1
(D) Edirect(soil1)	[t.y-1]		0.00E+00		0.00E+00	mol.s-1
(D) Edirect(soil2)	[t.y-1]		4.85E-03		6.15E-07	mol.s-1
(D) Edirect(soil3)	[t.y-1]	1E-20	4.85E-03		1.27E-24	mol.s-1
(A) PRODUCTION	[t.y-1]		4.65E+00		6.15E-04	mol.s-1
(A) POPULATION	[inh]		1.33E+07		1.33E+07	inh
(A) EMISfact(air)	[%]	0.1		0.1	1.00E-03	-
(A) EMISfact(water)	[%]	0.1		0.1	1.00E-03	-
(A) EMISfact(soil1)	[%]			0	0.00E+00	-
(A) EMISfact(soil2)	[%]	0.1		0.1	1.00E-03	-
(A) EMISfact(soil3)	[%]			0.1	1.00E-03	-
EMISSIONS VIA SEWAGE TREATMENT PLANT						
(D) Estp(air)	[t.y-1]	1E-20	4.85E-04		1.27E-24	mol.s-1
(D) Estp(water)	[t.y-1]	1E-20	9.70E-04		1.27E-24	mol.s-1
(D) Estp(susp)	[t.y-1]	1E-20	3.84E-07		1.27E-24	mol.s-1
(D) Estp(soil2)	[t.y-1]	1E-20	2.91E-03		1.27E-24	mol.s-1
(A) CONCstp(water)	[g.l-1]		1.77E-02		7.09E-02	mol.m-3
(A) CONCstp(susp)	[g.kg(d)-1]		1.12E-01		4.47E-04	mol.kg-1
(A) CONCstp(sludge)	[g.kg(d)-1]		8.35E+01		3.34E-01	mol.kg-1
(A) EFFLUENT(stp)	[m3.d-1]		1.50E-01		1.74E-06	m3.s-1
(A) SOLIDS(stp)	[kg(d).d-1]		9.55E-02		1.11E-06	kg.s-1
(A) SUSPeff(stp)	[mg.l-1]		4.00E+01		4.00E-02	kg.m-3
(A) STPcapacity	[eq]	1	1.26E+07		1.00E+00	eq
(A) STPload	[kg.d-1]		1.33E-02		6.15E-07	mol.s-1
(A) ACTIVEtime	[d.y-1]			365	1.00E+00	-
(A) FR(effstp)	[-]			0.2	2.00E-01	-
(A) FR(sludgestp)	[-]			0.6	6.00E-01	-
(A) FR(volatstp)	[-]			0.1	1.00E-01	-
IMPORT						
(D) IMPORT(air)	[t.y-1]	1E-20	1.81E+08		1.27E-24	mol.s-1
(A) AIRinflow	[m3.s-1]		1.10E+09		1.10E+09	m3.s-1
(A) CONCimp(air)	[g.m-3]		5.21E-03		2.09E-05	mol.m-3
(D) IMPORT(water)	[t.y-1]	1E-20	1.52E+07		1.27E-24	mol.s-1
(A) WATERinflow	[m3.s-1]		2.60E+03		2.60E+03	m3.s-1
(A) CONCimp(water)	[g.l-1]		1.85E-01		7.41E-01	mol.m-3
(D) IMPORT(susp)	[t.y-1]	1E-20	5.57E+03		1.27E-24	mol.s-1
(A) SUSPimport	[mg.l-1]	37		4E+01	3.70E-02	kg.m-3
(A) CONCimp(susp)	[g.kg(d)-1]		1.17E+00		4.68E-03	mol.kg-1

TRANSFORMATION PROCESSES			Formula	Value	Used	
(D) kdeg(air)	[d-1]	4.28E-03	4.28E-03		1.02E-08	s-1
(A) krad(OH)	[d-1]			4E-03	5.01E-08	s-1
(D) kdeg(water)	[d-1]	6.93E-04	6.93E-04		8.02E-09	s-1
(A) kdeg(test)	[d-1]		6.93E-04		6.93E-04	d-1
(A) BACT(test)	[cfu.ml-1]			4E+04	4.00E+04	cfu.ml-1
(A) BACT(water)	[cfu.ml-1]			4E+04	4.00E+04	cfu.ml-1
(D) kdeg(sed)	[d-1]	3.47E-02	1.52E-04		4.02E-07	s-1
(A) BACT(sedwater)	[cfu.ml-1]		2.25E+09	5E+09	2.25E+09	cfu.ml-1
(A) FRdisslvd(sed)	[mol %]		3.37E+01		3.37E-01	-
(D) kdeg(soil1)	[d-1]	3.47E-02	6.82E-03		4.02E-07	s-1
(D) kdeg(soil2)	[d-1]	3.47E-02	6.82E-03		4.02E-07	s-1
(D) kdeg(soil3)	[d-1]		6.82E-03		7.90E-08	s-1
(A) BACT(soilwater)	[cfu.ml-1]		3.50E+06	2E+06	3.50E+06	cfu.ml-1
(A) FRdisslvd(soil)	[mol %]		1.13E+01		1.13E-01	-

INTERMEDIA TRANSFER PROCESSES			Formula	Value	Used	
AIR/WATER and AIR/SOIL EXCHANGE						
(D) DRYDEPaerosol	[m(air).s-1]		1.23E-05		1.23E-05	m.s-1
(A) FRass(aerosol)	[-]		1.23E-02		1.23E-02	-
(A) AEROSOLdeprate	[cm.s-1]	0.1		1E-01	1.00E-03	m.s-1
(D) WASHOUT	[m(air).s-1]		9.05E-04		9.05E-04	m.s-1
(A) RAINrate	[mm.y-1]	700		8E+02	2.41E-08	m.s-1
(A) SCAVratio	[-]		3.76E+04		3.76E+04	-
(A) COLLECTeff	[-]	20000		2E+05	2.00E+05	-
(D) GASABS(water)	[m(air).s-1]		1.37E-03		1.37E-03	m.s-1
(D) VOLAT(water)	[m(water).s-1]		3.90E-06		3.90E-06	m.s-1
(A) kaw(air)	[m.s-1]	1.39E-03	4.24E-03	1E-03	1.39E-03	m.s-1
(A) kaw(water)	[m.s-1]	1.39E-05	5.00E-05	1E-05	1.39E-05	m.s-1
(D) GASABS(soil1)	[m(air).s-1]		2.46E-05		2.46E-05	m.s-1
(D) VOLAT(soil1)	[m(soil).s-1]		1.97E-10		1.97E-10	m.s-1
(D) GASABS(soil2)	[m(air).s-1]		2.46E-05		2.46E-05	m.s-1
(D) VOLAT(soil2)	[m(soil).s-1]		1.97E-10		1.97E-10	m.s-1
(D) GASABS(soil3)	[m(air).s-1]		2.46E-05		2.46E-05	m.s-1
(D) VOLAT(soil3)	[m(soil).s-1]		1.97E-10		1.97E-10	m.s-1
(A) kasl(air)	[m.s-1]		1.39E-03	1E-03	1.39E-03	m.s-1
(A) kasl(soilair)	[m.s-1]	5.56E-06		6E-06	5.56E-06	m.s-1
(A) kasl(soilwater)	[m.s-1]	5.56E-10		6E-10	5.56E-10	m.s-1
SUSP/WATER and BIO/WATER PARTITIONING						
(D) TRANS(susp-wat)	[m(susp)3.s-1]		1.65E+01		1.65E+01	m3.s-1
(D) TRANS(wat-susp)	[m(wat)3.s-1]		4.08E+01		4.08E+01	m3.s-1
(A) EQUtime(susp)	[hr]			1E+01	3.60E+04	s
(D) TRANS(bio-wat)	[m(bio)3.s-1]		2.19E-01		2.19E-01	m3.s-1
(D) TRANS(wat-bio)	[m(wat)3.s-1]		6.92E-01		6.92E-01	m3.s-1
(A) EQUtime(bio)	[hr]		1.00E+02		3.60E+05	s
WATER/SEDIMENT EXCHANGE						
(D) GROSSsedrate	[m(sed).s-1]		8.68E-10		8.68E-10	m.s-1
(A) SETTLvelocity	[m(water).s-1]	2.89E-05		3E-05	2.89E-05	m.s-1
(D) RESUSPrate	[m(sed).s-1]		8.46E-10		8.46E-10	m.s-1
(A) PROD(susp)	[kg(d).d-1]			0E+00	0.00E+00	kg.s-1
(A) NETsedrate	[m.s-1]		2.16E-11		2.16E-11	m.s-1
(D) ADSORB(sed)	[m(water).s-1]		2.75E-08		2.75E-08	m.s-1
(D) DESORB(sed)	[m(sed).s-1]		1.16E-08		1.16E-08	m.s-1
(A) kws(water)	[m.s-1]	2.78E-06		3E-06	2.78E-06	m.s-1
(A) kws(sed)	[m.s-1]	2.78E-08		3E-08	2.78E-08	m.s-1
SOIL TO WATER TRANSFER						
(D) RUNOFF(soil1)	[m(soil).s-1]		3.39E-09		3.39E-09	m.s-1
(D) RUNOFF(soil2)	[m(soil).s-1]		3.39E-09		3.39E-09	m.s-1
(D) RUNOFF(soil3)	[m(soil).s-1]		3.39E-09		3.39E-09	m.s-1
(A) FRACrun(soil1)	[-]	0.5		5E-01	5.00E-01	-
(A) FRACrun(soil2)	[-]	0.5		5E-01	5.00E-01	-
(A) FRACrun(soil3)	[-]			5E-01	5.00E-01	-
(A) EROSION(soil1)	[mm.y-1]			0E+00	0.00E+00	m.s-1
(A) EROSION(soil2)	[mm.y-1]			0E+00	0.00E+00	m.s-1
(A) EROSION(soil3)	[mm.y-1]			0E+00	0.00E+00	m.s-1
TRANSPORT FROM SYSTEM						
(D) BURIAL(sed)	[m(sed).s-1]		2.16E-11		2.16E-11	m.s-1
(D) LEACH(soil1)	[m(soil).s-1]		6.10E-09		6.10E-09	m.s-1
(D) LEACH(soil2)	[m(soil).s-1]		6.10E-09		6.10E-09	m.s-1
(D) LEACH(soil3)	[m(soil).s-1]		6.10E-09		6.10E-09	m.s-1
(A) FRACinf(soil1)	[-]	0.9		4E-01	9.00E-01	-
(A) FRACinf(soil2)	[-]	0.9		4E-01	9.00E-01	-
(A) FRACinf(soil3)	[-]	0.9		4E-01	9.00E-01	-

APPENDIX 3: Results literature review on chemical-specific input data

Aldrin

Water solubility in mg/l	temp. in °C	reference
0.02	20	Suntio et al, 1988
0.2	25	Mackay & Shiu, 1981
0.017	25	,,
0.02	20	Howard, 1991

Vapour pressure in Pa	temp. in °C	reference
5×10^{-3}	20	Suntio et al., 1988
8×10^{-4}	25	Mackay & Shiu, 1981
5×10^{-3}	20	Howard, 1991

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
1.4-4.2	25	value recommended	Mackay & Shiu, 1981
1.42	20	calculated	Suntio et al., 1988
1.46 - 2.8	25	calculated, 3 references	,,
38	20-25	calculated	,,
50	20	experimental value	,,
50.26	-	Warner et al., EPA, 1987	Howard, 1991
79.2	20	calculated with data from Suntio et al., 1988	
91.23	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

Biodegradation in soil.

DT50	temp. in °C	remarks	reference
some weeks	-	on soil, other processes not excluded	Butijn & Koeman, 1977
0.3-14 years[a]	-	*in soil*, ,,	,,
43-63 days	-	sandy loam, darkness	Howard, 1991

a upper value is very high: total aldrin + dieldrin (+ metabolites?) has probably been measured

Volatilization from soil.

IPCS (1989). data from lab studies:
Helene et al. (1981) reported 31% loss from a highly humic soil after 120 days and 62% from a soil of low organic matter (conc in soil, % moisture and %OM?)
Howard, 1991: pag. 16

Carbofuran

Water solubility in mg/l	temp. in °C	reference
650	20	Suntio et al., 1988
700	-	Howard, 1991

Vapour pressure in Pa	temp. in °C	reference
1.5×10^{-3}	20	Suntio et al., 1988
1.1×10^{-3}	25	Howard, 1991

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
5.56×10^{-4}	20	calculated with data from Suntio et al., 1988	
3.78×10^{-4}	-	calculated with data from Howard, 1991	
5.1×10^{-4}	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

Biodegradation in soil.

DT50	temp. in °C	remarks	reference
28 (42) days	25 (20)	two silt loams, a clay loam and an or-	RIVM/ACT, 1993
> 378 (> 560)	25 (20)	ganic soil were tested at 25 °C. (Data	,,
49 (73) d	25 (20)	converted to 20 °C.) Sampling up to	,,
13 (19) d	25 (20)	378 days.	,,
60 (89) d	25 (20)		,,
35 d	20	loam, incubation for 84 days	,,
14 (16) d	22 (20)	silty clay loam, incubation for 21 days	,,

The degradation rate might be influenced by pH: at higher pH values degradation is more rapid.

Volatilization from soil.
Howard, 1991: volatilization is expected to be insignificant.

Chlordane

Water solubility in mg/l	temp. in °C	reference
0.05	20	Suntio et al., 1988
0.1 (tech)	25	Howard, 1991
0.056 (75:25=cis:trans)	25	,,

Vapour pressure in Pa	temp. in °C	reference
1.1×10^{-3}	20	Suntio et al., 1988
6.1×10^{-2} (tech)	25	Howard, 1991
1.3×10^{-3} (refined)	-	,,

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
4.92	25	experimental value, Warner et al., 1980	Suntio et al., 1988
87.7-134	25	experimental value, Atlas et al., 1982	,,
9.12	25	calculated, Mabey et al., 1982	,,
2.92-9.5	-	calculated; Callahan et al., 1979	,,
4.91	-	from Suntio et al., 1988	Howard, 1991
7.4	20	calculated with data from Suntio et al., 1988	
9.02	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

Biodegradation in soil.

DT50	temp. in °C	remarks	reference
3.3 years	-	field conditions; better data lacking	Howard, 1991

Volatilization from soil.
Howard, 1991: chlordane can volatile significantly from soil surfaces, incorporation into the soil greatly restricts the volatilization.

Chlorpyrifos

Water solubility in mg/l	temp. in °C	reference
0.3	20	Suntio et al., 1988
0.4	23	Mackay and Shiu, 1981
1.12	24	Howard, 1991

Vapour pressure in Pa	temp. in °C	reference
1.5×10^{-3}	20	Suntio et al., 1988
2.5×10^{-3}	25	Mackay and Shiu, 1981
2.5×10^{-3}	25	Howard, 1991

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
1.49	20	calculated from data from Suntio et al., 1988	
0.79		,, ,, Howard, 1991	
1.75	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

Biodegradation in soil.

DT50	temp. in °C	remarks	reference
11-141 (16-210) d	25 (20)	om 0.49-6.12%; cat 2, data used in RIVM conclusions, because no better data were available	RIVM/ACT, 1988
4 and 12 weeks	-	clay loam and silt loam, resp.	Howard, 1991
1 and 2.5 weeks	-	sandy loam and organic soil, resp.	,,

p,p'-DDD

Water solubility in mg/l	temp. in °C	reference
0.05	20	Suntio et al., 1988

Vapour pressure in Pa	temp. in °C	reference
10^{-4}	20	Suntio et al., 1988

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
0.63	20	calculated from data from Suntio et al., 1988	
0.64	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

p,p'-DDE

Water solubility in mg/l	temp. in °C	reference
0.04	20	Suntio et al., 1988

Vapour pressure in Pa	temp. in °C	reference
10^{-3}	20	Suntio et al., 1988

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
7.63	20	calculated from data from Suntio et al., 1988	
2.2	20-25	calculated, Thibodeaux, 1979	Suntio et al., 1988
1.95-241	-	calculated, Callahan et al., 1979	Suntio et al., 1988
121.8	-	experimental, Atlas et al., 1982	Suntio et al., 1988
7.95	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

p,p'-DDT

(Suntio et al. en Mackay and Siu: p,p' of o,p' niet genoemd)

Water solubility in mg/l	temp. in °C	reference
0.003	20	Suntio et al., 1988
0.0012	20	Mackay and Shiu, 1981
0.0055	20	,,
0.0031	20	,,
0.001	25	,,

Vapour pressure in Pa	temp. in °C	reference
2×10^{-5}	20	Suntio et al., 1988
1.34×10^{-5}	25	Mackay and Shiu, 1981
2.53×10^{-5}	20	„

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
1.5-9.1	25	recommended value	Mackay and Shiu, 1981
6.02	20-25	calculated, Thibodeaux, 1979	Suntio et al., 1988
3.94	25	calculated, Mackay et al., 1975	Suntio et al., 1988
2.22	20	calculated with data from Suntio et al., 1988	
2.36	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

Biodegradation in soil.

DT50	temp. in °C	remarks	reference
5-8 years	field?	mixed into soil, no further data	IPCS, 1989
16-20 days	field?	surface application, no further data	„

(ACT documentation: when 1 mg/kg was applied in a sandy loam and an organic soil, 89% and 76% respectively was degraded after 8 weeks.)

Dieldrin

Water solubility in mg/l	temp. in °C	reference
0.17	20	Suntio et al., 1988
0.25	25	Mackay & Shiu, 1981
0.2	25	„
0.17	20	Howard, 1991

Vapour pressure in Pa	temp. in °C	reference
5×10^{-4}	20	Suntio et al., 1988
2.4×10^{-5} - 3.9×10^{-4}	20	Mackay & Shiu, 1981 (6 references)
6.6×10^{-4}	25	,, (from Edwards, 1966)
5×10^{-4}	20	Howard, 1991

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
0.9 -1.3	25	value recommended	Mackay & Shiu, 1981
0.02 - 21.3	20-25	calculated, 6 references	Suntio et al., 1988
1.07 - 5.84	20-25	experimental, 3 references	,,
5.88	25	Warner et al., EPA, 1987	Howard, 1991
0.94	20	calculated with data from Suntio et al., 1988	
1.12	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

Biodegradation in soil

DT50	temp. in °C	remarks	reference
some weeks		on soil; other processe not excluded	Butijn & Koeman, 1977
1-8 years		in soil; ,, ,,	,,
48 weeks	27	0.64 mg/kg; field conditions	ACT archives
7 years	-	field; no biodegrad. occurred in lab tests	Howard, 1991

Volatilization from the soil

ACT archives, from Verschueren (1983):
89% disappeared from a sandy loam soil after 60 days at 25 °C, and 34.2% from sand.
IPCS (1989): dieldrin was measured in dust at conc's of 3 ng/g dust (Cincinnatti) and 2.2 ng/ g dust (Barbados).

Aerosol.
Howard, 1991: dieldrin is probably associated with particulate matter in air.

Endosulfan

Water solubility in mg/l	temp. in °C	reference
0.15	20	Suntio et al., 1988
0.51 (α)[a]	20	Howard, 1991
0.45 (ß)[a]	20	,,

a Technical endosulfan is composed of 64-76% α-endosulfan and 29-32% ß-endosulfan.

Vapour pressure in Pa	temp. in °C	reference
1.1×10^{-3}	20	Suntio et al., 1988
1.3×10^{-3}	25	Howard, 1991

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
1.09	25	calculated	Suntio et al., 1988
1.1	-	approximate-calcuiated from average water solubility of α- and ß-isomers	Howard, 1991
2.29	20	calculated with data from Suntio et al., 1988	
2.98	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

Biodegradation in soil.

DT50	temp. in °C	remarks	reference
1.1 weeks (α)	20	sandy loam, hydrolysis was not excluded	Howard, 1991
2.2 weeks (ß)	20	,, ,,	,,
60 days (α)	-	field study	IPCS, 1984
900 days (ß)	-	field study	,,

Volatilization from soil.
Howard, 1991: no data, but little volatilization from soil is expected in view of the high soil- sorption coefficient.
Aerosol.
Howard, 1991: adsorption of endosulfan on atmospheric particulate matter occurred.

Endrin

Water solubility in mg/l	temp. in °C	reference
0.23	20	Suntio et al., 1988
0.25	25	Howard, 1991

Vapour pressure in Pa	temp. in °C	reference
2×10^{-5}	20	Suntio et al, 1988
4×10^{-4}	20	Howard, 1991

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
1.8×10^{-4}	25	calculated	Suntio et al., 1988
0.76	-	calculated	Howard, 1991
2.77×10^{-2}	20	calculated with data from Suntio et al., 1988	
3.3×10^{-2}	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

Biodegradation in soil.

DT50	temp. in °C	remarks	reference
2.2-12 years		in soil	Butijn & Koeman, 1977
< 20 - 80 days		in soil, several studies	U.S. Department, 1990
4-14 years, or more		several studies, other processes not excluded	Howard, 1991

Volatilization from soil.
Howard, 1991: With the three-compartment model EXAMS a half-life for volatilization from a model pond of greater than 14 years was estimated.

Aerosol.
Howard, 1991: in the atmosphere endrin is expected to be mainly associated with particulate matter.

Fenthion

Water solubility in mg/l	temp. in °C	reference
50	20	Suntio et al., 1988

Vapour pressure in Pa	temp. in °C	reference
4×10^{-3}	20	Suntio et al., 1988

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
2.1×10^{-2}	20	calculated from data from Suntio et al., 1988	
2.2×10^{-2}	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

α-HCH

Water solubility in mg/l	temp. in °C	reference
1	20	Suntio et al., 1988
2	-	Howard, 1991; IPCS, 1992
1.5	20	C. doc, 1988

Vapour pressure in Pa	temp. in °C	reference
3×10^{-3}	20	Suntio et al., 1988
6×10^{-3}	25	Howard, 1991
2.67	20	IPCS, 1992
7.2×10^{-4}	20	C. doc, 1988

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
0.55	22-25	calculated, Mabey et al., 1982	Suntio et al., 1988
1.07	25	calc. from water sol and vap pr	Howard, 1991
0.65	-		C. doc, 1988
0.73	20	calculated from data from Suntio et al., 1988	
0.87	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

Biodegradation in soil.

DT50	temp. in °C	remarks	reference
179 days	-	sandy loam 6.5% om, 5000 mg/kg	C. doc, 1988; IPCS, 1992
83 days	-	sandy loam 6.5% om, 4000 mg/kg	,, ,,
125 days	-	6.8% om	,, ,,
< 70 days	-	clay, 15 mg/kg	IPCS, 1992

Volatilization from soil.
(RIVM/ACT archives, 1984: Evaporation occurs, more easily from a damp soil than from a dry soil. Rainfall leads to the compound being washed out.)
Aerosol.
Howard, 1991: Based on the vapour pressure, α-HCH is expected to exist in both the vapor and particulate matter and aerosols in the air.

ß-HCH

Water solubility in mg/l	temp. in °C	reference
0.1	20	Suntio et al., 1988
1.5	20	IPCS, 1992
0.2	28	,,
0.2	20	C. doc, 1988

Vapour pressure in Pa	temp. in °C	reference
4×10^{-5}	20	Suntio et., 1988
0.67	20	IPCS,1992
3.8×10^{-5}	20	C. doc, 1988

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
0.018	20-25	calculated, Mabey et al., 1982	Suntio et al., 1988
0.051	-		C. doc, 1988
9.7×10^{-2}	20	calculated from data from Suntio et al., 1988	
0.12	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

Biodegradation in soil.

DT50	temp. in °C	remarks	reference
91 days	-	6.8% om, 20 mg/kg	C. doc, 1988; IPCS, 1992
> 40 weeks	5-17	no degrad. after 40 weeks	C. doc, 1988; IPCS, 1992
< 70 days	-	clay, 15 mg/kg	IPCS, 1992

Volatilization from soil.
RIVM/ACT archives, 1984: the compound is not readily vapourised. Degradation is slow, and occurs predominantly under anaerobic conditions.

Lindane

Water solubility in mg/l	temp. in °C	reference
6.5	20	Suntio et al., 1988
7.3	25	Mackay and Shiu, 1981; C. doc, 1988
7.8	25	,,
7.3	-	Howard, 1991
2	-	,,
10	20	IPCS, 1991

Vapour pressure in Pa	temp. in °C	reference
3×10^{-3}	20	Suntio et al., 1988
8.39×10^{-3}	25	Mackay and Shiu, 1981
$1.25\text{-}4.35 \times 10^{-3}$	20	,, (4 references)
4	20	,,
7.4×10^{-3}	25	Howard, 1991
1.25×10^{-3}	20	C. doc, 1988
4.3×10^{-3}	20	IPCS, 1991

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
0.05	20	calculated, Lyman et al., 1982	Suntio et al., 1988
0.2	20-25	,, , Thibodeaux, 1979	,,
0.73	25	,, , Mabey et al., 1982	,,
0.05	25	,, , Mackay et al., 1975	,,
0.3-0.34	25	recommended value	Mackay and Shiu, 1981
0.3	25	calculated value	Howard, 1991
0.5	-		C. doc, 1988
0.11	20	calculated from data from Suntio et al., 1988	
0.13	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

Biodegradation in soil. (lindane)

DT50	temp. in °C	remarks	reference
980 days	24.5	extrapolated, sampling up to 336 d	RIVM/ACT, 1991
529 days	15	extrapolated, sampl. 28 d, cat. 2	,,
276 days	-	5.1% om	C. doc, 1988
endless	35	6.8% om	,,
100 days	25		,,
106-720 days	22	lab or field not mentioned	,,
12-174 days	-	several studies and soils, %om?	IPCS, 1991

Volatilization from soil.

RIVM/ACT archives, 1991: 1.2 mg/kg of a 16.7% EC formulation was applied to sandy loam (pH 7.5, o.m. 1.9%) in the dark at 25 °C. After 8 days 15.7% was volatilized and 83% was recovered in the soil (100% RH). Comparable studies 2-4% per day dissipated by volatilization.
(Evaporation occurred, more easily from a damp soil than from a dry soil. Rainfall leads to the compound being washed out.)

Heptachlor

Water solubility in mg/l	temp. in °C	reference
0.1	20	Suntio et al., 1988
0.18	-	Howard, 1991
0.056	-	IPCS, 1984

Vapour pressure in Pa	temp. in °C	reference
3×10^{-2}	20	Suntio et al., 1988
5.3×10^{-2}	25	Howard, 1991

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
150	-	Warner et al., EPA, 1987	Howard, 1991
92.46	20	calculated from data from Suntio et al., 1988	
112.01	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

Biodegradation in soil.

DT50	temp. in °C	remarks	reference
0.4 - 0.8 year	-	field; no better data available	Howard, 1991

Volatilization from soil.
Howard, 1991: after 167 days 7% of the heptachlor incorporated 7.5 cm in the soil had volatilized.
When applied on soil, evaporation is much faster, depending on the soil moisture.

Heptachlor epoxide

Water solubility in mg/l	temp. in °C	reference
0.2	-	Howard, 1991

Vapour pressure in Pa	temp. in °C	reference
2.6×10^{-3}	-	Howard, 1991; value estimated

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
3.24	-	Warner et al., EPA, 1987	Howard, 1991
5.06	20	calculated from data from Howard, 1991	

Biodegradation.
Howard, 1991: In a sandy loam at 28 °C 12% was converted after 12 weeks.

Aerosols
Howard, 1991: Based on the vapour pressure, heptachlor epoxide is expected to exist in both the vapor and particulate matter and aerosols in the air.

Hexachlorobenzene

DT50	temp. in °C	remarks	reference
1-6 years	-	no biodegradation at all was observed in some studies	C. doc, 1991
1530	-	no significant biodegradation was noted in other tests, volatilization is the major loss mechanism	Howard, 1989

Volatilization from the soil.
Criteria document, 1991: Only volatilization from the top soil layers plays an important role in the dissappearing from the soil.

Pentachlorobenzene

DT50	temp. in °C	remarks	reference
0.5-1 year	-	no test data are given; in other studies no aerobic biodegradation was observed	C. doc, 1991
194, 345 days	-	conc. equivalent to 10 kg/ha	IPCS, 1991

Volatilization from the soil.
See hexachlorobenzene.

Pentachlorophenol

Water solubility in mg/l	temp. in °C	reference
12	20	Suntio et al., 1988
14	20	Howard, 1991
0.14[a]	20	C. doc, 1991

a solubility of the non-dissociated form (pH = 4)

Vapour pressure in Pa	temp. in °C	reference
2×10^{-3}	20	Suntio et al., 1988
1.5×10^{-2}	25	Howard, 1991
1.3×10^{-2}	-	C. doc, 1991

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
0.28	-	calc from water sol and vap pr	Howard, 1991
3.47×10^{-2}	20	calculated from data from Suntio et al., 1988	
4.4×10^{-2}	20	calc from subcooled liquid sol.and vap pr	Suntio et al., 1988

Biodegradation in soil.

DT50	temp. in °C	remarks	reference
weeks to months	-	several studies, no further data	Howard, 1991
7-14 days	-	several soils, 100 mg/kg	IPCS, 1987
>= 11 days	-	no further data	C. doc, 1991
30 (5-120) days	-	several sudies, no test data	,,

Volatilization from soil.
Criteria document, 1991: evaporation from soil is insignificant.
Aerosol.
Howard, 1991: PCP associates with particulate matter in the air.

Quintozene

Water solubility in mg/l	temp. in °C	reference
0.032	25	Howard, 1991
0.44	20	IPCS, 1984; ACT data

Vapour pressure in Pa	temp. in °C	reference
0.32	25	Howard, 1991
6.7×10^{-3}	20	IPCS, 1984; ACT data
1.8	25	IPCS, 1984

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
2918	-		Howard, 1991

Biodagradation in soil.

DT50	temp. in °C	remarks	reference
135 days	25	100 mg/kg, 0.34% om, soil layer 1 cm	ACT data, 1979
270 days	25	100 mg/kg, 22.4% om, ,,	,,
38 days	20	5 mg/kg, 3.7% om, applied as emulsion	,,
19 days	30	1000 mg/kg, greenhouse soil 9.2% om	,,
150 days	30	1000 mg/kg, loamy sand 3% om	,,

Thiram

Water solubility in mg/l	temp. in °C	reference
30	25	Howard, 1991; RIVM/ACT, 1993

Vapour pressure in Pa	temp. in °C	reference
10^{-3}	25	Howard, 1991
$< 10^{-4}$	25	RIVM/ACT, 1993

Henry coeff. in Pa m^3/mol	temp. in °C	remarks	reference
$< 8 \times 10^{-3}$	25		Howard, 1991
8×10^{-3}	20	calculated from data from Howard, 1991	

Biodegradation in soil.

DT50	temp. in °C	remarks	reference
8 days	-	autoclaved sandy loam inoculated with Pseudomonas aeruginosa	Howard, 1991
7-38 days	20	cat. 2, no better data available	RIVM/ACT, 1993

Volatilization from soil.
Howard, 1991: thiram should not volatilize from both wet and dry soil surfaces, considering the H coeff., the soil adsorption coeff. (672) and the vapour pressure.

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Henry coefficient:

Heptachlor epoxide: Warner et al. (1987) EPA/600/D-87/229, PB 87-212684

Quintozene: Dixon et al. (1985) EPA/450/3-85-007, PB 85-204527

APPENDIX 4: Results additional database-search on chemical-specific input data

Aldrin

```
IRPTC-database

file: 01.01 IDENT   rn : 142
systematic name:1,4:5,8-Dimethanonaphthalene,1,2,3,4,10,10-hexachloro-1,
                4,4a,5,8,8a-hexahydro-,(1.alpha.,4.alpha.,4a.beta.,5.alp
                ha.,8.alpha.,8 a.beta.)-
common name     :aldrin
cas no          :309-00-2           rtecs no       :IO2100000
molfm           :C12H8CL6
molwt           :364.90
mp              :104C
den             :1.6G/ML
vp              :1.0E-5KPA(7.5E-5MMHG) AT 20C
n-octoh:aq      :27E-6G/L AT 27C
fatsol          :VERY SOLUBLE IN MOST ORGANIC SOLVENTS
particle        :CRYSTALS
colour          :COLORLESS(AG); BROWN(TG)
odour           :ODOURLESS
impurities      :IN THE TECHNICAL PRODUCT: ISODRIN; CHLORDANE;
                 HEXACHLOROCYCLOPENTADIENE; HEXACHLOROBUTADIENE;
                 OCTACHLOROCYCLOPENTENE; HEXACHLOROETHANE;
                 BICYCLOHEPTADIENE; TOLUENE (!IARMB8 5,-,1974)
hazard class    :UN HAZ CLASS 6.1
                 PACK GROUP II,III
                 IMO CLASS 6.1
synonyms        :1,4:5,8-dimethanonaphthalene,1,2,3,4,10,10-hexachloro-1,
                 4,4a,5,8,8a-hexahydro-,endo,exo-; ent 15949; hhdn;
                 octalene;


MEDCHEM

         Measured    Estimate
logP      6.50         5.406

LOCAL NAME  ALDRIN
ACTIVITY TYPE  INSECTICIDE

LOGP        6.50
SOLV PAIR   Octanol
REFERENCE   De Bruijn,J., Busser,F., Seinen,W. & Hermens,J.,
            Environ. Tox. Chem., (1989) 8, 499
FOOTNOTE    Both Phases Analyzed
...  2      Slow-stir method (ref. 2129)
SEL         *

LOGPSTAR    6.50
```

ASTER

CAS : 309-00-2
NAME : 1,2,3,4,10,10-Hexachloro-1,4,4a,5,8,8a-hexahydro-(1a,4a,4ab,5a,8a,8ab)-1,4:5,8-dimethanonaphthalene
SMILES: ClC(=C(Cl)Cl(Cl)C2C3C=4)C(Cl)(C1(Cl)Cl)C2C(C4)C3

#	Property	Value and Units		Source	Method Error	
1	Mol Wgt.	364.9	g/mole	Calc.		
2	Parachor	590.		Calc.	????	
3	Mol Ref.	77.1		Calc.	Av. % Error = 5	
4	Mol Vol.	273.	cm^3/g.m	Calc.	????	
5	LogP	6.50		User	????	
6	Melt Pt.	103.	C	ASTER		
7	Boil Pt.	409.	C @760mm	Calc.	Av. % Error = 7.4 K	
8	V.Press.	2.66E-09	mm of Hg	Calc.	Av. % Error = 47.0	
9	Ht. Vpr.	1.40E+04	cal/mole	Calc.	Av. % Error = 1.85	
10	Sol. H2O	2.90E-08	moles/L	Recalc	????	
11	pKa					
12	FH TMOA	24.0	MOA num.	Recalc	Neurotoxicant: Cyclo	

Carbofuran

IRPTC-database

file: 01.01 IDENT rn : 224
systematic name:7-Benzofuranol,2,3-dihydro-2,2-dimethyl-,methylcarbamate
common name :carbofuran
cas no :1563-66-2 rtecs no :FB9450000
molfm :C12H15NO3
molwt :221.28
mp :153-154C
state :SOLID
den :1.2G/ML
vp :3E-6KPA(2E-5MMHG) AT 33C
n-octoh:aq :700E-3G/L AT 25C
colour :COLOURLESS
odour :SLIGHT PHENOL
synonyms :2,3-dihydro-2,2-dimethyl-7-benzofuranyl methylcarbamate; carbamic acid,methyl-,2,3-dihydro-2,2-dimethyl-7-benzofuranyl ester; curaterr; furadan;

MEDCHEM

	Measured	Estimate
logP	2.32	2.323

LOCAL NAME CARBOFURAN
LOCAL NAME FURADAN
ACTIVITY TYPE INSECTICIDE
REFERENCE EPA-600/2-81-011

LOGP 2.32
SOLV PAIR Octanol
REFERENCE Metcalf,R. & Lu,P., EPA Report , In Press
SEL *

LOGPSTAR 2.32

ASTER

CAS : 1563-66-2
NAME : 2,3-Dihydro-2,2-dimethyl-7-benzofuranol, Methylcarbamate
SMILES: O(C(C1)(C)C)-c(c1cc2)c(c2)OC(=O)NC

#	Property	Value and Units		Source	Method Error
1	Mol Wgt.	221.3	g/mole	Calc.	
2	Parachor	484.		Calc.	????
3	Mol Ref.	58.6		Calc.	Av. % Error = 5
4	Mol Vol.	210.	cm^3/g.m	Calc.	????
5	LogP	2.32		User	????
6	Melt Pt.	152.	C	ASTER	
7	Boil Pt.	292.	C @760mm	Calc.	Av. % Error = 7.4 K
8	V.Press.	2.91E-04	mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.37E+04	cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	7.43E-04	moles/L	Recalc	R**2 = .93
11	pKa				
12	FH TMOA	3.00	MOA num.	Recalc	Carbamate mediated A

Chlordane

IRPTC-database

file: 01.01 IDENT rn : 120
systematic name:4,7-Methano-1H-indene,1,2,4,5,6,7,8,8-octachloro-2,3,3a,4,7,7a-hexahydro-
cas no :57-74-9 rtecs no :PB9800000
molfm :C10H6C18
molwt :409.76
mp :106-107C
bp :175C
state :LIQUID, VISCOUS
fl :0.1-0.8KG/M3
den :1.59-1.63G/ML
vp :1E-6KPA(1E-5MMHG) FOR TG
pow :6
n-octoh:aq :9E-6G/L AT 25C
fatsol :SOLUBLE IN MOST ORGANIC SOLVENTS INCLUDING PETROLEUM OILS
colour :AMBER
odour :ODOURLESS; CEDAR-LIKE FOR TG
additives :ORIGINALLY TECHNICAL CHLORDANE COMPRISED 60-75% CHLORDANE ISOMERS, THE REMAINDER BEING RELATED TO ENDO-COMPOUNDS INCLUDING HEPTACHLOR, NONACHLOR, DIELS-ALDER ADDUCT OF CYCLOPENTADIENE AND PENTACHLOROCYCLOPENTADIENE, HEXACHLOROCYCLOPENTADIENE, OCTACHLOROCYCLOP ENTADIENE
impurities :COMMERCIAL PRODUCT MAY CONTAIN 25-40% OF HEXACHLOROPENTADIENE, HEPTACHLOR, CHLORDENE, NONACHLOR, ETC(APPROXIMATELY 20 SUBSTANCES ALTOGETHER)
hazard class :UN HAZ CLASS 6.1
UN TOX GROUP III
comments :VOLATILITY IS 0.2MG/M3. LOSES ITS CHLORINE IN PRESENCE OF ALKALINE REAGENTS AND SHOULD NOT BE FORMULATED WITH ANY SOLVENT, CARRIER, DILUENT OR EMULSIFIER, WHICH HAS AN ALKALINE REACTION. CORROSIVE TO IRON, ZINC AND VARIOUS PROTECTIVE COATINGS.
synonyms :4,7-methanoindan,1,2,4,5,6,7,8,8-octachloro-3a,4,7,7a-tetrahydro-; chlorindan; ent 9932; m 140; octachloro-4,7-methanotetrahydroindane; toxichlor;

MEDCHEM

	Measured	Estimate
logP	n/a	5.802

ASTER

CAS : 57-74-9
NAME : 1,2,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-hexahydro-4,7-methano-1H-indene
SMILES: ClC(C(Cl)C1)C(C1C2(Cl)C=3Cl)C(Cl)(C3Cl)C2(Cl)Cl

#	Property	Value and Units	Source	Method Error
1	Mol Wgt.	409.8 g/mole	Calc.	
2	Parachor	626.	Calc.	????
3	Mol Ref.	80.2	Calc.	Av. % Error = 5
4	Mol Vol.	294. cm^3/g.m	Calc.	????
5	LogP	5.80	User	????
6	Melt Pt.	103. C	ASTER	
7	Boil Pt.	419. C @760mm	Calc.	Av. % Error = 7.4 K
8	V.Press.	1.05E-09 mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.44E+04 cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	1.87E-07 moles/L	Recalc	????
11	pKa			
12	FH TMOA	24.0 MOA num.	Recalc	Neurotoxicant: Cyclo

Chlorpyrifos

IRPTC-database

file: 01.01 IDENT rn : 297
systematic name:Phosphorothioic acid,O,O-diethyl O-(3,5,6-trichloro-2-pyridinyl)ester
common name :chlorpyrifos
cas no :2921-88-2 rtecs no :TF6300000
molfm :C9H11CL3NO3PS
molwt :350.6
mp :42.5-43C
state :SOLID, CRYSTALLINE
vp :1.87E-5MMHG AT 25C
n-octoh:aq :2E-3G/L AT 35C
fatsol :790G/KG OCTANES,430G/KG METHANOL; READILY SOLUBLE IN MOST OTHER ORGANIC SOLVENTS
colour :COLOURLESS
odour :MILD MERCAPTAN
synonyms :chlorpyriphos; dursban; ent 27311; phosphorothioic acid,O,O-diethyl O-(3,5,6-trichloro-2-pyridyl)ester;

MEDCHEM

	Measured	Estimate
logP	5.27	4.442

LOCAL NAME CHLORPYRIFOS
LOCAL NAME DURSBAN
ACTIVITY TYPE INSECTICIDE
REFERENCE EPA-600/2-81-011

LOGP 5.27
SOLV PAIR Octanol
REFERENCE De Bruijn,J., Busser,F., Seinen,W. & Hermens,J.,
Environ. Tox. Chem., (1989) 8, 499
FOOTNOTE Both Phases Analyzed
... 2 Slow-stir method (ref. 2129)
SEL *

LOGPSTAR 5.27

ASTER

CAS : 2921-88-2
NAME : Chlorpyriphos
SMILES: Cl-c(nc(c1Cl)OP(=S)(OCC)OCC)c(Cl)c1

#	Property	Value and Units		Source	Method Error
1	Mol Wgt.	350.6	g/mole	Calc.	
2	Parachor	627.		Calc.	????
3	Mol Ref.	77.8		Calc.	Av. % Error = 5
4	Mol Vol.				
5	LogP	5.27		User	????
6	Melt Pt.	42.0	C	ASTER	
7	Boil Pt.	379.	C @760mm	Calc.	Av. % Error = 7.4 K
8	V.Press.	4.44E-08	mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.71E+04	cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	2.75E-06	moles/L	Recalc	????
11	pKa	-3.78	@ 25 C.	Calc.	
12	FH TMOA	4.00	MOA num.	Recalc	OP mediated AChE inh

DDD

IRPTC-database

file: 01.01 IDENT rn : 25
systematic name:Benzene,1,1'-(2,2-dichloroethylidene)bis(4-chloro-
common name :ddd
cas no :72-54-8 rtecs no :KI0700000
molfm :C14H10CL4
molwt :320.04
mp :110C
den :1.5G/ML
rvden :11
n-octoh:aq :INSOLUBLE
colour :COLOURLESS
impurities :O,P'-TDE
synonyms :dichlorodiphenyl dichloroethane; dilene;
ethane,1,1-dichloro-2,2-bis(p-chlorophenyl)-; me-1,700;
p,p'-DDD; rhothane; tde;

MEDCHEM

	Measured	Estimate
logP	6.22	6.060

LOCAL NAME DDD

LOGP 6.22
SOLV PAIR Octanol
REFERENCE De Bruijn,J., Busser,F., Seinen,W. & Hermens,J., Environ. Tox. Chem., (1989) 8, 499
FOOTNOTE Both Phases Analyzed
... 2 Slow-stir method (ref. 2129)
SEL *

LOGPSTAR 6.22

ASTER

CAS : 72-54-8
NAME : 1,1'-(2,2-Dichloroethylidene)bis(4-chlorobenzene)
SMILES: Cl-c(ccc1C(-c(ccc2Cl)cc2)C(Cl)Cl)cc1

#	Property	Value and Units		Source	Method Error
1	Mol Wgt.	320.0	g/mole	Calc.	
2	Parachor	610.		Calc.	????
3	Mol Ref.	79.1		Calc.	Av. % Error = 5
4	Mol Vol.	252.	cm^3/g.m	Calc.	????
5	LogP	6.22		User	????
6	Melt Pt.	110.	C	ASTER	
7	Boil Pt.	397.	C @760mm	Calc.	Av. % Error = 7.4 K
8	V.Press.	8.06E-09	mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.54E+04	cal/mole	Calc	Av. % Error = 1.85
10	Sol. H2O	5.31E-08	moles/L	Recalc	????
11	pKa				
12	FH TMOA	25.0	MOA num.	Recalc	Neurotoxicant: DDT-t

DDE

IRPTC-database

file: 01.01 IDENT rn : 1523
systematic name:Benzene,1,1'-(dichloroethenylidene)bis(4-chloro-
common name :dde
cas no :72-55-9 rtecs no :KV9450000
synonyms :4.4'-DDE;
ethylene,1,1-dichloro-2,2-bis(p-chlorophenyl)-;
p,p'-DDE;

MEDCHEM

	Measured	Estimate
logP	6.96	6.936

LOCAL NAME DDE

LOGP	6.96
SOLV PAIR	Octanol
REFERENCE	De Bruijn,J., Busser,F., Seinen,W. & Hermens,J., Environ. Tox. Chem., (1989) 8, 499
FOOTNOTE	Both Phases Analyzed
... 2	Slow-stir method (ref. 2129)
SEL	*

LOGPSTAR 6.96

ASTER

CAS : 72-55-9
NAME : 1,1'-(Dichloroethenylidene)bis(4-chlorobenzene)
SMILES:

#	Property	Value and Units	Source	Method Error
1	Mol Wgt.			
2	Parachor			
3	Mol Ref.			
4	Mol Vol.			
5	LogP	6.96	User	????
6	Melt Pt.	89.0 C	ASTER	
7	Boil Pt.			
8	V.Press.			
9	Ht. Vpr.			
10	Sol. H2O	1.14E-08 moles/L	Recalc	????
11	pKa			
12	FH TMOA			

DDT

IRPTC-database

```
file: 01.01 IDENT   rn : 26
systematic name:Benzene,1,1'-(2,2,2-trichloroethylidene)bis(4-chloro-
common name    :ddt
cas no         :50-29-3            rtecs no       :KJ3325000
molfm          :C14H9CL5
molwt          :354.48
mp             :108-109C
bp             :260C
den            :1.6G/ML
vp             :2.5E-8KPA(1.9E-7MMHG) AT 20C
n-octoh:aq     :1.2E-6G/L AT 25C
fatsol         :SOLUBLE IN AROMATIC AND CHLORINATED SOLVENTS
colour         :COLOURLESS
taste          :TASTELESS
odour          :ODOURLESS, SLIGHT AROMATIC
impurities     :O,P'-DDT; P,P'-TDE; O,P'-TDE; P,P-DDE; O,P'-DDE;
                1-(P-CHLOROPHENYL)-2,2,2-TRICHLORO-ETHANOL; O,O'-DDT;
                BIS-(P-CHLOROPHENYL)SULPHONE; M,P'-DDT !WHOEC* 9,23,1979
                !IARMB8 5,86,1974
hazard class   :EUR ADR CLASS 6.1
                EUR RID CLASS 6.1
                IMO CLASS 6.1
                UN HAZ CLASS 6.1
                UN TOX GROUP III
synonyms       :4,4'-dichlorodiphenyltrichloroethane; agritan; arkotine;
                bosan supra; bovidermol; chlorophenothane; citox;
                clofenotane; deoval; detox; detoxan; dicophane; dodat;
                dykol; ent 1,506; estonate;
                ethane,1,1,1-trichloro-2,2-bis(p-chlorophenyl)-;
                gesafid; gesarol; ivoran; neocid; p,p'-DDT;
                pentachlorin; trichlorobis(4-chlorophenyl)ethane;
```

MEDCHEM

	Measured	Estimate
logP	6.91	6.763

```
LOCAL NAME  DDT
ACTIVITY TYPE  INSECTICIDE
REFERENCE   EPA-600/2-81-011

LOGP        6.91
SOLV PAIR   Octanol
REFERENCE   De Bruijn,J., Busser,F., Seinen,W. & Hermens,J.,
            Environ. Tox. Chem., (1989) 8, 499
FOOTNOTE    Both Phases Analyzed
...  2      Slow-stir method (ref. 2129)
SEL         *

LOGPSTAR    6.91
```

ASTER

CAS : 50-29-3
NAME : 1,1'-(2,2,2-Trichloroethylidene)bis(4-chlorobenzene)
SMILES: Cl-c(ccc1C(-c(ccc2Cl)cc2)C(Cl)(Cl)Cl)cc1

#	Property	Value and	Units	Source	Method Error
1	Mol Wgt.	354.5	g/mole	Calc.	
2	Parachor	648.		Calc.	????
3	Mol Ref.	84.0		Calc.	Av. % Error = 5
4	Mol Vol.	270.	cm^3/g.m	Calc.	????
5	LogP	6.91		User	????
6	Melt Pt.	108.	C	ASTER	
7	Boil Pt.	260.	C @760mm	ASTER	
8	V.Press.	2.52E-03	mm of Hg	Calc.	Av. % Error = 39.0
9	Ht. Vpr.	1.21E+04	cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	8.76E-09	moles/L	Recalc	????
11	pKa				
12	FH TMOA	25.0	MOA num.	Recalc	Neurotoxicant: DDT-t

Dieldrin

IRPTC-database

file: 01.01 IDENT rn : 62
systematic name:1,4:5,8-DIMETHANONAPHTHALENE,1,2,3,4,10,10-HEXACHLORO-6,
7-EPOXY-1,4,4A,5,6,7,8,8A-OCTAHYDRO-,ENDO,EXO-
common name :dieldrin
cas no :60-57-1 rtecs no :IO1750000
molfm :C12H8CL6O
molwt :380.90
mp :176-177C
fl :NONE
den :1.8G/ML
rvden :13.2
vp :4.1E-7KPA(3.1E-6MMHG) AT 20C
n-octoh:aq :0.25E-3G/L AT 25C
fatsol :MODERATELY SOLUBLE IN BENZENE & ACETONE
hazard class :EUR ADR CLASS 6.1
EUR RID CLASS 6.1
IMO CLASS 6.1
UN HAZ CLASS 6.1
UN TOX GROUP II
synonyms :1,4:5,8-dimethanonaphthalene,1,2,3,4,10,10-hexachloro-6,
7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-,endo,exo-;
dieldrex; ent 16,225; heod; illoxol; octalox;

MEDCHEM

	Measured	Estimate
logP	5.20	3.626

LOCAL NAME ENDRIN
ACTIVITY TYPE INSECTICIDE
REFERENCE EPA-600/2-81-011

LOGP 5.20
SOLV PAIR Octanol
REFERENCE De Bruijn,J., Busser,F., Seinen,W. & Hermens,J., Environ. Tox. Chem., (1989) 8, 499
FOOTNOTE Both Phases Analyzed
... 2 Slow-stir method (ref. 2129)
SEL *

LOGPSTAR 5.20

ASTER

CAS : 60-57-1
NAME : Dieldrin
SMILES: O(C1C(C2)C3C(Cl)(C=4Cl)C5(Cl)Cl)C1C2C3C5(Cl)C4Cl

#	Property	Value and Units		Source	Method Error
1	Mol Wgt.	380.9	g/mole	Calc.	
2	Parachor	588.		Calc.	????
3	Mol Ref.	77.0		Calc.	Av. % Error = 5
4	Mol Vol.	266.	cm^3/g.m	Calc.	????
5	LogP	5.20		User	????
6	Melt Pt.	177.	C	ASTER	
7	Boil Pt.	417.	C @760mm	Calc.	Av. % Error = 7.4 K
8	V.Press.	1.28E-09	mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.44E+04	cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	2.02E-07	moles/L	Recalc	????
11	pKa				
12	FH TMOA	24.0	MOA num.	Recalc	Neurotoxicant: Cyclo

Endosulfan

IRPTC-database

```
file: 01.01 IDENT   rn : 112
systematic name:6,9-Methano-2,4,3-benzodioxathiepin,6,7,8,9,10,10-hexach
                loro-1,5,5a,6,9,9a-hexahydro-,3-oxide
common name    :endosulfan
cas no         :115-29-7            rtecs no       :RB9275000
molfm          :C9H6CL6O3S
molwt          :406.9
mp             :70-100C FOR TG
state          :SOLID, CRYSTALLINE
den            :1.745 AT 20C
vp             :1E-6KPA(1E-5MMHG) AT 25C
pow            :3.55(ALPHA), 3.62(BETA)
n-octoh:aq     :INSOLUBLE
fatsol         :MODERATELY SOLUBLE IN MOST ORGANIC SOLVENTS
colour         :BROWNISH FOR TG
odour          :TERPENE-LIKE
hazard class   :UN HAZ CLASS 6.1
definition     :MIXTURE OF 2 STEREOISOMERS; .ALPHA. AND .BETA.
comments       :ENDOSULFAN IS SENSITIVE TO MOISTURE, ACIDS, ALKALIS.
                STABLE TO SUNLIGHT.
synonyms       :5-norbornene-2,3-dimethanol,1,4,5,6,7,7-hexachloro-,cycl
                icsulfite; benzoepin; beosit; bio 5,462; chlorthiepin;
                endosulphan; ent 23,979; hildan; malix; thimul; thiodan;
                thiodan 35; thionex;
```

not in MEDCHEM

ASTER

```
CAS   :      115-29-7
NAME  : 6,7,8,9,10,10-Hexachloro-1,5,5a,6,9,9a-hexahydro-6,9-methano
-2,4,3-benzodioxathiepin, 3-Oxide
SMILES: S(=O)(OCC1C(Cl)(C=2Cl)C3(Cl)Cl)OCC1C3(Cl)C2Cl
```

#	Property	Value and Units		Source	Method Error
1	Mol Wgt.	406.9	g/mole	Calc.	
2	Parachor	612.		Calc.	????
3	Mol Ref.	77.2		Calc.	Av. % Error = 5
4	Mol Vol.	287.	cm^3/g.m	Calc.	????
5	LogP	3.60		User	????
6	Melt Pt.	106.	C	ASTER	
7	Boil Pt.	430.	C @760mm	Calc.	Av. % Error = 7.4 K
8	V.Press.	3.59E-10	mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.60E+04	cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	6.31E-05	moles/L	Recalc	R**2 = .93
11	pKa				
12	FH TMOA	24.0	MOA num.	Recalc	Neurotoxicant: Cyclo

Endrin

IRPTC-database

```
file: 01.01 IDENT   rn : 104
systematic name:1,4:5,8-DIMETHANONAPHTHALENE,1,2,3,4,10,10-HEXACHLORO-6,
                7-EPOXY-1,4,4A,5,6,7,8,8A-OCTAHYDRO-,ENDO,ENDO-
common name     :endrin
cas no          :72-20-8              rtecs no      :IO1575000
molfm           :C12H8CL6O
molwt           :380.90
mp              :235C, TG>200C DCP
bp              :DCP
state           :SOLID
fl              :NON FLAMMABLE
den             :1.7
vp              :2.6XE-8KPA (2XE-7MMHG) AT 25C
pow             :5.63
n-octoh:aq      :0.25E-3G/L AT 25C
fatsol          :BENZENE 13.8, ACETONE 17, CARBON TETRACHLORIDE 3.3,
                 HEXANE7.1(ALL IN G/0.1L 25C)
particle        :CRYSTALLINE (PURE), POWDER (TG)
colour          :WHITE (PURE), LIGHT TAN (TG)
additives       :HEXAMETHYLENE TETRAMINE (AS STABILISER)
impurities      :LESS THAN 0.4%. FREE ACID (AS HCL) AND LESS THAN 0.1%
                 WATER.
hazard class    :UN HAZ CLASS 6.1
                 PACK GROUP I,II,III
                 IMO CLASS 6.1
                 PACK GROUP I,II,III
comments        :SLIGHTLY CORROSIVE TO METALS. STABLE IN THE PRESENCE OF
                 MOST ALKALI, UNSTABLE IN THE PRESENCE OF STRONG ACIDS,
                 IN SUNLIGGHT AND WHEN HEATED. CONTACT WITH STRONG
                 OXIDIZERS MAY CAUSE FIRES AND EXPLOSIONS. TOXIC GASES
                 AND VAPORS (HYDROGEN CHLORIDE, OTHER VOLATILE
                 CHLORINATED COMPOUNDS, AND CARBON MONOXIDE).
synonyms        :1,4:5,8-dimethanonaphthalene,1,2,3,4,10,10-hexachloro-6,
                 7-epoxy-1,4,4a,5,6,7,8,8a-octahydro-,endo,endo-; endrex;
                 endricol; hexadrin; mendrin; oktanex;
```

MEDCHEM

	Measured	Estimate
logP	5.20	3.626

```
LOCAL NAME  ENDRIN
ACTIVITY TYPE  INSECTICIDE
REFERENCE   EPA-600/2-81-011

LOGP        5.20
SOLV PAIR   Octanol
REFERENCE   De Bruijn,J., Busser,F., Seinen,W. & Hermens,J.,
            Environ. Tox. Chem., (1989) 8, 499
FOOTNOTE    Both Phases Analyzed
...  2      Slow-stir method (ref. 2129)
SEL         *

LOGPSTAR    5.20
```

ASTER

CAS : 72-20-8
NAME : Endrin
SMILES: O(C1C(C2)C3C(Cl)(C=4Cl)C5(Cl)Cl)C1C2C3C5(Cl)C4Cl

#	Property	Value and Units	Source	Method Error
1	Mol Wgt.	380.9 g/mole	Calc.	
2	Parachor	588.	Calc.	????
3	Mol Ref.	77.0	Calc.	Av. % Error = 5
4	Mol Vol.	266. cm^3/g.m	Calc.	????
5	LogP	5.20	User	????
6	Melt Pt.			
7	Boil Pt.	417. C @760mm	Calc.	Av. % Error = 7.4 K
8	V.Press.	1.28E-09 mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.44E+04 cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	2.48E-06 moles/L	Recalc	????
11	pKa			
12	FH TMOA	24.0 MOA num.	Recalc	Neurotoxicant: Cyclo

Fenthion

IRPTC-database

file: 01.01 IDENT rn : 392
systematic name:Phosphorothioic acid,O,O-dimethyl O-(3-methyl-4-(methylthio)phe nyl)ester
common name :fenthion
cas no :55-38-9 rtecs no :TF9625000
molfm :C10H15O3PS2
molwt :278.34
bp :87C
state :LIQUID
den :1.250
vp :3E-5MMHG AT 20C
n-octoh:aq :55E-3G/L PRACTICALLY INSOLUBLE
fatsol :SOLUBLE IN METHANOL, ETHANOL, ETHER, ACETONE AND MANY OTHER ORGANIC SOLVENTS
odour :SLIGHT ORDOUR-LIKE
definition :ORGANOPHOSPHORUS INSECTICIDE
synonyms :baycid; baytex; ent 25.540; entex; lebaycid; mpp; phosphorothioic acid,O,O-dimethyl O-(4-methylthio)-m-tolyl)ester; queletox; spotton;

MEDCHEM

	Measured	Estimate
logP	4.09	3.907

LOCAL NAME FENTHION
LOCAL NAME BAYTEX
ACTIVITY TYPE INSECTICIDE
REFERENCE EPA-600/2-81-011

LOGP 4.09
SOLV PAIR Octanol
REFERENCE Bowman,B.T. & Sans,W.W., J. Environ. Sci. Health, (1983) B18 (6), 667
SEL *

LOGPSTAR 4.09

ASTER

CAS : 55-38-9
NAME : Phosphorothioic acid, O,O-Dimethyl O-(3-methyl-4-(methylthio
)phenyl ester
SMILES: S(C)-c(ccc1OP(=S)(OC)OC)c(c1)C

#	Property	Value and Units	Source	Method Error
1	Mol Wgt.	278.3 g/mole	Calc.	
2	Parachor	575.	Calc.	????
3	Mol Ref.	71.8	Calc.	Av. % Error = 5
4	Mol Vol.			
5	LogP	4.09	User	????
6	Melt Pt.			
7	Boil Pt.	355. C @760mm	Calc.	Av. % Error = 7.4 K
8	V.Press.	3.67E-07 mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.61E+04 cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	5.75E-05 moles/L	Recalc	????
11	pKa			
12	FH TMOA	4.00 MOA num.	Recalc	OP mediated AChE inh

Alpha-HCH

IRPTC-database

file: 01.01 IDENT rn : 813
systematic name:Cyclohexane,1,2,3,4,5,6-hexachloro-,(1.alpha.,2.alpha.,3
.beta.,4.alpha.,5.beta.,6.beta.)-
common name :.alpha.-hch
cas no :319-84-6 rtecs no :GV3500000
molfm :C6H6CL6
molwt :290.82
mp :158C
bp :288C
state :SOLID
den :1.87
vp :4XE-6KPA (2.8XE-5MMHG) AT 20C
pow :3.82
n-octoh:aq :1MG/L AT 20C
fatsol :SOLUBLE IN ACETONE, BENZENE, ETHYL ALCOHOL AND ETHER
particle :CRYSTALLINE, MONOCLINIC OR PRISMS
colour :COLOURLESS
odour :PERSISTANT, ACRID
comments :FOR VP THE VALUE 0.02MMHG AT 20C IS ALSO REPORTED.
RATHER STABLE; DOES NOT OXIDISE OR HYDROLYZE, STABLE
TOWARD AIR, MOISTURE AND STRONG ACIDS. UNSTABLE IN
PRESENCE OF ALKALI. SOME SOURCES FEEL THAT THE NAME
BENZENE HEXACHLORIDE SHOULD NOT BE USED FOR HCH.
synonyms :.alpha.-1,2,3,4,5,6-hexachlorocyclohexane; .alpha.-BHC;
.alpha.-benzenehexachloride; .alpha.-hexachloran;
.alpha.-hexachlorane; .alpha.-hexachlorcyclohexane;
.alpha.-hexachlorocyclohexane; .alpha.-lindane;
cyclohexane,1,2,3,4,5,6-hexachloro,.alpha.;

MEDCHEM

	Measured	Estimate
logP	3.72	3.752

LOCAL NAME HEXACHLOROCYCLOHEXANE, ALPHA ISOMER

LOGPSTAR 3.80

LOGP 3.80
SOLV PAIR Octanol
REFERENCE Kurihara,N., Matazaemon,U., Fujita,T. & Nakajima, M., Pest. Biochem. Physiol., (1973) 2, 383
SEL *

LOGP 3.78
SOLV PAIR Octanol
REFERENCE De Bruijn,J., Busser,F., Seinen,W. & Hermens,J., Environ. Tox. Chem., (1989) 8, 499
FOOTNOTE Both Phases Analyzed
... 2 Slow-stir method (ref. 2129)

ASTER

CAS : 319-84-6
NAME : 1,2,3,4,5,6-Hexachloro(1a,2a,3b,4a,5b,6b)cyclohexane
SMILES: ClC(C(Cl)C(Cl)Cl)C(Cl)Cl

#	Property	Value and Units		Source	Method Error
1	Mol Wgt.	290.8	g/mole	Calc.	
2	Parachor	464.		Calc.	????
3	Mol Ref.	56.9		Calc.	Av. % Error = 5
4	Mol Vol.	224.	cm^3/g.m	Calc.	????
5	LogP	3.72		User	????
6	Melt Pt.	158.	C	ASTER	
7	Boil Pt.	301.	C @760mm	Calc.	Av. % Error = 7.4 K
8	V.Press.	1.64E-04	mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.25E+04	cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	1.56E-05	moles/L	Recalc	R**2 = .93
11	pKa				
12	FH TMOA	24.0	MOA num.	ASTER	Neurotoxicant: Cyclo

Beta-HCH

IRPTC-database

```
file: 01.01 IDENT   rn : 814
systematic name:Cyclohexane,1,2,3,4,5,6-hexachloro-,(1.alpha.,2.beta.,3.
              alpha.,4.beta.,5.alpha.,6.beta.)-
common name    :.beta.hch
cas no         :319-85-7            rtecs no       :GV4375000
molfm          :C6H6CL6
molwt          :290.82
mp             :311.7C SUB
bp             :60C AT 0.58MMHG
state          :SOLID
den            :1.89
vp             :3.7XE-8KPA(2.8XE-7MMHG) AT 20C
pow            :3.80
n-octoh:aq     :0.2MG/L AT 20C,5MG/L AT 20C
fatsol         :READILY SOLUBLE IN ACETONE & CYCLOHEXANE;SLIGHTLY
                SOLUBLE IN CHLOROFORM,BENZENE
particle       :CUBIC CRYSTALS
colour         :COLOURLESS
comments       :THE VP 0.005MMHG AT 20C IS ALSO REPORTED. STABLE AT ROOM
                TEMPERATURE, TOWARD AIR, MOISTURE, STRONG ACIDS, AND
                OXIDATION. UNSTABLE IN PRESENCE OF ALKALI.
synonyms       :.beta.-1,2,3,4,5,6-hexachlorocyclohexane; .beta.-BHC;
                .beta.-benzene hexachloride; .beta.-hexachlorobenzene;
                .beta.-hexachlorocyclohexane;
                cyclohexane,1,2,3,4,5,6-hexachloro-,.beta.-;
```

MEDCHEM

	Measured	Estimate
logP	3.72	3.752

LOCAL NAME HEXACHLOROCYCLOHEXANE, BETA ISOMER

```
LOGP        3.78
SOLV PAIR   Octanol
REFERENCE   Kurihara,N., Matazaemon,U., Fujita,T. & Nakajima,
            M., Pest. Biochem. Physiol., (1973) 2, 383
SEL         *

LOGP        3.84
SOLV PAIR   Octanol
REFERENCE   De Bruijn,J., Busser,F., Seinen,W. & Hermens,J.,
            Environ. Tox. Chem., (1989) 8, 499
FOOTNOTE    Both Phases Analyzed
...  2      Slow-stir method (ref. 2129)

LOGPSTAR    3.78
```

ASTER

CAS : 319-85-7
NAME : 1,2,3,4,5,6-Hexachloro((1a,2b,3a,4b,5a,6b)cyclohexane
SMILES: ClC(C(Cl)C(Cl)C1Cl)C(Cl)C1Cl

#	Property	Value and Units		Source	Method Error
1	Mol Wgt.	290.8	g/mole	Calc.	
2	Parachor	464.		Calc.	????
3	Mol Ref.	56.9		Calc.	Av. % Error = 5
4	Mol Vol.	224.	cm^3/g.m	Calc.	????
5	LogP	3.78		User	????
6	Melt Pt.	297.	C	ASTER	
7	Boil Pt.	301.	C @760mm	Calc.	Av. % Error = 7.4 K
8	V.Press.	1.64E-04	mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.25E+04	cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	7.45E-07	moles/L	Recalc	????
11	pKa				
12	FH TMOA	24.0	MOA num.	ASTER	Neurotoxicant: Cyclo

Gamma-HCH

IRPTC-database

file: 01.01 IDENT rn : 233
systematic name:CYCLOHEXANE,1,2,3,4,5,6-HEXACHLORO-,GAMMA-ISOMER
common name :lindane
cas no :58-89-9 rtecs no :GV4900000
molfm :C6H6CL6
molwt :290.82
mp :112.9C
bp :323.4C
state :SOLID
fl :NON-FLAMMABLE
den :1.85
vp :1.25E-6KPA(9.4E-6MMHG) AT 20C
pow :3.72
n-octoh:aq :10E-3G/L AT 20C
fatsol :SOLUBLE IN ACETONE 43.5, BENZENE 28.9, CHCL3 24.0, ETHER 20.8, ALL G/100G AT 20C
particle :CRYSTALLINE
colour :WHITE
odour :SLIGHTLY MUSTY, FAINT
impurities :HEPTACHLOROCYCLOHEXANE, OTHER ISOMERS OF HCH.
hazard class :UN HAZ CLASS 6.1
PACK GROUP III
IMO CLASS 6.1
PACK GROUP III
comments :FOR VP 3.26XE-5 MMHG AT 20C IS ALSO REPORTED. CORROSIVE TO ALUMINIUM. STABLE TO LIGHT, AIR, HEAT, CARBON DIOXIDE AND STRONG ACIDS. UNSTABLE IN THE PRESENCE OF ALKALI OR ON PROLONGED EXPOSURE TO HEAT. DECOMPOSES IN THE PRESENCE OF CERTAINPOWDERED METALS SUCH AS IRON, ALUMINIUM AND ZINC.DECOMPOSITION PRODUCTS: PHOSGENE, HYDROGEN CHLORIDE AND CARBON MONOXIDE
synonyms :.gama.cid; .gamma.benzene hexachloride; .gamma.-HCH; .gamma.-bhc; .gamma.-hexachloran; .gamma.-hexachlorane; .gamma.-hexachlorocyclohexane; .gamma.-lindane; .gamma.1,2,3,4,5,6-hexachlorocyclohexane; aalindan; aficide; agrocide; agrocide wp; ameisenmittel merck; aparasin; aphtiria; aplidal; arbitex; bbh; bexol; bhc; celanex; chloresene; codechine; dbh; detmol-extrakt; devoran; dol granule; drill tox-spezial aglukon; ent 7,796; entomoxan; gammexane; gexane; hcch; hch; heclotox; hexa; hexachloran; hexachlorane; hexaverm; hexicide; hexyclan; hgi; hortex; jacutin; kokotine; kwell; lendine; lentox; lidenal; lindatox; lindosep; lintox; lorexane; milbol 49; mszycol; neo-scabicidol; nexen fb; nexit; nexit-stark; nicochloran; omnitox; ovadziak; pedraczak; pflanzol;

MEDCHEM

	Measured	Estimate
logP	3.72	3.752

LOCAL NAME LINDANE
LOCAL NAME HEXACHLOROCYCLOHEXANE, GAMMA ISOMER
ACTIVITY TYPE ANTIPARASITIC (TOPICAL)

LOGP 3.72
SOLV PAIR Octanol
REFERENCE Kiso,M., Fujita,T., Kurihara,N., Uchida,M. Tanaka K. & Nakajima,M., Pest. Biochem. Physiol., (1978) 8, 33
SEL *

LOGP 3.69
SOLV PAIR Octanol
REFERENCE De Bruijn,J., Busser,F., Seinen,W. & Hermens,J., Environ. Tox. Chem., (1989) 8, 499
FOOTNOTE Both Phases Analyzed
... 2 Slow-stir method (ref. 2129)

LOGPSTAR 3.72

ASTER

CAS : 58-89-9
NAME : (1a,2a,3b,4a,5a,6b)-1,2,3,4,5,6-Hexachlorocyclohexane
SMILES: ClC(C(Cl)C(Cl)Cl)C(Cl)Cl

#	Property	Value and Units		Source	Method Error
1	Mol Wgt.	290.8	g/mole	Calc.	
2	Parachor	464.		Calc.	????
3	Mol Ref.	56.9		Calc.	Av. % Error = 5
4	Mol Vol.	224.	cm^3/g.m	Calc.	????
5	LogP	3.72		User	????
6	Melt Pt.	113.	C	ASTER	
7	Boil Pt.	323.	C @760mm	ASTER	
8	V.Press.	3.59E-05	mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.30E+04	cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	3.96E-05	moles/L	Recalc	R**2 = .93
11	pKa				
12	FH TMOA	24.0	MOA num.	ASTER	Neurotoxicant: Cyclo

Heptachlor

IRPTC-database

```
file: 01.01 IDENT   rn : 187
systematic name:4,7-Methano-1H-indene,1,4,5,6,7,8,8-heptachloro-3a,4,7,7
                a-tetra hydro-
common name    :heptachlor
cas no         :76-44-8            rtecs no       :PC0700000
molfm          :C10H5CL7
molwt          :373.30
mp             :95-96C
bp             :135-145C AT 1MMHG
state          :SOLID
den            :1.7G/ML
vp             :4E-5KPA(3E-4MMHG) AT 25C
pow            :5.44
n-octoh:aq     :56E-6G/L AT 25-29C
fatsol         :ETHANOL (45GL), ACETONE (750G/L), BENZENE (1060G/L)
colour         :COLOURLESS, WHITE
odour          :MILD CAMPHOR-LIKE
impurities     :HEXACHLOROCYCLOPENTADIENE; TRANS(GAMMA)CHLORDANE 21%
                (TG); NONACHLOR 5% (TG); CHLORDENE ISOMERS 1% (TG)
hazard class   :EUR ADR CLASS 6.1
                EUR RID CLASS 6.1
                IMO CLASS 6.1
                UN HAZ CLASS 6.1
                UN TOX GROUP III
synonyms       :3-chlorochlordene;
                4,7-methanoindene,1,4,5,6,7,8,8-heptachloro-3a,4,7,7a-te
                trahydro-; aahepta; agroceres; e 3314; ent 15,152; gpkh;
                heptachlorane; rhodiachlor;
```

MEDCHEM

	Measured	Estimate
logP	n/a	4.925

ASTER

```
CAS   :       76-44-8
NAME  : 1,4,5,6,7,8,8-Heptachloro-3a,4,7,7a-tetrahydro-4,7-methano-1
H-indene
SMILES: ClC(C=C1)C(ClC2(Cl)C=3Cl)C(Cl)(C3Cl)C2(Cl)Cl
```

#	Property	Value and Units		Source	Method Error	
1	Mol Wgt.	373.3	g/mole	Calc.		
2	Parachor	578.		Calc.	????	
3	Mol Ref.	74.9		Calc.	Av. % Error = 5	
4	Mol Vol.	270.	cm^3/g.m	Calc.	????	
5	LogP	4.93		User	????	
6	Melt Pt.	95.0	C	ASTER		
7	Boil Pt.	404.	C @760mm	Calc.	Av. % Error = 7.4 K	
8	V.Press.	4.43E-09	mm of Hg	Calc.	Av. % Error = 47.0	
9	Ht. Vpr.	1.39E+04	cal/mole	Calc.	Av. % Error = 1.85	
10	Sol. H2O	2.30E-06	moles/L	Recalc	????	
11	pKa					
12	FH TMOA	24.0	MOA num.	Recalc	Neurotoxicant: Cyclo	

Heptachlor epoxide

IRPTC-database

```
file: 01.01 IDENT   rn : 198
systematic name:2,5-Methano-2H-indeno(1,2-b)oxirene,2,3,4,5,6,7,7-heptac
                hloro-1
                a,1b,5,5a,6,6a-hexahydro-,(1a.alpha.,1b.beta.,2.alpha.,5
                .alpha.,5a.beta.,6.beta.,6a.alpha.)-
common name     :heptachlor epoxide
cas no          :1024-57-3          rtecs no       :PB9450000
molfm           :C10H5CL7O
molwt           :389.30
mp              :157-159C
state           :SOLID
vp              :3.99E-5PKA(3E-4MMHG) AT 25C
pow             :4.60
n-octoh:aq      :0.350E-3G/L,0.200E-3G/L AT 25C
comments        :SOME SUSCEPTIBILITY TO OXIDATION BY OZONE.
synonyms        :4,7-methanoindan,1,4,5,6,7,8,8-heptachloro-2,3-epoxy-3a,
                 4,7,7a-tetrahydro-; ent 25,584; epoxyheptachlor; hce;
```

MEDCHEM

	Measured	Estimate
logP	n/a	3.495

ASTER

```
CAS   :       00-00-0
NAME  :
SMILES: ClC(C1OC12)C(C2C3(Cl)C=4Cl)C(Cl)(C4Cl)C3(Cl)Cl
```

#	Property	Value and Units		Source	Method Error
1	Mol Wgt.	389.3	g/mole	Calc.	
2	Parachor	576.		Calc.	????
3	Mol Ref.	74.8		Calc.	Av. % Error = 5
4	Mol Vol.	263.	cm^3/g.m	Calc.	????
5	LogP	3.49		User	????
6	Melt Pt.				
7	Boil Pt.	412.	C @760mm	Calc.	Av. % Error = 7.4 K
8	V.Press.	2.11E-09	mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.43E+04	cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	3.10E-04	moles/L	Recalc	????
11	pKa				
12	FH TMOA	24.0	MOA num.	Recalc	Neurotoxicant: Cyclo

Hexachlorobenzene

IRPTC-database

file: 01.01 IDENT rn : 199
systematic name:Benzene,hexachloro-
common name :hexachlorobenzene
cas no :118-74-1 rtecs no :DA2975000
molfm :C6CL6
molwt :284.76
mp :231C
bp :326, 322C SUB
state :SOLID, CRYSTALLINE
fp :242C
fl :FLAMMABLE
den :2.044 AT 23C
rvden :9.8
vp :1.5E-6KPA(1.09E-5MMHG) AT 20C
pow :6.18
n-octoh:aq :1E-5G/L AT 25C
fatsol :SPARINGLY SOLUBLE IN COLD ALCOHOL; SOLUBLE IN BENZENE, CHLOROFORM AND ETHER
particle :CRYSTALLINE AS NEEDLES
colour :WHITE
odour :SPECIFIC, UNPLEASANT
impurities :HEXACHLOROBUTADIENE IF HCB IS DERIVED FROM TAR. HEPTA-AND OCTACHLORODIBENZOFURANS AND OCTACHLORODIBENZO-PARA-DIOXIN HAVE BEEN FOUND IN COMMERCIAL HCB. TG IN US CONTAINS 1.8% PENTACHLOROBENZENE AND 0.2%. 1,2,4,5-TETRACHLOROBENZENE.
hazard class :UN HAZ CLASS 6.1
PACK GROUP III
IMO CLASS 6.1
PACK GROUP III
comments :FOR FP THE VALUE 116.7C IS ALSO REPORTED. FOR DENSITY THE VALUE AT 20C IS ALSO REPORTED. COMBUSTIBLE WHEN EXPOSED TO HEAT OR FLAME. WHEN HEATED TO DECOMPOSITION EMITS HIGHLY TOXIC FUMES OF CHLORINE. VIOLENT REACTION WITH DIMETHYLFORMAMIDE. VERY STABLE; NON REACTIVE. SUBLIMABLE. TO FIGHT FIRE, USE CO2, DRY CHEMICAL.
synonyms :amatin; anticarie; bunt-cure; bunt-no-more; co-op hexa; hcb; julin's carbon chloride; no bunt; no bunt 40; no bunt 80; no bunt liquid; pentachlorophenyl chloride; perchlorobenzene; sanocide; snieciotox;

MEDCHEM

	Measured	Estimate
logP	5.73	5.700

LOCAL NAME HEXACHLOROBENZENE

ACTIVITY TYPE FUNGICIDE
REFERENCE EPA-600/2-81-011

LOGP 5.73
SOLV PAIR Octanol
REFERENCE De Bruijn,J., Busser,F., Seinen,W. & Hermens,J., Environ. Tox. Chem., (1989) 8, 499
FOOTNOTE Both Phases Analyzed
... 2 Slow-stir method (ref. 2129)
SEL *

LOGPSTAR 5.73

ASTER

CAS : 118-74-1
NAME : Hexachlorobenzene
SMILES: Cl-c(c(Cl)c(Cl)c1Cl)c(Cl)c1Cl

#	Property	Value and Units		Source	Method Error
1	Mol Wgt.	284.8	g/mole	Calc.	
2	Parachor	430.		Calc.	????
3	Mol Ref.	55.5		Calc.	Av. % Error = 5
4	Mol Vol.	182.	cm^3/g.m	Calc.	????
5	LogP	5.73		User	????
6	Melt Pt.	230.	C	ASTER	
7	Boil Pt.	326.	C @760mm	Calc.	Av. % Error = 7.4 K
8	V.Press.	4.35E-06	mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.34E+04	cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	1.62E-08	moles/L	ASTER	
11	pKa				
12	FH TMOA	31.0	MOA num.	Recalc	Nonpolar narcosis

Pentachlorobenzene

IRPTC-database

file: 01.01 IDENT rn : 3464
systematic name:Benzene,pentachloro-
common name :pentachlorobenzene
cas no :608-93-5 rtecs no :DA6640000

MEDCHEM

	Measured	Estimate
logP	5.18	5.227

LOCAL NAME PENTACHLOROBENZENE

LOGP	5.18
SOLV PAIR	Octanol
REFERENCE	De Bruijn,J., Busser,F., Seinen,W. & Hermens,J., Environ. Tox. Chem., (1989) 8, 499
FOOTNOTE	Both Phases Analyzed
... 2	Slow-stir method (ref. 2129)
SEL	*

LOGPSTAR 5.18

ASTER

CAS : 608-93-5
NAME : Pentachlorobenzene
SMILES: Cl-c(c(Cl)c(Cl)c1)c(Cl)c1Cl

#	Property	Value and Units		Source	Method Error
1	Mol Wgt.	250.3	g/mole	Calc.	
2	Parachor	392.		Calc.	????
3	Mol Ref.	50.6		Calc.	Av. % Error = 5
4	Mol Vol.	165.	cm^3/g.m	Calc.	????
5	LogP	5.18		User	????
6	Melt Pt.	86.0	C	ASTER	
7	Boil Pt.	277.	C @760mm	ASTER	
8	V.Press.	8.21E-04	mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.22E+04	cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	3.30E-06	moles/L	ASTER	
11	pKa				
12	FH TMOA	31.0	MOA num.	Recalc	Nonpolar narcosis

Pentachlorophenol

IRPTC-database

file: 01.01 IDENT rn : 92
systematic name:Phenol,pentachloro-
common name :pentachlorophenol
cas no :87-86-5 rtecs no :SM6300000
molfm :C6HCL5O
molwt :266.32
mp :191C
bp :310C DCP
den :2.0 G/ML
vp :1.5E-5KPA(1.1E-4MMHG) AT 20C
pow :5.01
n-octoh:aq :14E-3G/L AT 20C
colour :LIGHT TAN, WHITE
odour :PHENOLIC, PUNGENT
impurities :TETRACHLOROPHENOL(4.4%) ; HIGHER CHLORINATED PHENOXYPHENOLS(6.2%); TRICHLOROPHENOL (<0.1%); POLYCHLORINATED DIBENZO-P-DIOXINS; POLYCHLORINATED DIBENZOFURANS; HEXACHLOROBENZENE(TG)!IARMB820,304,79
hazard class :EUR ADR CLASS 6.1
EUR RID CLASS 6.1
IMO CLASS 6.1
UN HAZ CLASS 6.1
UN TOX GROUP III
comments :THRESHOLD LEVEL FOR MAN FOR TASTE = 30UG/L, FOR ODOUR = 1600UG/L (REF. !ABWQC*,81-117764,-,1980,EPA,AMBIANT WATER QUALI TY CRITERIA)
synonyms :dowicide 7; fungifen; grundier arbezol; lauxtol; liroprem; pcp; permasan; santophen 20;

MEDCHEM

	Measured	Estimate
logP	5.12	4.323

LOCAL NAME PENTACHLOROPHENOL
ACTIVITY TYPE HERBICIDE
... 2 PRESERVATIVE(WOOD)
REFERENCE EPA-600/2-81-011

LOGPSTAR 5.12

LOGP 5.12
SOLV PAIR Octanol
REFERENCE Nikaitani,D. & Hansch,C., Pomona College, Unpublished Analysis
FOOTNOTE Using HCl
SEL *
pH 1.4

ASTER

CAS : 87-86-5
NAME : Pentachlorophenol
SMILES: Cl-c(c(Cl)c(Cl)c1O)c(Cl)c1Cl

#	Property	Value and Units		Source	Method Error
1	Mol Wgt.	266.3	g/mole	Calc.	
2	Parachor	410.		Calc.	????
3	Mol Ref.	52.2		Calc.	Av. % Error = 5
4	Mol Vol.	172.	cm^3/g.m	Calc.	????
5	LogP	5.12		User	????
6	Melt Pt.	174.	C	ASTER	
7	Boil Pt.	337.	C @760mm	Calc.	Av. % Error = 7.4 K
8	V.Press.	1.82E-06	mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.49E+04	cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	2.66E-07	moles/L	Recalc	????
11	pKa	4.70	@ 25 C.	Calc.	
12	FH TMOA	41.0	MOA num.	Recalc	Uncoupler of oxidati

Quintozene

IRPTC-database

file: 01.01 IDENT rn : 341
systematic name:Benzene,pentachloronitro-
common name :quintozene
cas no :82-68-8 rtecs no :DA6650000
molfm :C6CL5NO2
molwt :295.32
mp :144C
bp :328C
state :SOLID
den :1.718
vp :1.77E-3KPA AT 25C
n-octoh:aq :INSOLUBLE 0.44E-3G/L AT 20C
fatsol :SOLUBLE IN ETHANOL(2%), BENZENE, CARBON DISULFIDE, CHLOROFORM AND KETONE
particle :CRYSTALLINE
colour :COLOURLESS
odour :MUSTY
impurities :TG 97-99% PURE. MAIN IMPURITIES: 1.5% HEXACHLOROBENZENE TOGETHER WITH LESSER AMOUNTS OF PENTACHLOROBENZENE AND TETRACHLORONITROBENZENE
comments :FORMULATIONS: 1.4-99% DUSTS, 35-75% WP, 2 EC, 10% GRANULES, 0.75-1.63% PASTES. OFTEN FORMULATED IN COMBINATION WITH OTHER PESTICIDES
synonyms :batrilex; botrilex; brassicol; fartox; folosan; gc3944-3-4; kobutol; pcnb; pentachloronitrobenzene; pentagen; quintocene; terrachlor; terraclor; terrafun; tilcarex;

MEDCHEM

	Measured	Estimate
logP	4.22	4.570

LOCAL NAME PENTACHLORONITROBENZENE
ACTIVITY TYPE FUNGICIDE (SOIL)
REFERENCE Merck Index, 11th Ed.
LOCAL NAME QUINTOZENE

LOGP 4.22
SOLV PAIR Octanol
REFERENCE Kanazawa,J., Pestic. Sci., (1981) 12, 417
SEL *

LOGPSTAR 4.22

ASTER

CAS : 82-68-8
NAME : Pentachloronitrobenzene
SMILES: Cl-c(c(Cl)c(Cl)c1N(=O)=O)c(Cl)c1Cl

#	Property	Value and Units		Source	Method Error
1	Mol Wgt.	295.3	g/mole	Calc.	
2	Parachor	444.		Calc.	????
3	Mol Ref.	56.1		Calc.	Av. % Error = 5
4	Mol Vol.	193.	cm^3/g.m	Calc.	????
5	LogP	4.22		User	????
6	Melt Pt.	144.	C	ASTER	
7	Boil Pt.	367.	C @760mm	Calc.	Av. % Error = 7.4 K
8	V.Press.	1.22E-07	mm of Hg	Calc.	Av. % Error = 47.0
9	Ht. Vpr.	1.56E+04	cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	5.48E-06	moles/L	Recalc	R**2 = .93
11	pKa				
12	FH TMOA	31.0	MOA num.	Recalc	Nonpolar narcosis

Thiram

IRPTC-database

file: 01.01 IDENT rn : 133
systematic name:Thioperoxydicarbonic diamide(((H2N)C(S))2S2),tetramethyl-
common name :thiram
cas no :137-26-8 rtecs no :JO1400000
molfm :N2S4C6H12
molwt :240.44
den :1.3G/ML
n-octoh:aq :30E-3G/L
fatsol :SLIGHTLY SOLUBLE IN ETHANOL, DIETHYL ETHER, ACETONE, CHLOROFORM
colour :COLOURLESS
hazard class :UN HAZ CLASS 6.1
synonyms :accelerator thiuram; aceto tetd; arasan; arasan 42-S; arasan 70; arasan 75; arasan-m; arasan-sf; disulfide,bis(dimethylthiocarbamoyl); ekagom tb; fernacol; fernasan; fernasan a; fernide; hermal; heryl; kregasan; mercuram; methyl thiram; methyl tuads; nobecutan; normersan; panoram 75; polyram ultra; pomarsol; pomarsol forte; pomasol; puralin; rezifilm; royal tmtd; sadoplon; spotrete; tersan; tersan 75; tetramethylthioperoxydicarbonic diamide; tetramethylthiuram bisulfide; tetramethylthiuram disulfide; tetramethylthiuram disulphide; tetrasipton; thillate; thiosan; thiotox; thiram 75; thiram b; thirasan; thiurad; thiuram; thiuram d; thiuram disulfide,tetramethyl-; thiuram m; thiuramyl; thylate; tiuramyl; tmtd; tmtds; trametan; tridipam; tripomol; tuads; tuex; tulisan; vulcafor tmtd;

MEDCHEM

	Measured	Estimate
logP	n/a	1.764

ASTER

CAS : 137-26-8
NAME : Tetramethylthioperoxydicarbonicdiamide
SMILES: S=C(SSC(=S)N(C)C)N(C)C

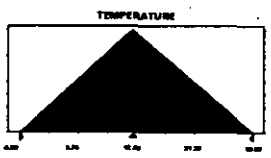
#	Property	Value and Units		Source	Method Error
1	Mol Wgt.	240.4	g/mole	Calc.	
2	Parachor	500.		Calc.	????
3	Mol Ref.	68.5		Calc.	Av. % Error = 5
4	Mol Vol.	238.	cm^3/g.m	Calc.	????
5	LogP	1.76		User	????
6	Melt Pt.				
7	Boil Pt.	110.	C @760mm	ASTER	
8	V.Press.	24.0	mm of Hg	Calc.	Av. % Error = 2.5
9	Ht. Vpr.	7.94E+03	cal/mole	Calc.	Av. % Error = 1.85
10	Sol. H2O	4.17E-02	moles/L	Recalc	????
11	pKa				
12	FH TMOA	31.0	MOA num.	Recalc	Nonpolar narcosis

APPENDIX 5: Chosen ranges of uncertainty for non chemical-specific input data

Assumption: TEMPERATURE **Cell: H19**

Triangular distribution with parameters:

Minimum	-5.00
Likeliest	12.00
Maximum	30.00

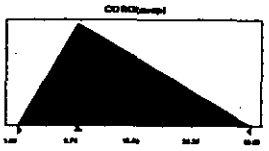


Selected range is from -5.00 to 30.00

Assumption: CORG(susp) **Cell: H22**

Triangular distribution with parameters:

Minimum	3.00
Likeliest	10.00
Maximum	30.00

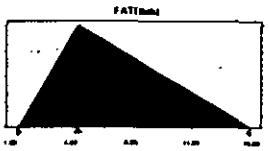


Selected range is from 3.00 to 30.00

Assumption: FAT(fish) **Cell: H25**

Triangular distribution with parameters:

Minimum	1.50
Likeliest	5.00
Maximum	15.00

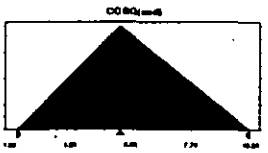


Selected range is from 1.50 to 15.00

Assumption: CORG(sed) **Cell: H28**

Triangular distribution with parameters:

Minimum	1.00
Likeliest	5.00
Maximum	10.00

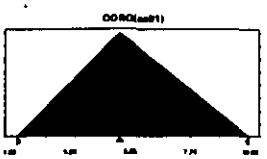


Selected range is from 1.00 to 10.00

Assumption: CORG(soil1) **Cell: H31**

Triangular distribution with parameters:

Minimum	1.00
Likeliest	5.00
Maximum	10.00

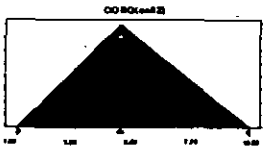


Selected range is from 1.00 to 10.00

Assumption: CORG(soil2) **Cell: H34**

Triangular distribution with parameters:

Minimum	1.00
Likeliest	5.00
Maximum	10.00

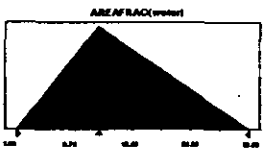


Selected range is from 1.00 to 10.00

Assumption: AREAFRAC(water) **Cell: H51**

Triangular distribution with parameters:

Minimum	3.00
Likeliest	12.50
Maximum	30.00

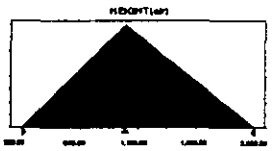


Selected range is from 3.00 to 30.00

Assumption: HEIGHT(air) **Cell: H55**

Triangular distribution with parameters:

Minimum	200.00
Likeliest	1,000.00
Maximum	2,000.00



Selected range is from 200.00 to 2,000.00

Assumption: DEPTH(water) **Cell: H56**

Triangular distribution with parameters:

Minimum	1.00
Likeliest	3.00
Maximum	10.00

Selected range is from 1.00 to 10.00

Assumption: DEPTH(sed) **Cell: H61**

Triangular distribution with parameters:

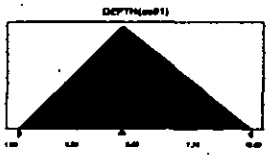
Minimum	1.00
Likeliest	3.00
Maximum	5.00

Selected range is from 1.00 to 5.00

Assumption: DEPTH(soil1) **Cell: H63**

Triangular distribution with parameters:

Minimum	1.00
Likeliest	5.00
Maximum	10.00

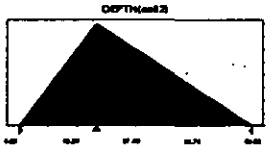


Selected range is from 1.00 to 10.00

Assumption: DEPTH(soil2) **Cell: H64**

Triangular distribution with parameters:

Minimum	5.00
Likeliest	20.00
Maximum	50.00

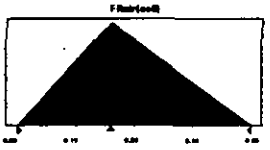


Selected range is from 5.00 to 50.00

Assumption: FRair(soil) **Cell: H66**

Triangular distribution with parameters:

Minimum	0.00
Likeliest	0.20
Maximum	0.50



Selected range is from 0.00 to 0.50

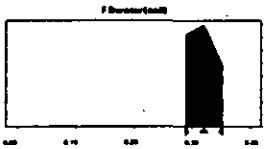
Correlated with:

FRwater(soil) (H67)	-0.77

Assumption: FRwater(soil) **Cell: H67**

Triangular distribution with parameters:

Minimum	0.00
Likeliest	0.40
Maximum	0.50



Selected range is from 0.36 to 0.44

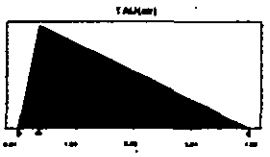
Correlated with:

FRair(soil) (H66)	-0.77

Assumption: TAU(air) **Cell: H70**

Triangular distribution with parameters:

Minimum	0.04
Likeliest	0.40
Maximum	4.00



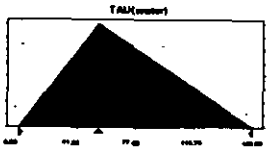
Selected range is from 0.04 to 4.00

Assumption: TAU(water) **Cell: H72**

Triangular distribution with parameters:

Minimum	5.00
Likeliest	54.54
Maximum	150.00

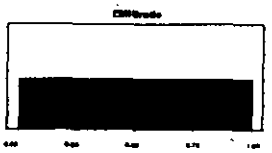
Selected range is from 5.00 to 150.00



Assumption: EMISratio **Cell: H78**

Uniform distribution with parameters:

Minimum	0.00
Maximum	1.00

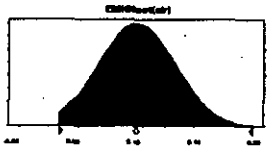


Assumption: EMISfact(air) **Cell: H86**

Normal distribution with parameters:

Mean	0.10
Standard Dev.	0.05

Selected range is from 0.00 to +Infinity

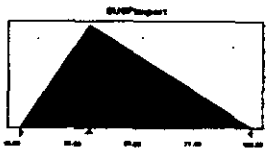


Assumption: SUSPimport **Cell: H118**

Triangular distribution with parameters:

Minimum	10.00
Likeliest	37.00
Maximum	100.00

Selected range is from 10.00 to 100.00

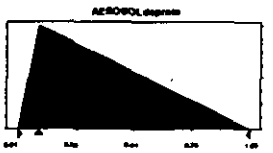


Assumption: AEROSOLdeprate **Cell: H143**

Triangular distribution with parameters:

Minimum	0.01
Likeliest	0.10
Maximum	1.00

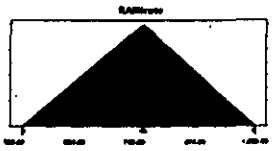
Selected range is from 0.01 to 1.00



Assumption: RAINrate **Cell: H145**

Triangular distribution with parameters:

Minimum	500.00
Likeliest	760.00
Maximum	1,000.00



Selected range is from 500.00 to 1,000.00

Assumption: COLLECTeff **Cell: H147**

Triangular distribution with parameters:

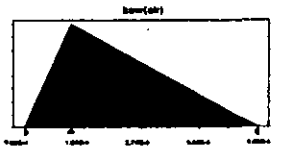
Minimum	60,000.00
Likeliest	200,000.00
Maximum	600,000.00

Selected range is from 60,000.00 to 600,000.00

Assumption: kaw(air) **Cell: H150**

Triangular distribution with parameters:

Minimum	5.00E-04
Likeliest	1.39E-03
Maximum	5.00E-03

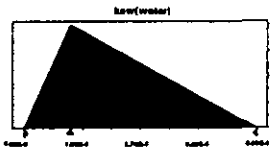


Selected range is from 5.00E-4 to 5.00E-3

Assumption: kaw(water) **Cell: H151**

Triangular distribution with parameters:

Minimum	5.00E-06
Likeliest	1.39E-05
Maximum	5.00E-05

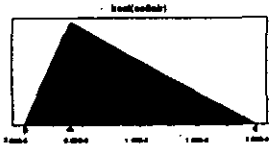


Selected range is from 5.00E-6 to 5.00E-5

Assumption: kasl(soilair) **Cell: H159**

Triangular distribution with parameters:

Minimum	2.00E-06
Likeliest	5.56E-06
Maximum	2.00E-05

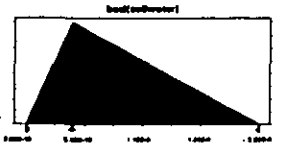


Selected range is from 2.00E-6 to 2.00E-5

Assumption: kasl(soilwater) **Cell: H160**

Triangular distribution with parameters:

Minimum	2.00E-10
Likeliest	5.56E-10
Maximum	2.00E-09

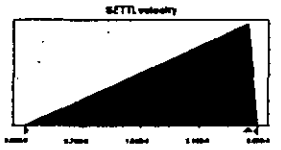


Selected range is from 2.00E-10 to 2.00E-9

Assumption: SETTLvelocity **Cell: H172**

Triangular distribution with parameters:

Minimum	3.00E-06
Likeliest	2.89E-05
Maximum	3.00E-05

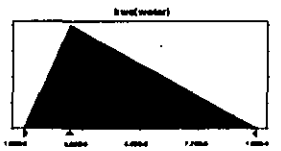


Selected range is from 3.00E-6 to 3.00E-5

Assumption: kws(water) **Cell: H178**

Triangular distribution with parameters:

Minimum	1.00E-06
Likeliest	2.78E-06
Maximum	1.00E-05



Selected range is from 1.00E-6 to 1.00E-5

Assumption: kws(sed) **Cell: H179**

Triangular distribution with parameters:

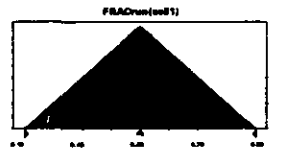
Minimum	1.00E-08
Likeliest	2.78E-08
Maximum	1.00E-07

Selected range is from 1.00E-8 to 1.00E-7

Assumption: FRACrun(soil1) **Cell: H185**

Triangular distribution with parameters:

Minimum	0.10
Likeliest	0.50
Maximum	0.90

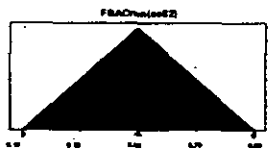


Selected range is from 0.10 to 0.90

Assumption: FRACrun(soil2) **Cell: H186**

Triangular distribution with parameters:

Minimum	0.10
Likeliest	0.50
Maximum	0.90



Selected range is from 0.10 to 0.90

End of Assumptions

APPENDIX 6: Steady-state model output for Thiram

SIMPLEBOX STEADY-STATE OUTPUT

TABLE 1: ANALYSIS REPORT

DOCUMENTATION

Model version	SimpleBox vs 1.1 (950101); Excel-version
Model files	SIMBOX11.xls(950101); INTEGRAT.exe(940617)
Date and time of analysis	01/26/95 17:27
Analyst	D. van de Meent
Description of the analysis	Calculation steady-state AIR-SOIL concentration ratio for Thiram

DATA USED

COMPOUND	Thiram		SYSTEM	NETHERLANDS	
MOL WEIGHT	250	g.mol-1	SYSTEM AREA	37975	km2
LOG KOW	1.80	-	AREA WATER	4746.875	km2
VAPOR PRESSURE	8.00E-03	Pa	AREA NATURAL SOIL	15760	km2
SOLUBILITY	3.00E-02	g.l-1	AREA AGRICULTURAL SOIL	17089	km2
HENRY'S LAW CONSTANT	6.67E-02	Pa.m3.mol-1	AREA OTHER SOIL	379.75	km2
KP (suspended matter)	6.31E+00	l.kg-1	RESIDENCE TIME AIR	0.40	d
KP (sediment)	3.15E+00	l.kg-1	RESIDENCE TIME WATER	54.5	d
KP (natural soil)	3.15E+00	l.kg-1	EFFLUENT STP	2.81E+06	m3.d-1
KP (agricultural soil)	3.15E+00	l.kg-1	DILUTION FACTOR	1.74E+09	[-]
KP (other soil)	3.15E+00	l.kg-1	SLUDGE PRODUCTION STP	9.55E-02	kg.d-1
DEGRADATION RATE (air)	6.93E-03	d-1	QUALITY STANDARD (water)	1.85E-01	g.l-1
DEGRADATION RATE (water)	1.39E-02	d-1	QUALITY STANDARD (sediment)	5.85E-01	g.kg-1
DEGRADATION RATE (sediment)	3.47E-02	d-1	QUALITY STANDARD (soil)	5.85E-01	g.kg-1
DEGRADATION RATE (soil)	3.47E-02	d-1	QUALITY STANDARD (groundwater)	1.85E-01	g.l-1

FATE

* DIRECT EMISSION TO AIR	4.85E-03	t.y-1	* EXPORT WITH AIR	4.83E-03	t.y-1
* DIRECT EMISSION TO WATER	4.85E-03	t.y-1	* EXPORT WITH WATER	2.77E-03	t.y-1
* DIRECT EMISSION TO SOIL	4.85E-03	t.y-1	TOTAL EXPORT	7.60E-03	t.y-1
* EMISSION from STP to AIR	1.00E-20	t.y-1	* BURIAL IN SEDIMENT	1.17E-07	t.y-1
* EMISSION from STP to WATER	2.00E-20	t.y-1	* LEACHING TO GROUNDWATER	3.47E-04	t.y-1
* EMISSION with WWTP SLUDGE	1.00E-20	t.y-1	TOTAL ACCUMULATION	3.47E-04	t.y-1
TOTAL EMISSIONS	1.46E-02	t.y-1			
			* DEGRADATION in AIR	1.34E-05	t.y-1
* IMPORT with AIR	1.00E-20	t.y-1	* DEGRADATION in WATER	2.09E-03	t.y-1
* IMPORT with WATER	2.00E-20	t.y-1	* DEGRADATION in SEDIMENT	6.56E-05	t.y-1
TOTAL IMPORT	3.00E-20	t.y-1	* DEGRADATION in SOIL	4.44E-03	t.y-1
			TOTAL DEGRADATION	6.61E-03	t.y-1
RESIDENCE TIME	5.32E-02	y			

DISTRIBUTION & RISK

	CONCENTRATION		RISK QUOTIENT		DISTRIBUTION			
AIR	1.39E-13	g.m-3	2.6733E-11	-	5.29E-03	kg	0.7	%
* GAS PHASE	1.38E-13	g.m-3						
* AEROSOL	1.72E-15	g.m-3						
WATER	2.90E-11	g.l-1			4.13E-01	kg	53.4	%
* DISSOLVED	2.90E-11	g.l-1	1.5657E-10	-				
* PARTICULATE	3.21E-15	g.l-1						
SEDIMENT	2.60E-11	g.kg(wet)-1	6.2571E-11	-	5.16E-03	kg	0.7	%
* PORE WATER	1.53E-11	g.l-1						
* SOLID PHASE	4.83E-11	g.kg(dry)-1						
NATURAL SOIL	3.15E-12	g.kg(wet)-1	6.6981E-12	-	3.48E-03	kg	0.4	%
*PORE WATER / GROUNDWATER	1.24E-12	g.l-1						
*SOLID PHASE	3.92E-12	g.kg(dry)-1						
AGRICULTURAL SOIL	7.25E-11	g.kg(wet)-1	1.5402E-10	-	3.47E-01	kg	44.8	%
*PORE WATER / GROUNDWATER	2.85E-11	g.l-1						
*SOLID PHASE	9.01E-11	g.kg(dry)-1						
OTHER SOIL	1.06E-12	g.kg(wet)-1	2.2486E-12	-	2.81E-05	kg	0.0	%
*PORE WATER / GROUNDWATER	4.17E-13	g.l-1						
*SOLID PHASE	1.31E-12	g.kg(dry)-1						
TOTAL					7.74E-01	kg	100.0	%

WATER-AIR concentration ratio	2.08E+02	m3/L-1
WATER-AIR fugacity ratio	3.09E+00	-
SOIL-AIR concentration ratio	2.81E+01	m3/kg(dry)
SOIL-AIR fugacity ratio	2.81E-01	-

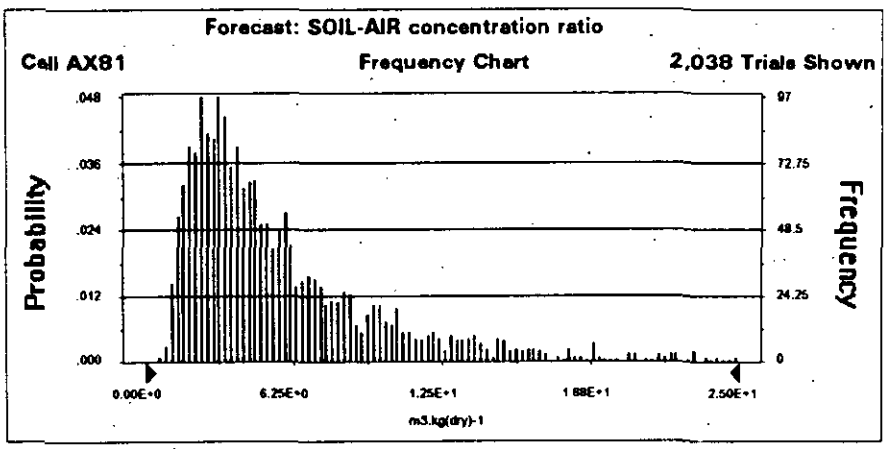
APPENDIX 7: Analysis reports Monte Carlo simulations soil-air concentration ratios

Aldrin

Summary:

Display Range is from 0.00E+0 to 2.50E+1 m3.kg(dry)-1
Entire Range is from 5.52E-1 to 1.10E+2 m3.kg(dry)-1
After 2,079 Trials, the Std. Error of the Mean is 1.49E-1

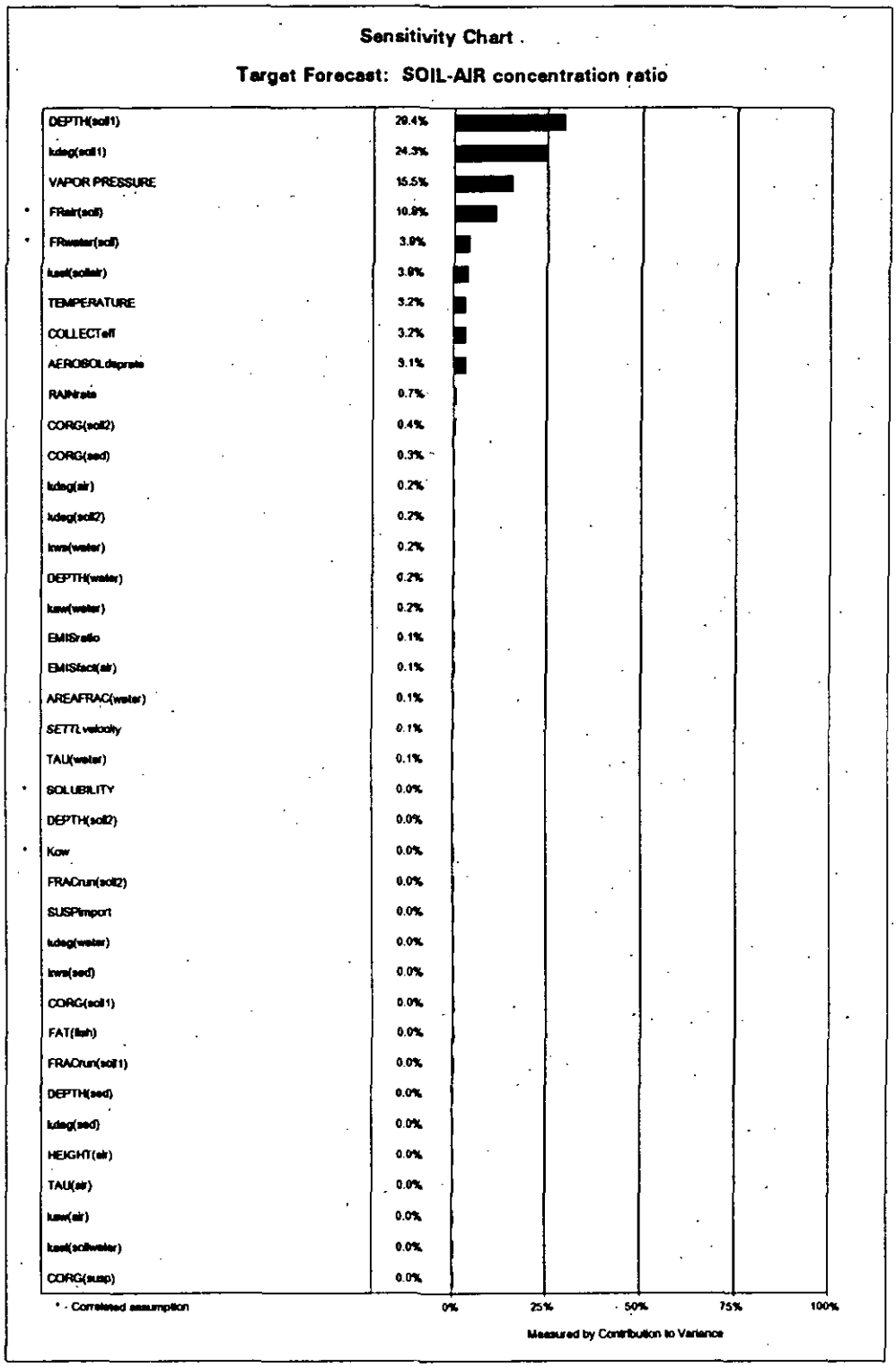
Statistics:	Value
Trials	2079
Mean	6.43E+00
Median (approx.)	4.48E+00
Mode (approx.)	3.28E+00
Standard Deviation	6.78E+00
Variance	4.60E+01
Skewness	5.06
Kurtosis	47.99
Coeff. of Variability	1.05
Range Minimum	5.52E-01
Range Maximum	1.10E+02
Range Width	1.09E+02
Mean Std. Error	1.49E-01



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	5.52E-01
2.5%	1.31E+00
5.0%	1.53E+00
50.0%	4.48E+00
95.0%	1.66E+01
97.5%	2.30E+01
100.0%	1.10E+02

Crystal Ball Report
Simulation started on 95/1/23 at 20:59:14
Simulation stopped on 95/1/23 at 21:16:07

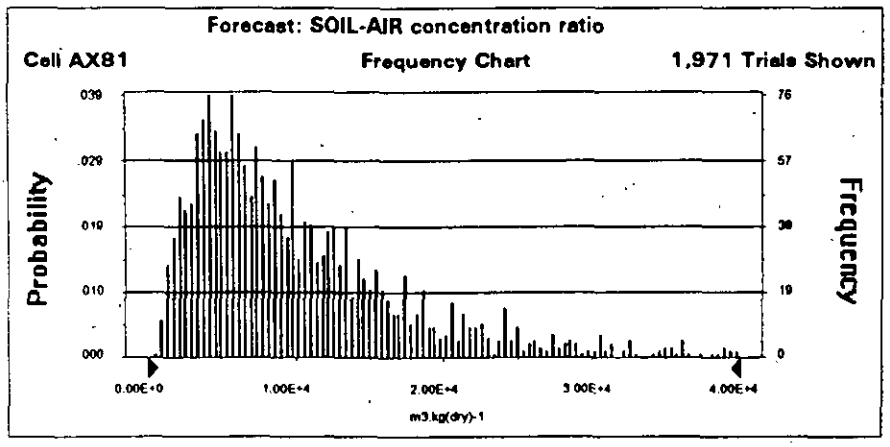


Carbofuran

Summary:

Display Range is from 0.00E+0 to 4.00E+4 m3.kg(dry)-1
Entire Range is from 5.73E+2 to 9.64E+4 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 2.09E+2

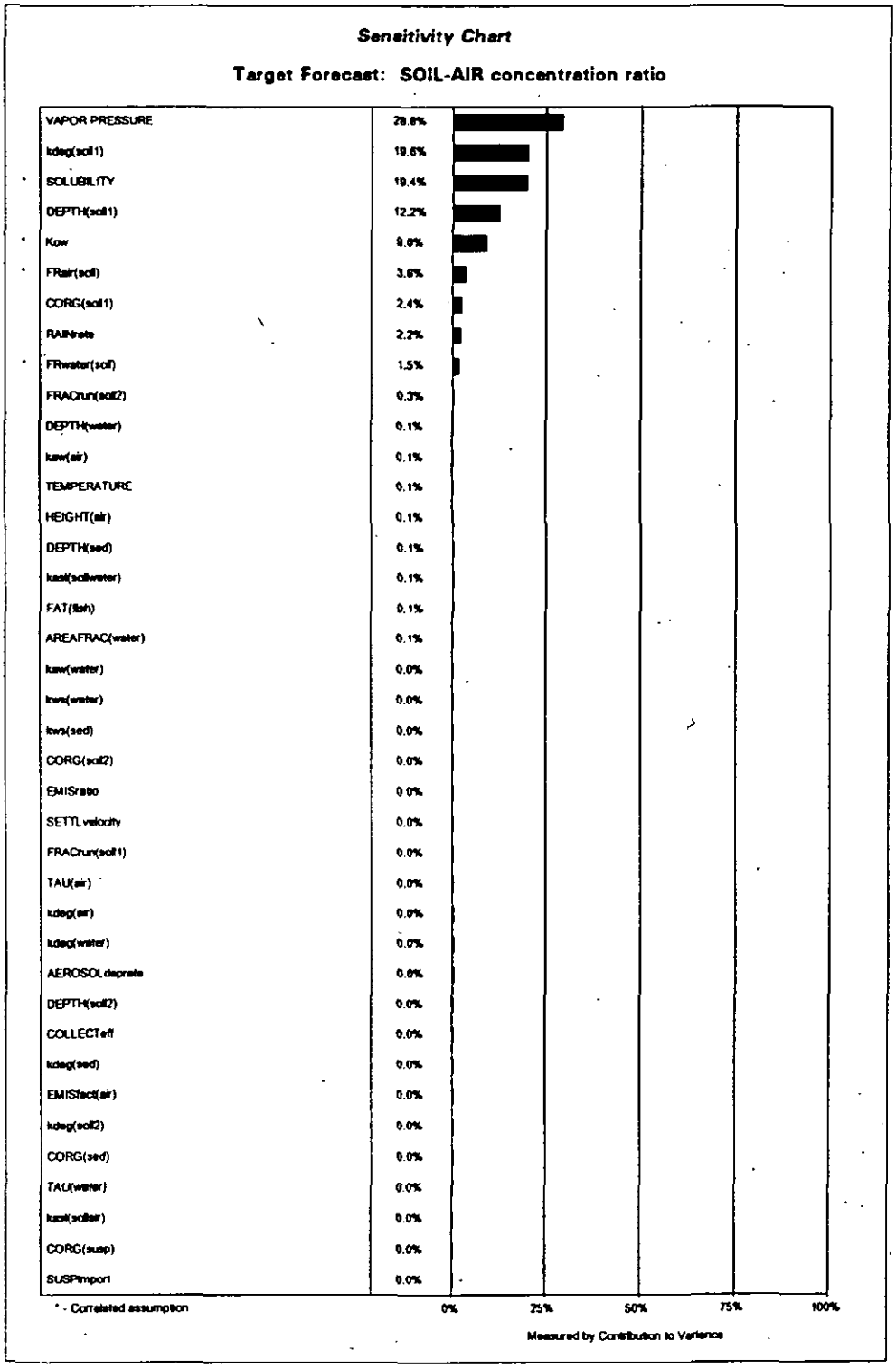
Statistics:	Value
Trials	2000
Mean	1.08E+04
Median (approx.)	8.31E+03
Mode (approx.)	3.93E+03
Standard Deviation	9.34E+03
Variance	8.72E+07
Skewness	3.07
Kurtosis	19.14
Coeff. of Variability	0.86
Range Minimum	5.73E+02
Range Maximum	9.64E+04
Range Width	9.58E+04
Mean Std. Error	2.09E+02



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	5.73E+02
2.5%	1.72E+03
5.0%	2.27E+03
50.0%	8.31E+03
95.0%	2.73E+04
97.5%	3.52E+04
100.0%	9.64E+04

Crystal Ball Report
Simulation started on 95/1/23 at 21:42:12
Simulation stopped on 95/1/23 at 21:53:55

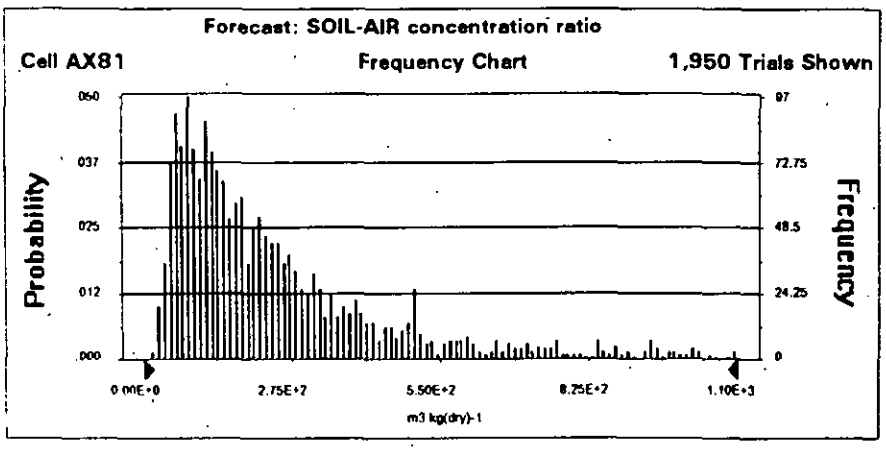


Chlorane

Summary:

Display Range is from 0.00E+0 to 1.10E+3 m3.kg(dry)-1
Entire Range is from 1.40E+1 to 4.20E+3 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 6.79E+0

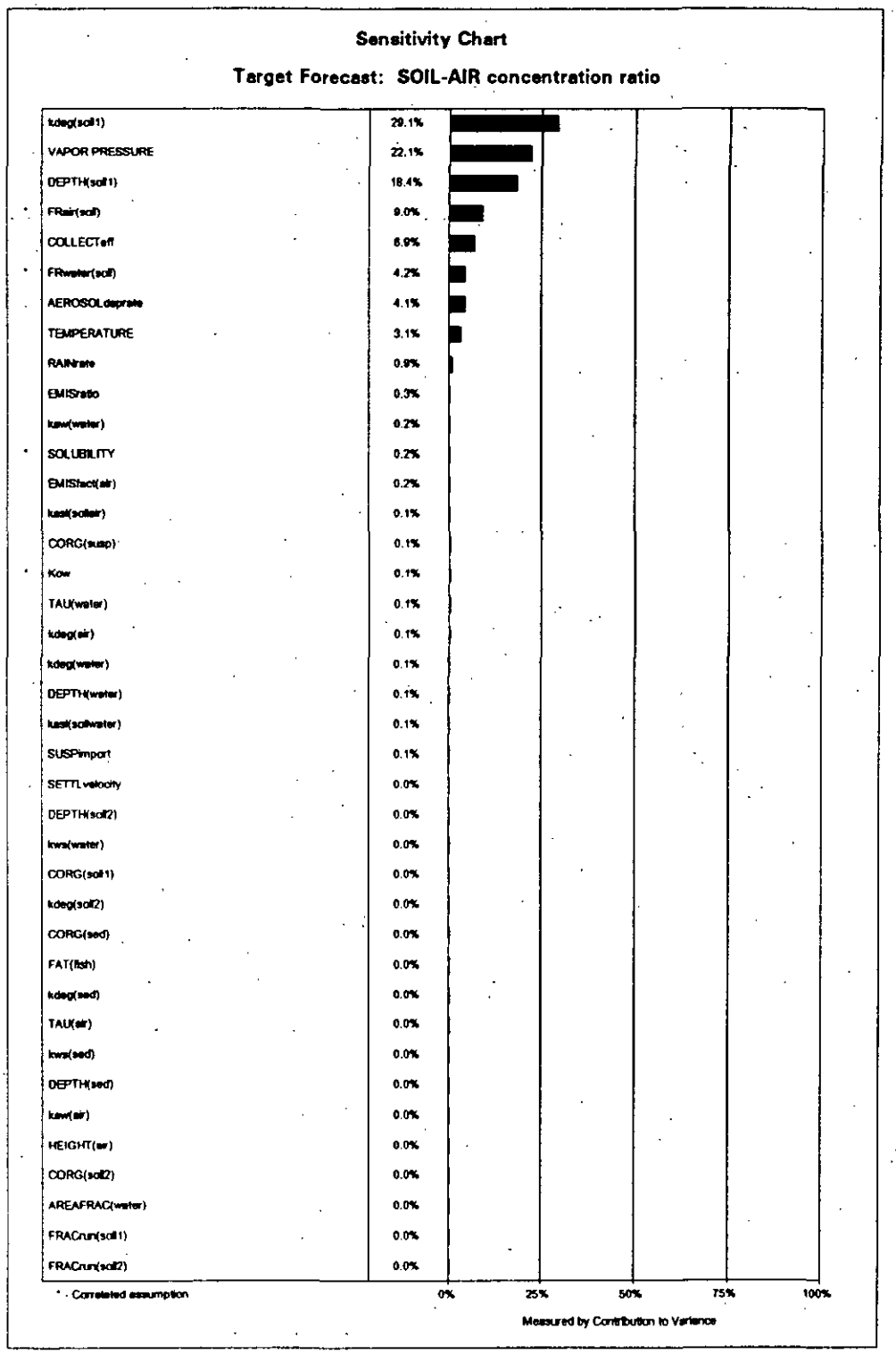
Statistics:	Value
Trials	2000
Mean	2.79E+02
Median (approx.)	1.84E+02
Mode (approx.)	7.68E+01
Standard Deviation	3.04E+02
Variance	9.23E+04
Skewness	3.70
Kurtosis	27.09
Coeff. of Variability	1.09
Range Minimum	1.40E+01
Range Maximum	4.20E+03
Range Width	4.19E+03
Mean Std. Error	6.79E+00



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	1.40E+01
2.5%	4.08E+01
5.0%	4.96E+01
50.0%	1.84E+02
95.0%	8.68E+02
97.5%	1.10E+03
100.0%	4.20E+03

Crystal Ball Report
Simulation started on 95/1/23 at 22:13:14
Simulation stopped on 95/1/23 at 22:28:17

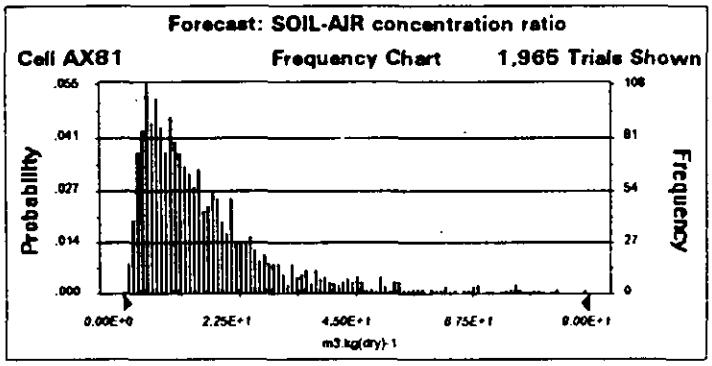


Chlorpyrifos

Summary:

Display Range is from 0.00E+0 to 9.00E+1 m3.kg(dry)-1
Entire Range is from 6.37E-1 to 4.51E+2 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 5.23E-1

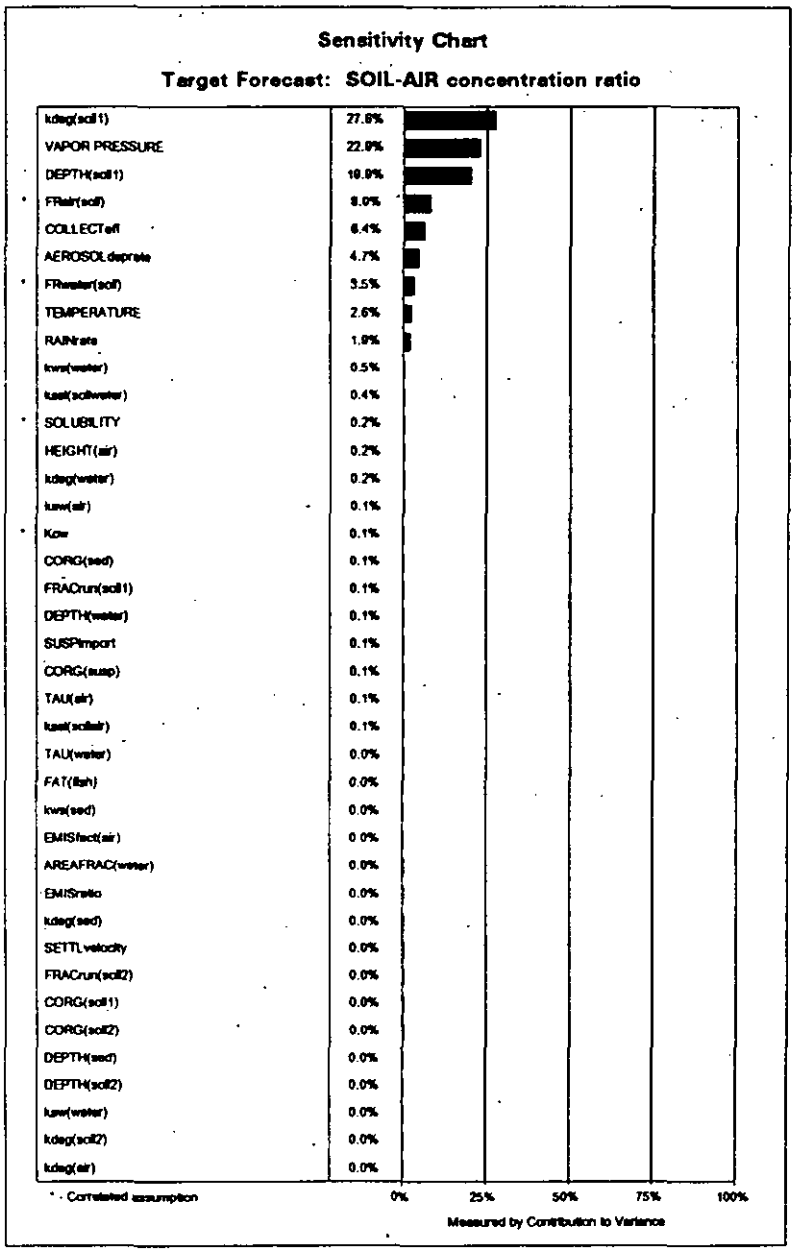
Statistics:	Value
Trials	2000
Mean	1.92E+01
Median (approx.)	1.28E+01
Mode (approx.)	7.39E+00
Standard Deviation	2.34E+01
Variance	5.46E+02
Skewness	6.16
Kurtosis	77.31
Coeff. of Variability	1.22
Range Minimum	6.37E-01
Range Maximum	4.51E+02
Range Width	4.50E+02
Mean Std. Error	5.23E-01



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	6.37E-01
2.5%	2.45E+00
5.0%	3.17E+00
50.0%	1.28E+01
95.0%	5.52E+01
97.5%	7.67E+01
100.0%	4.51E+02

Crystal Ball Report
Simulation started on 1/24/95 at 14:49:25
Simulation stopped on 1/24/95 at 15:05:60

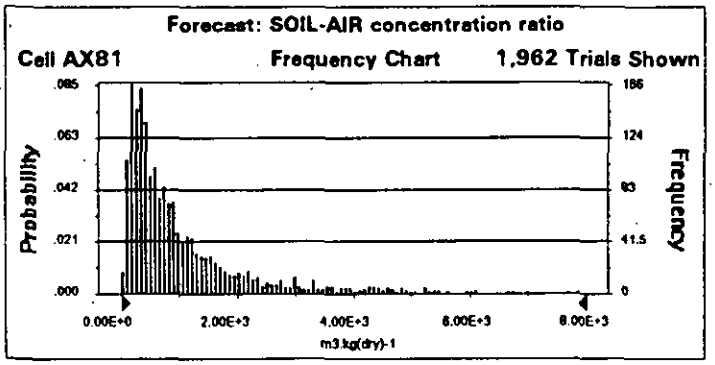


p,p'-DDD

Summary:

Display Range is from 0.00E+0 to 8.00E+3 m3.kg(dry)-1
Entire Range is from 4.49E+1 to 3.55E+4 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 5.20E+1

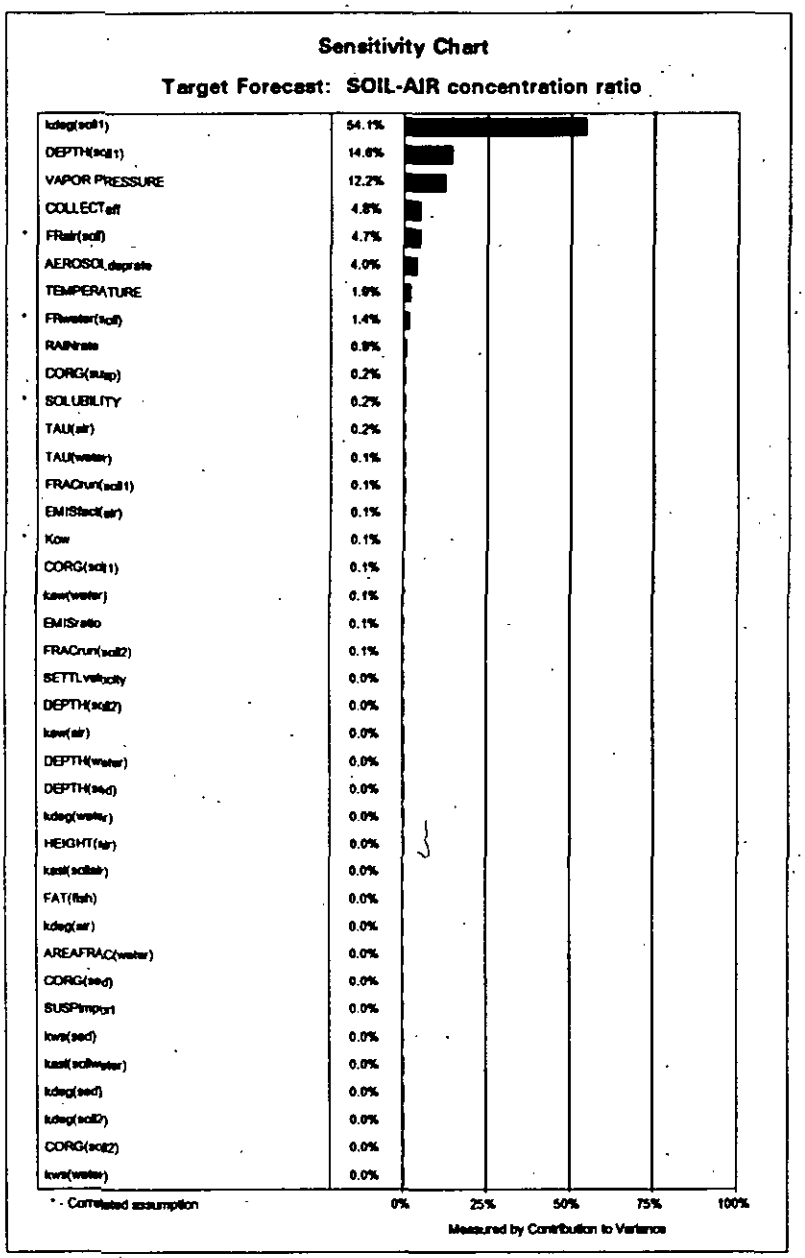
Statistics:	Value
Trials	2000
Mean	1.40E+03
Median (approx.)	7.08E+02
Mode (approx.)	2.22E+02
Standard Deviation	2.33E+03
Variance	5.42E+06
Skewness	5.99
Kurtosis	57.50
Coeff. of Variability	1.67
Range Minimum	4.49E+01
Range Maximum	3.55E+04
Range Width	3.55E+04
Mean Std. Error	5.20E+01



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	4.49E+01
2.5%	8.97E+01
5.0%	1.34E+02
50.0%	7.08E+02
95.0%	4.73E+03
97.5%	6.79E+03
100.0%	3.55E+04

Crystal Ball Report
Simulation started on 1/25/95 at 14:38:08
Simulation stopped on 1/25/95 at 14:50:03

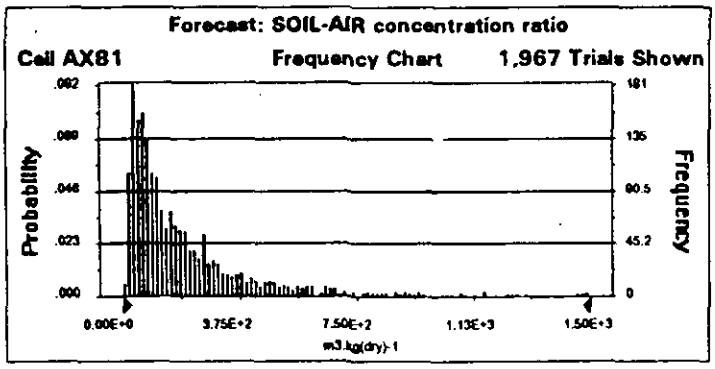


p,p'-DDE

Summary:

Display Range is from 0.00E+0 to 1.50E+3 m3.kg(dry)-1
Entire Range is from 7.51E+0 to 7.97E+3 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 9.47E+0

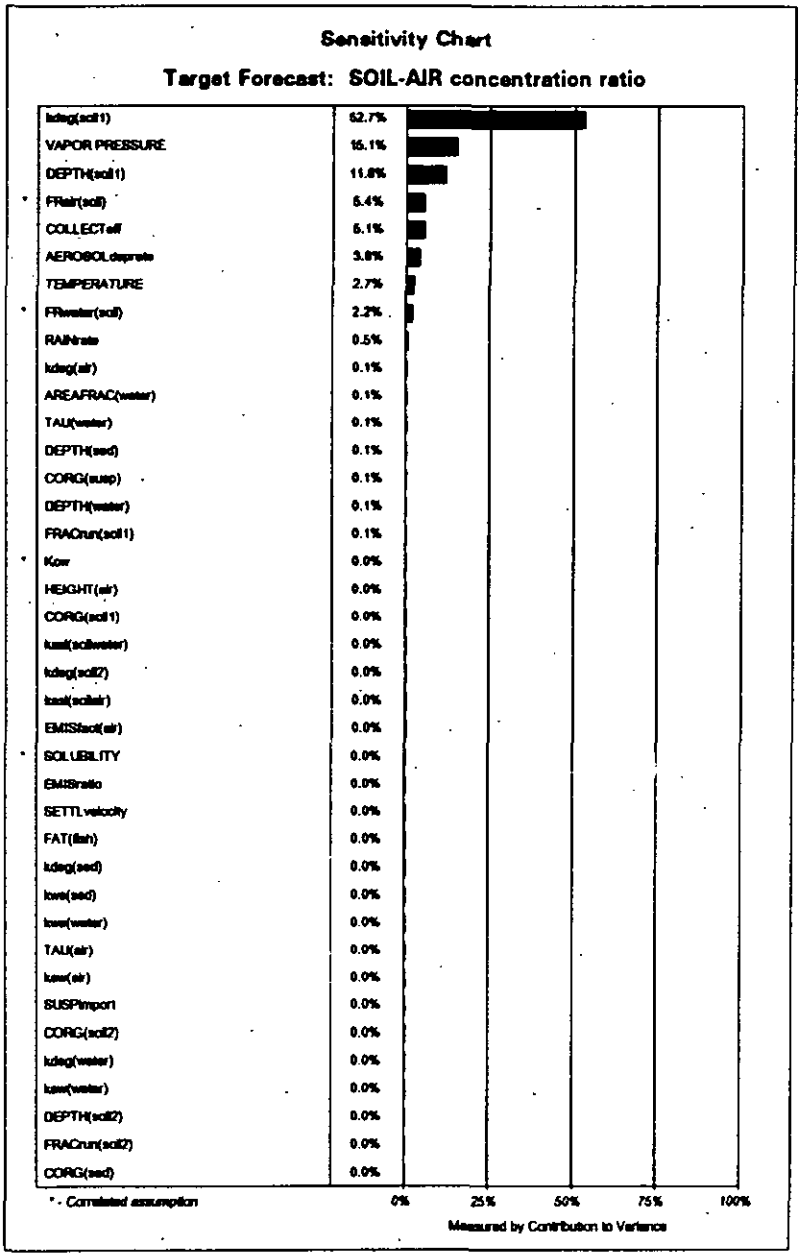
Statistics:	Value
Trials	2000
Mean	2.53E+02
Median (approx.)	1.31E+02
Mode (approx.)	4.73E+01
Standard Deviation	4.23E+02
Variance	1.79E+05
Skewness	7.03
Kurtosis	85.87
Coeff. of Variability	1.67
Range Minimum	7.51E+00
Range Maximum	7.97E+03
Range Width	7.96E+03
Mean Std. Error	9.47E+00



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	7.51E+00
2.5%	1.59E+01
5.0%	2.42E+01
50.0%	1.31E+02
95.0%	8.74E+02
97.5%	1.28E+03
100.0%	7.97E+03

Crystal Ball Report
Simulation started on 1/25/95 at 15:00:26
Simulation stopped on 1/25/95 at 15:13:08

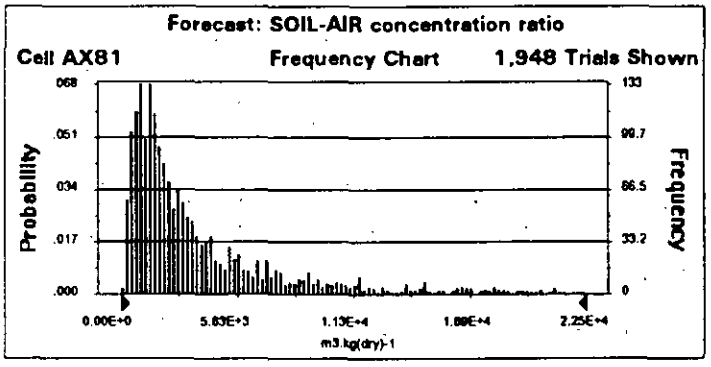


p,p'-DDT

Summary:

Display Range is from 0.00E+0 to 2.25E+4 m3.kg(dry)-1
Entire Range is from 1.38E+2 to 8.40E+4 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 1.48E+2

Statistics:	Value
Trials	2000
Mean	4.68E+03
Median (approx.)	2.45E+03
Mode (approx.)	1.40E+03
Standard Deviation	6.62E+03
Variance	4.38E+07
Skewness	4.49
Kurtosis	35.25
Coeff. of Variability	1.42
Range Minimum	1.38E+02
Range Maximum	8.40E+04
Range Width	8.39E+04
Mean Std. Error	1.48E+02



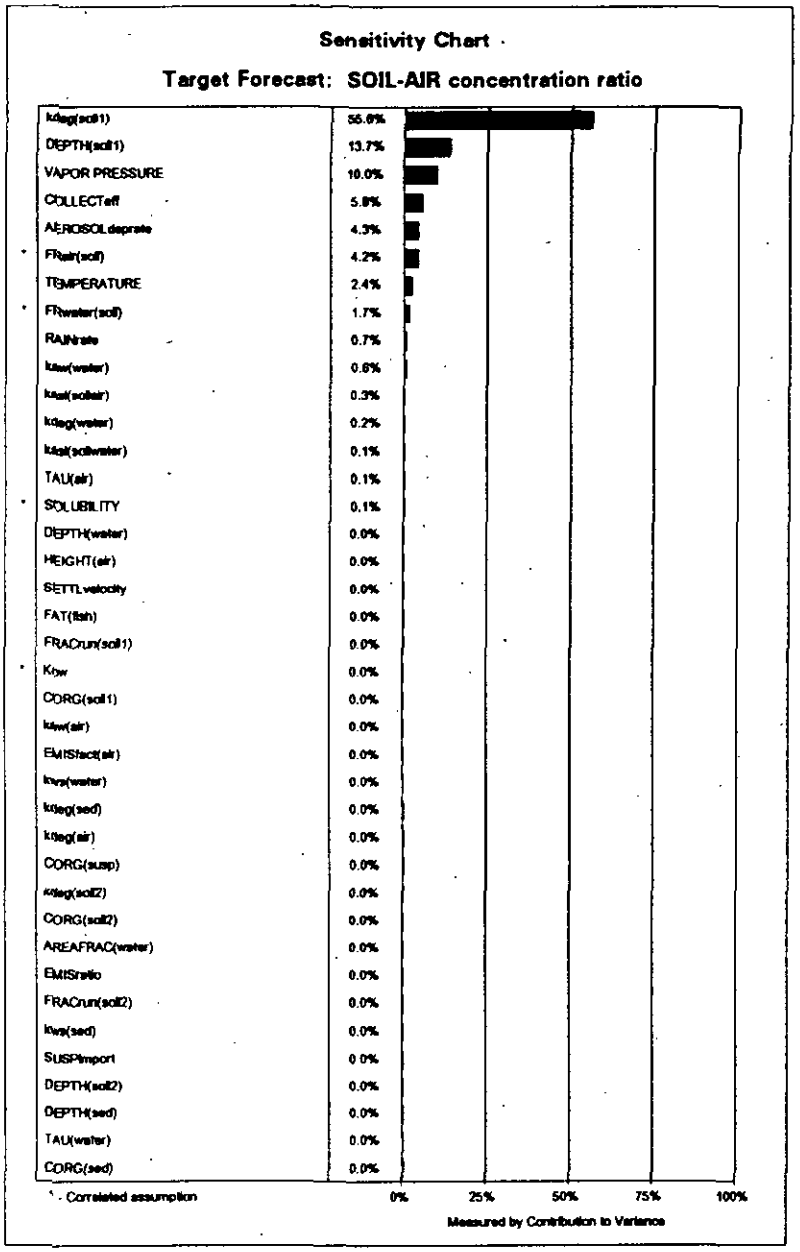
Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	1.38E+02
2.5%	3.88E+02
5.0%	5.25E+02
50.0%	2.45E+03
95.0%	1.67E+04
97.5%	2.27E+04
100.0%	8.40E+04

Crystal Ball Report

Simulation started on 1/24/95 at 17:39:40

Simulation stopped on 1/24/95 at 18:02:43

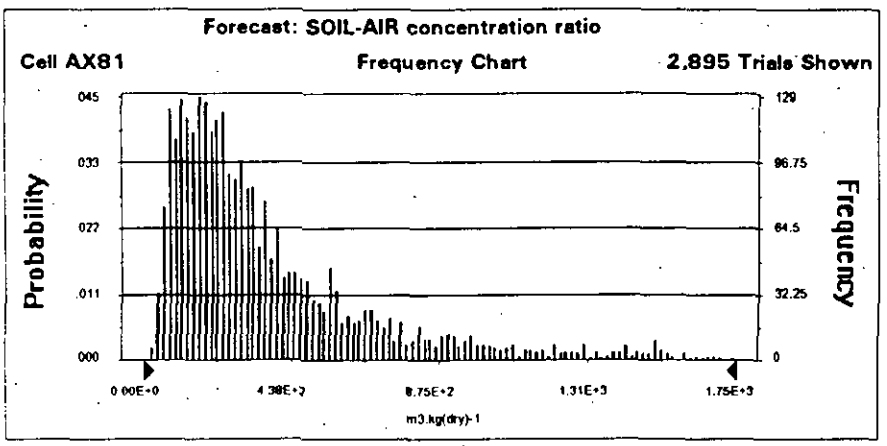


Dieldrin

Summary:

Display Range is from 0.00E+0 to 1.75E+3 m3.kg(dry)-1
Entire Range is from 2.21E+1 to 7.24E+3 m3.kg(dry)-1
After 2,949 Trials, the Std. Error of the Mean is 8.40E+0

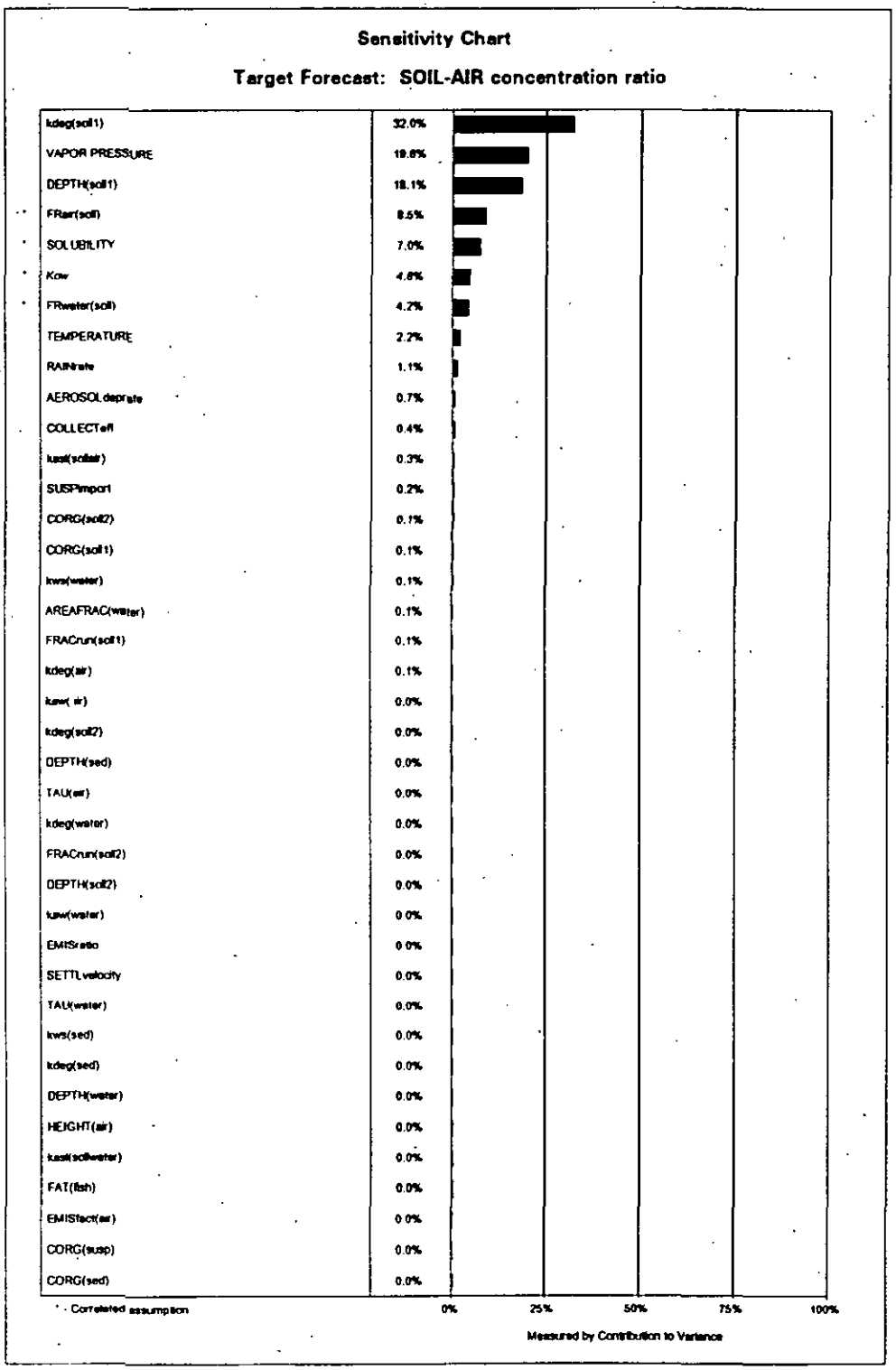
Statistics:	Value
Trials	2949
Mean	4.11E+02
Median (approx.)	2.76E+02
Mode (approx.)	1.30E+02
Standard Deviation	4.55E+02
Variance	2.07E+05
Skewness	4.58
Kurtosis	41.45
Coeff. of Variability	1.11
Range Minimum	2.21E+01
Range Maximum	7.24E+03
Range Width	7.21E+03
Mean Std. Error	8.37E+00



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	2.21E+01
2.5%	5.90E+01
5.0%	7.48E+01
50.0%	2.76E+02
95.0%	1.21E+03
97.5%	1.53E+03
100.0%	7.24E+03

Crystal Ball Report
Simulation started on 95/1/24 at 20:33:49
Simulation stopped on 95/1/24 at 21:03:29

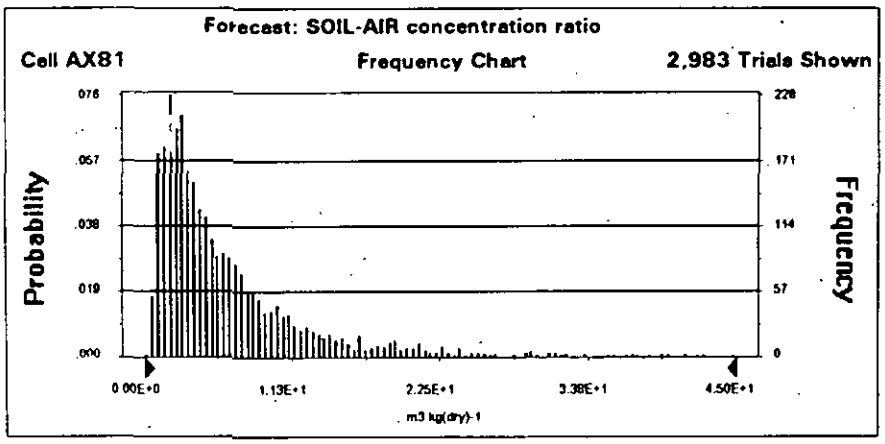


Endosulfan

Summary:

Display Range is from 0.00E+0 to 4.50E+1 m3.kg(dry)-1
Entire Range is from 4.28E-1 to 3.30E+2 m3.kg(dry)-1
After 3,013 Trials, the Std. Error of the Mean is 2.53E-1

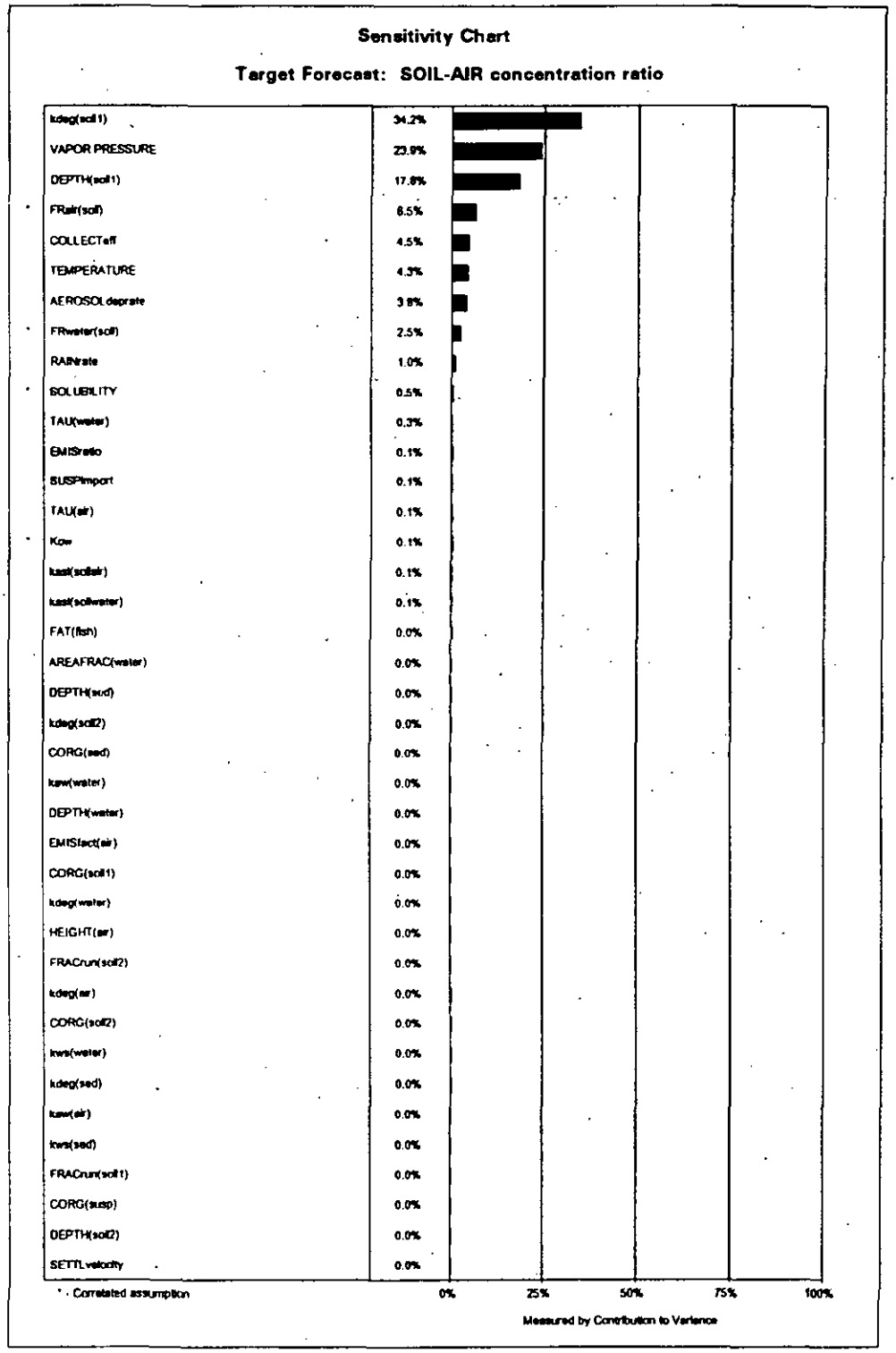
Statistics:	Value
Trials	3013
Mean	7.67E+00
Median (approx.)	4.57E+00
Mode (approx.)	2.07E+00
Standard Deviation	1.39E+01
Variance	1.92E+02
Skewness	13.57
Kurtosis	276.65
Coeff. of Variability	1.81
Range Minimum	4.28E-01
Range Maximum	3.30E+02
Range Width	3.29E+02
Mean Std. Error	2.53E-01



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	4.28E-01
2.5%	6.95E-01
5.0%	9.63E-01
50.0%	4.57E+00
95.0%	2.20E+01
97.5%	3.16E+01
100.0%	3.30E+02

Crystal Ball Report
Simulation started on 95/1/24 at 21:35:53
Simulation stopped on 95/1/24 at 22:04:26

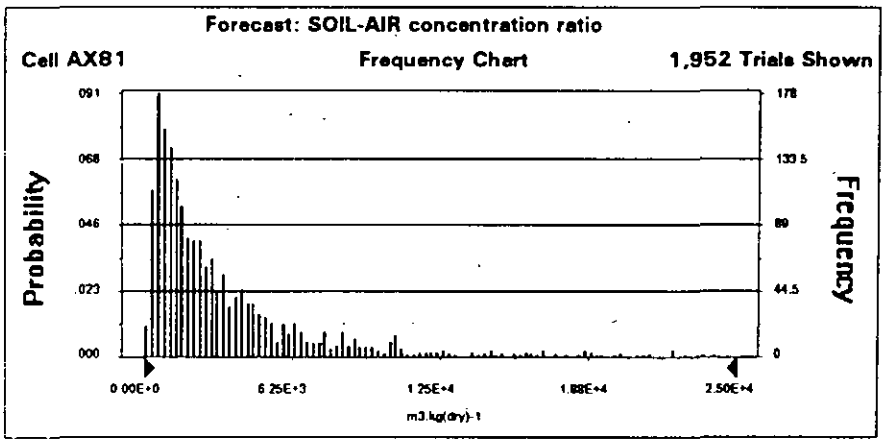


Endrin

Summary:

Display Range is from 0.00E+0 to 2.50E+4 m3.kg(dry)-1
Entire Range is from 1.24E+2 to 9.63E+4 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 1.61E+2

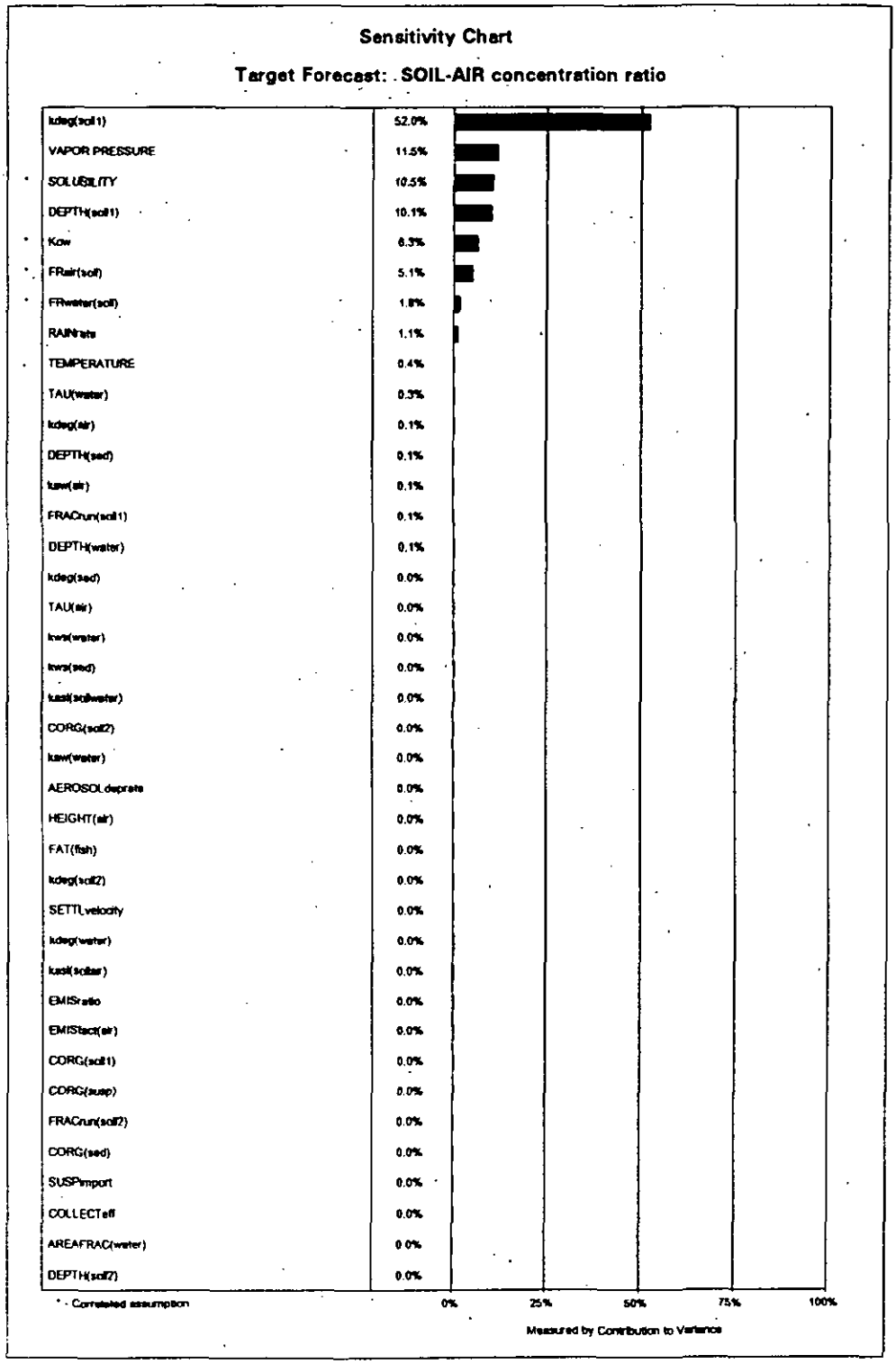
Statistics:	Value
Trials	2000
Mean	4.56E+03
Median (approx.)	2.27E+03
Mode (approx.)	6.05E+02
Standard Deviation	7.20E+03
Variance	5.19E+07
Skewness	4.79
Kurtosis	37.63
Coeff. of Variability	1.58
Range Minimum	1.24E+02
Range Maximum	9.63E+04
Range Width	9.61E+04
Mean Std. Error	1.61E+02



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	1.24E+02
2.5%	2.91E+02
5.0%	4.51E+02
50.0%	2.27E+03
95.0%	1.79E+04
97.5%	2.45E+04
100.0%	9.63E+04

Crystal Ball Report
Simulation started on 95/1/24 at 22:16:11
Simulation stopped on 95/1/24 at 22:35:40

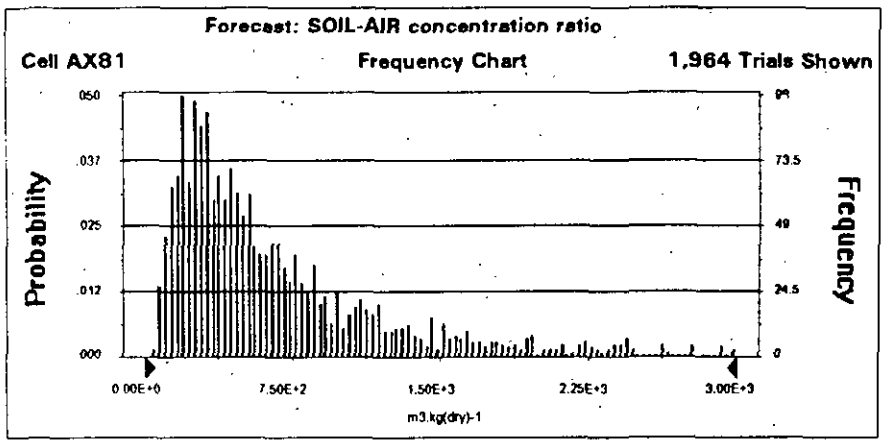


Fenthion

Summary:

Display Range is from 0.00E+0 to 3.00E+3 m3.kg(dry)-1
Entire Range is from 4.26E+1 to 1.11E+4 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 1.76E+1

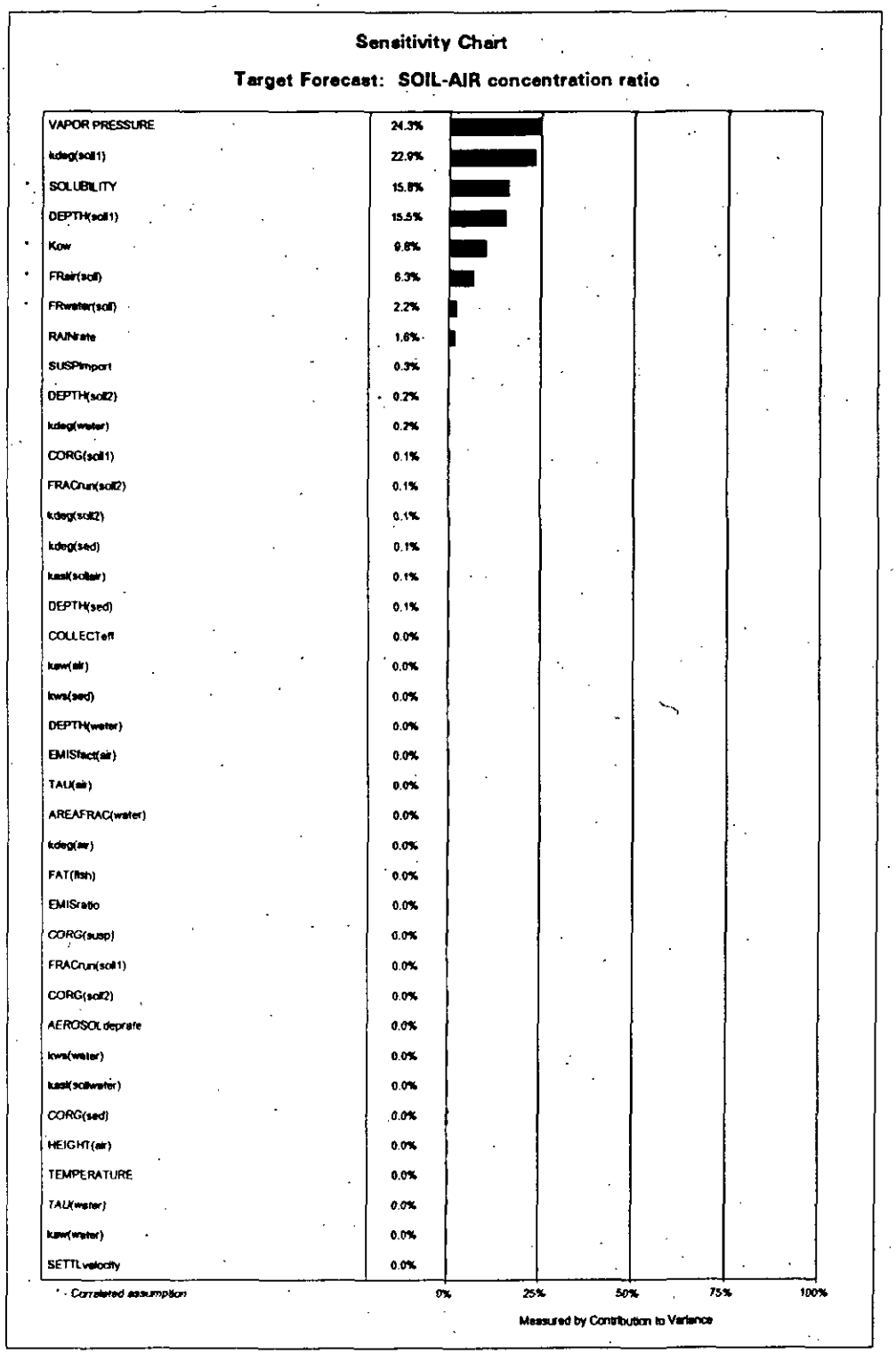
Statistics:	Value
Trials	2000
Mean	7.45E+02
Median (approx.)	4.98E+02
Mode (approx.)	3.19E+02
Standard Deviation	7.88E+02
Variance	6.21E+05
Skewness	3.99
Kurtosis	33.47
Coeff. of Variability	1.06
Range Minimum	4.26E+01
Range Maximum	1.11E+04
Range Width	1.10E+04
Mean Std. Error	1.76E+01



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	4.26E+01
2.5%	1.00E+02
5.0%	1.30E+02
50.0%	4.98E+02
95.0%	2.23E+03
97.5%	2.77E+03
100.0%	1.11E+04

Crystal Ball Report
Simulation started on 95/1/24 at 22:53:32
Simulation stopped on 95/1/24 at 23:12:58

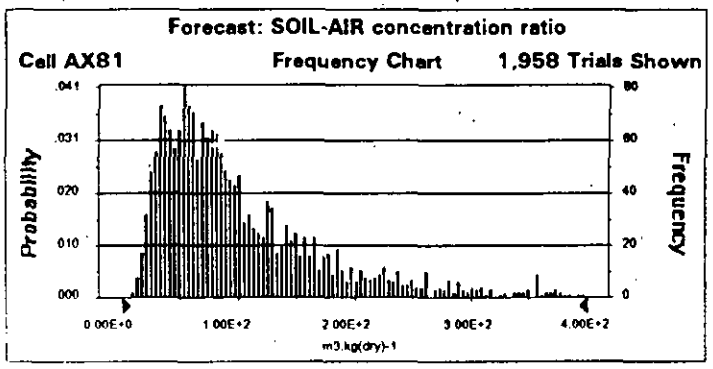


α-HCH

Summary:

Display Range is from 0.00E+0 to 4.00E+2 m3.kg(dry)-1
Entire Range is from 1.08E+1 to 1.64E+3 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 2.22E+0

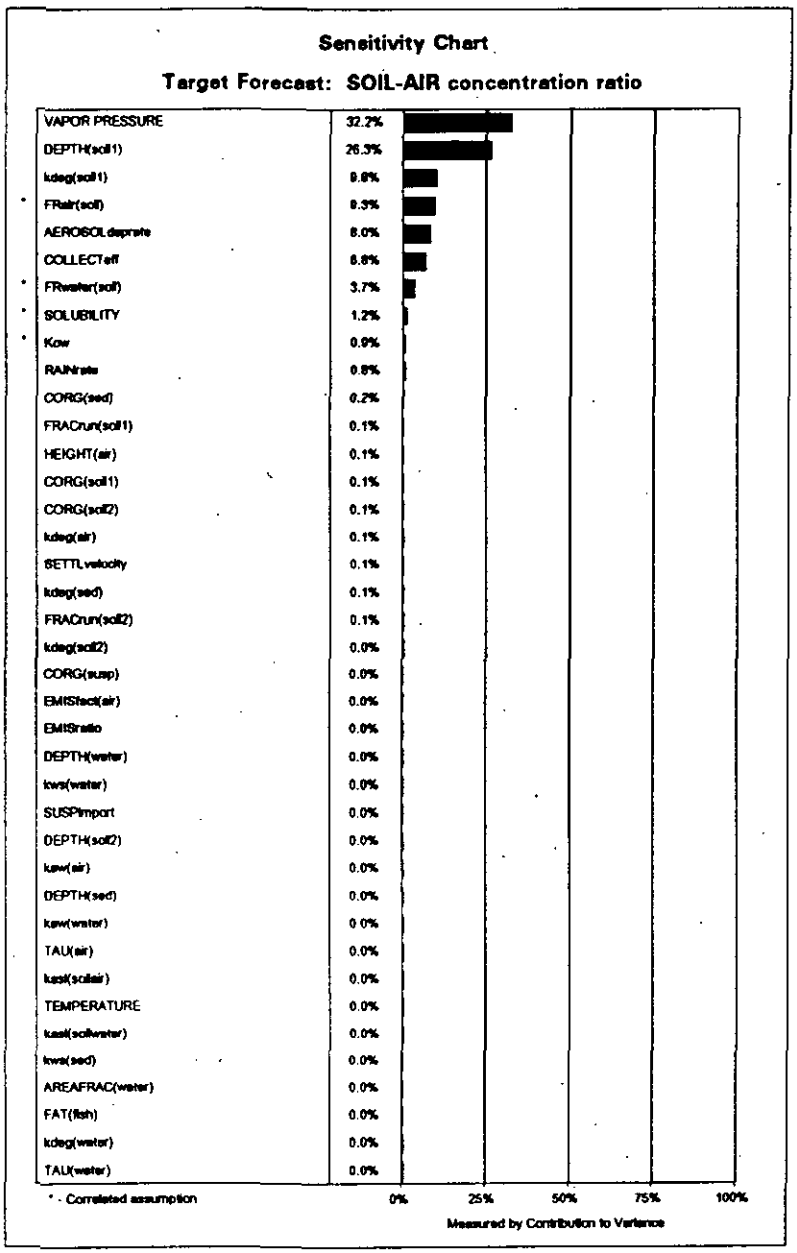
Statistics:	Value
Trials	2000
Mean	1.12E+02
Median (approx.)	8.27E+01
Mode (approx.)	5.16E+01
Standard Deviation	9.93E+01
Variance	9.86E+03
Skewness	3.95
Kurtosis	38.15
Coeff. of Variability	0.89
Range Minimum	1.08E+01
Range Maximum	1.64E+03
Range Width	1.63E+03
Mean Std. Error	2.22E+00



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	1.08E+01
2.5%	2.25E+01
5.0%	2.73E+01
50.0%	8.27E+01
95.0%	2.91E+02
97.5%	3.73E+02
100.0%	1.64E+03

Crystal Ball Report
Simulation started on 1/25/95 at 13:01:48
Simulation stopped on 1/25/95 at 13:25:32

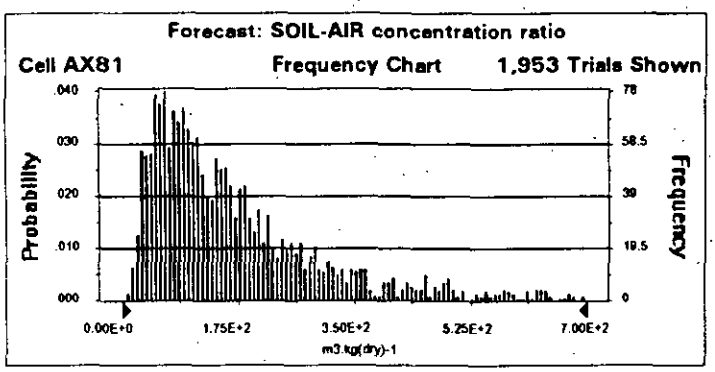


β-HCH

Summary:

Display Range is from 0.00E+0 to 7.00E+2 m3.kg(dry)-1
Entire Range is from 1.37E+1 to 2.91E+3 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 4.34E+0

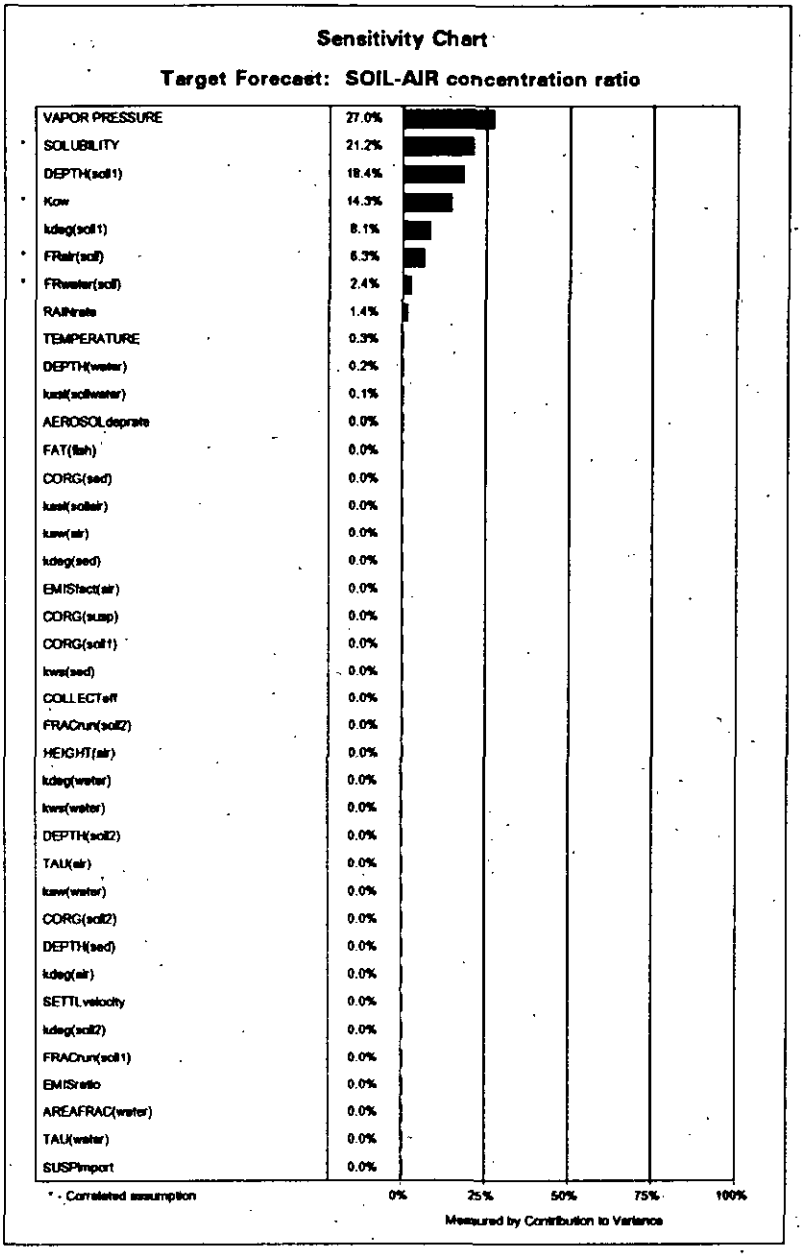
Statistics:	Value
Trials	2000
Mean	1.93E+02
Median (approx.)	1.38E+02
Mode (approx.)	5.72E+01
Standard Deviation	1.94E+02
Variance	3.76E+04
Skewness	3.95
Kurtosis	33.61
Coeff. of Variability	1.01
Range Minimum	1.37E+01
Range Maximum	2.91E+03
Range Width	2.90E+03
Mean Std. Error	4.34E+00



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	1.37E+01
2.5%	2.82E+01
5.0%	3.58E+01
50.0%	1.38E+02
95.0%	5.51E+02
97.5%	6.85E+02
100.0%	2.91E+03

Crystal Ball Report
Simulation started on 1/25/95 at 14:12:03
Simulation stopped on 1/25/95 at 14:22:51

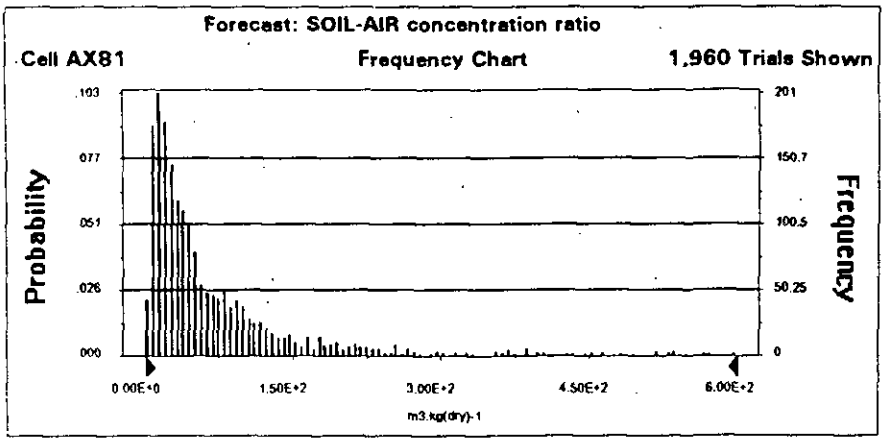


γ-HCH

Summary:

Display Range is from 0.00E+0 to 6.00E+2 m3.kg(dry)-1
Entire Range is from 1.54E+0 to 3.13E+3 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 4.06E+0

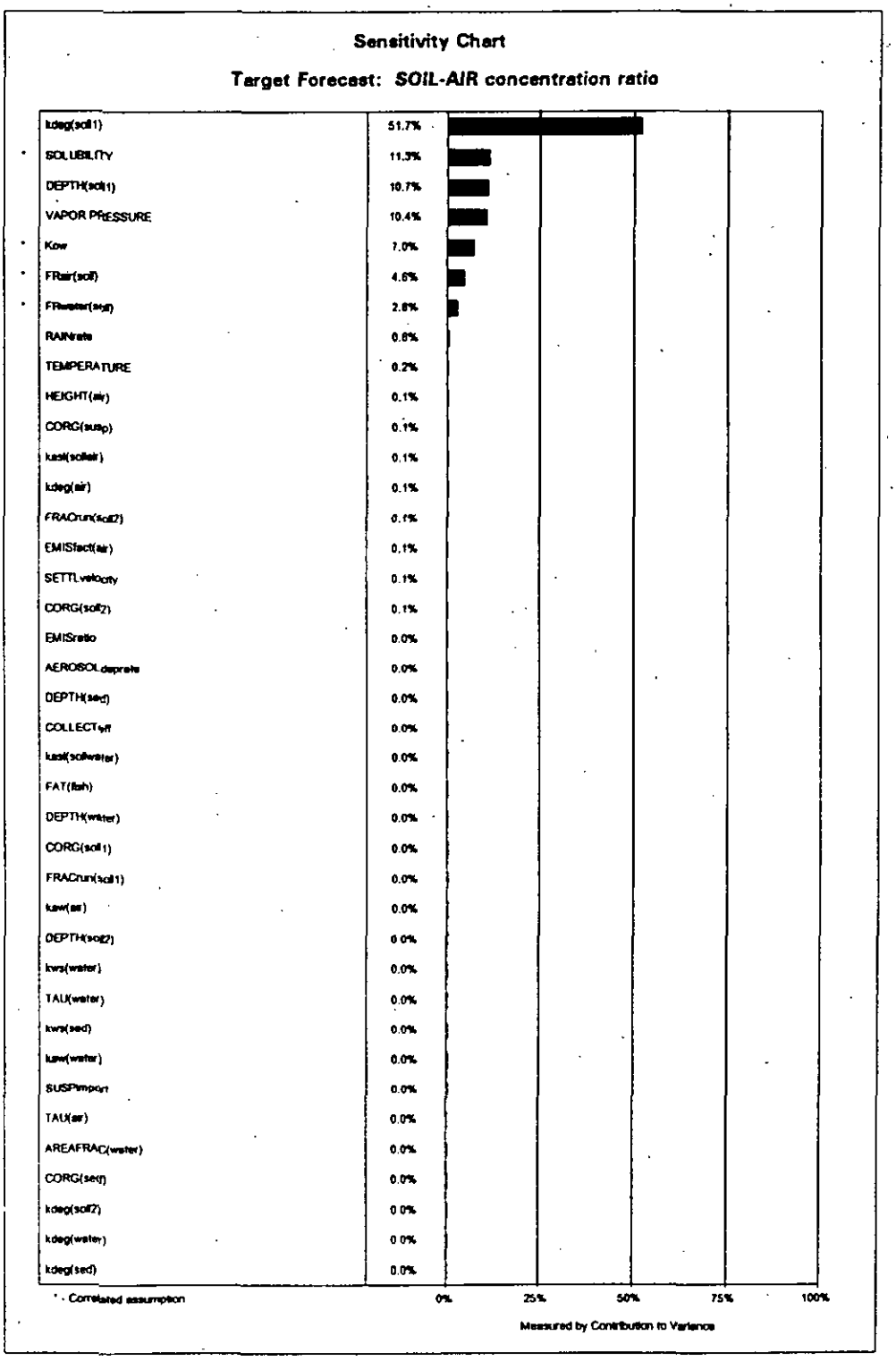
Statistics:	Value
Trials	2000
Mean	9.81E+01
Median (approx.)	4.33E+01
Mode (approx.)	1.72E+01
Standard Deviation	1.82E+02
Variance	3.30E+04
Skewness	6.55
Kurtosis	71.90
Coeff. of Variability	1.85
Range Minimum	1.54E+00
Range Maximum	3.13E+03
Range Width	3.12E+03
Mean Std. Error	4.06E+00



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	1.54E+00
2.5%	3.97E+00
5.0%	6.39E+00
50.0%	4.33E+01
95.0%	3.82E+02
97.5%	5.48E+02
100.0%	3.13E+03

Crystal Ball Report
Simulation started on 95/1/24 at 23:25:27
Simulation stopped on 95/1/24 at 23:45:19

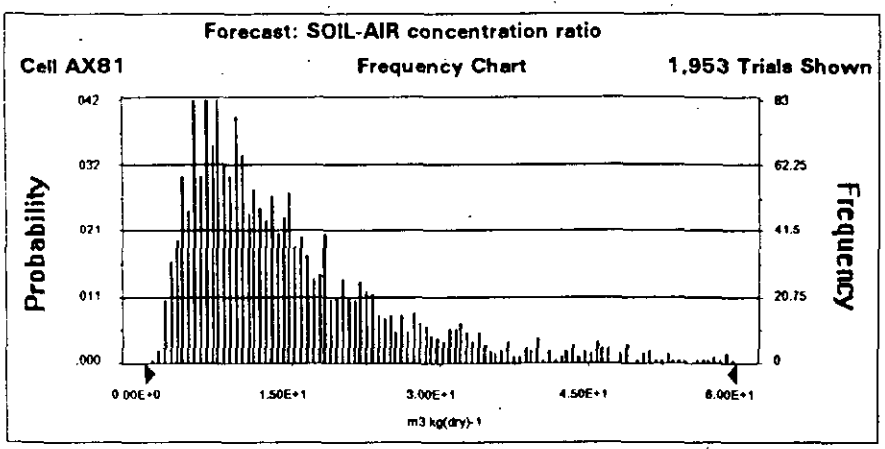


Heptachlor

Summary:

Display Range is from 0.00E+0 to 6.00E+1 m3.kg(dry)-1
Entire Range is from 1.12E+0 to 1.77E+2 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 3.54E-1

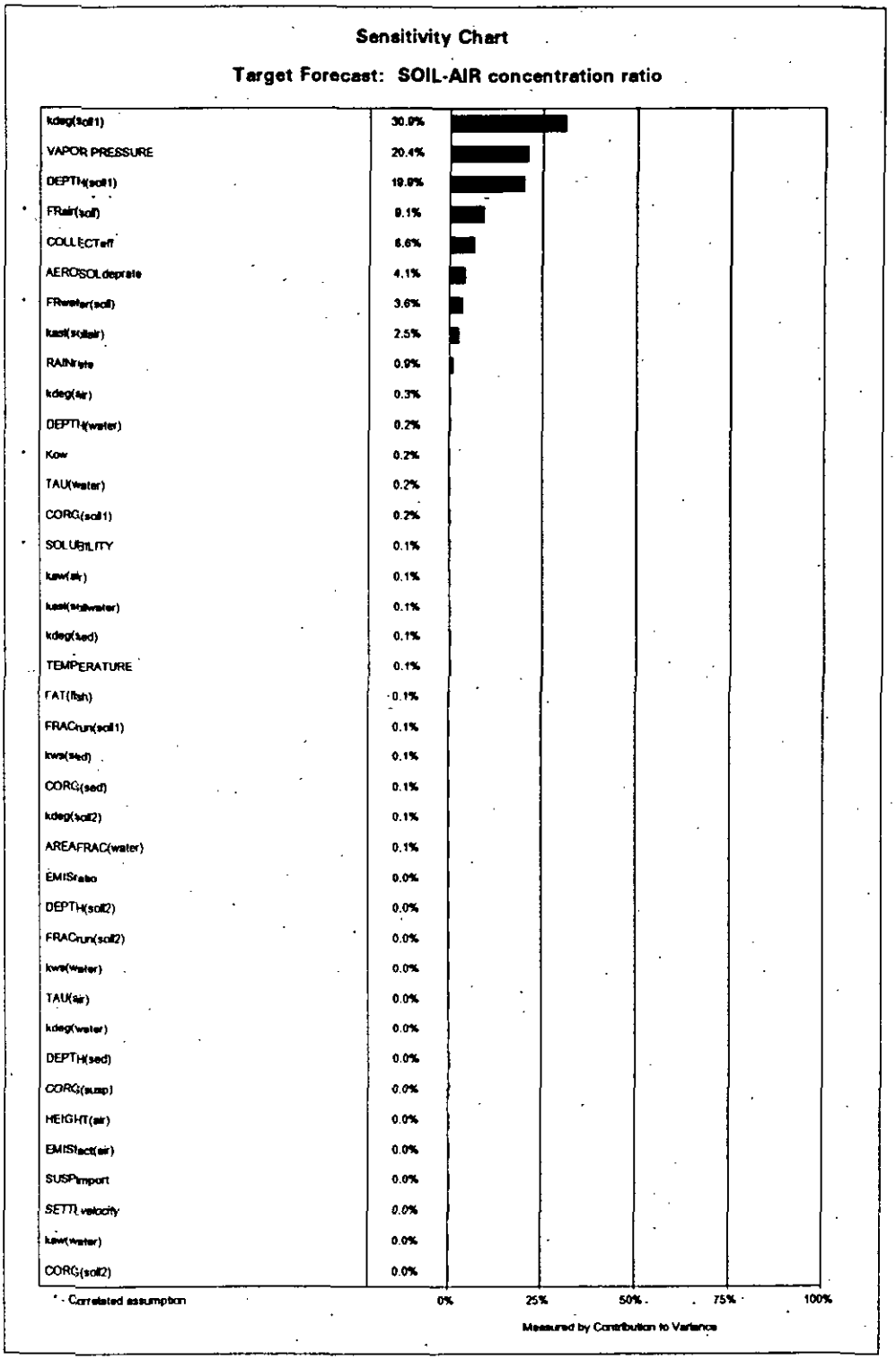
Statistics:	Value
Trials	2000
Mean	1.65E+01
Median (approx.)	1.21E+01
Mode (approx.)	7.26E+00
Standard Deviation	1.58E+01
Variance	2.51E+02
Skewness	3.63
Kurtosis	24.81
Coeff. of Variability	0.96
Range Minimum	1.12E+00
Range Maximum	1.77E+02
Range Width	1.75E+02
Mean Std. Error	3.54E-01



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	1.12E+00
2.5%	2.92E+00
5.0%	3.62E+00
50.0%	1.21E+01
95.0%	4.56E+01
97.5%	5.90E+01
100.0%	1.77E+02

Crystal Ball Report
Simulation started on 95/1/24 at 23:54:13
Simulation stopped on 95/1/25 at 0:13:54

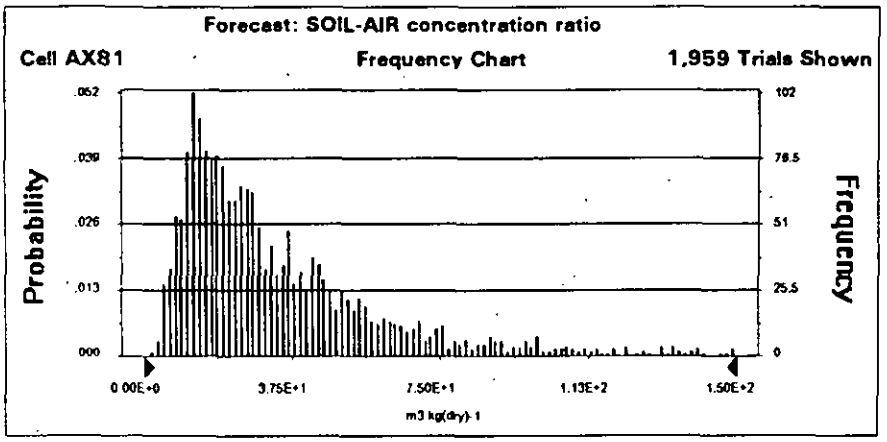


Heptachlor epoxide

Summary:

Display Range is from 0.00E+0 to 1.50E+2 m3.kg(dry)-1
Entire Range is from 2.64E+0 to 4.31E+2 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 7.74E-1

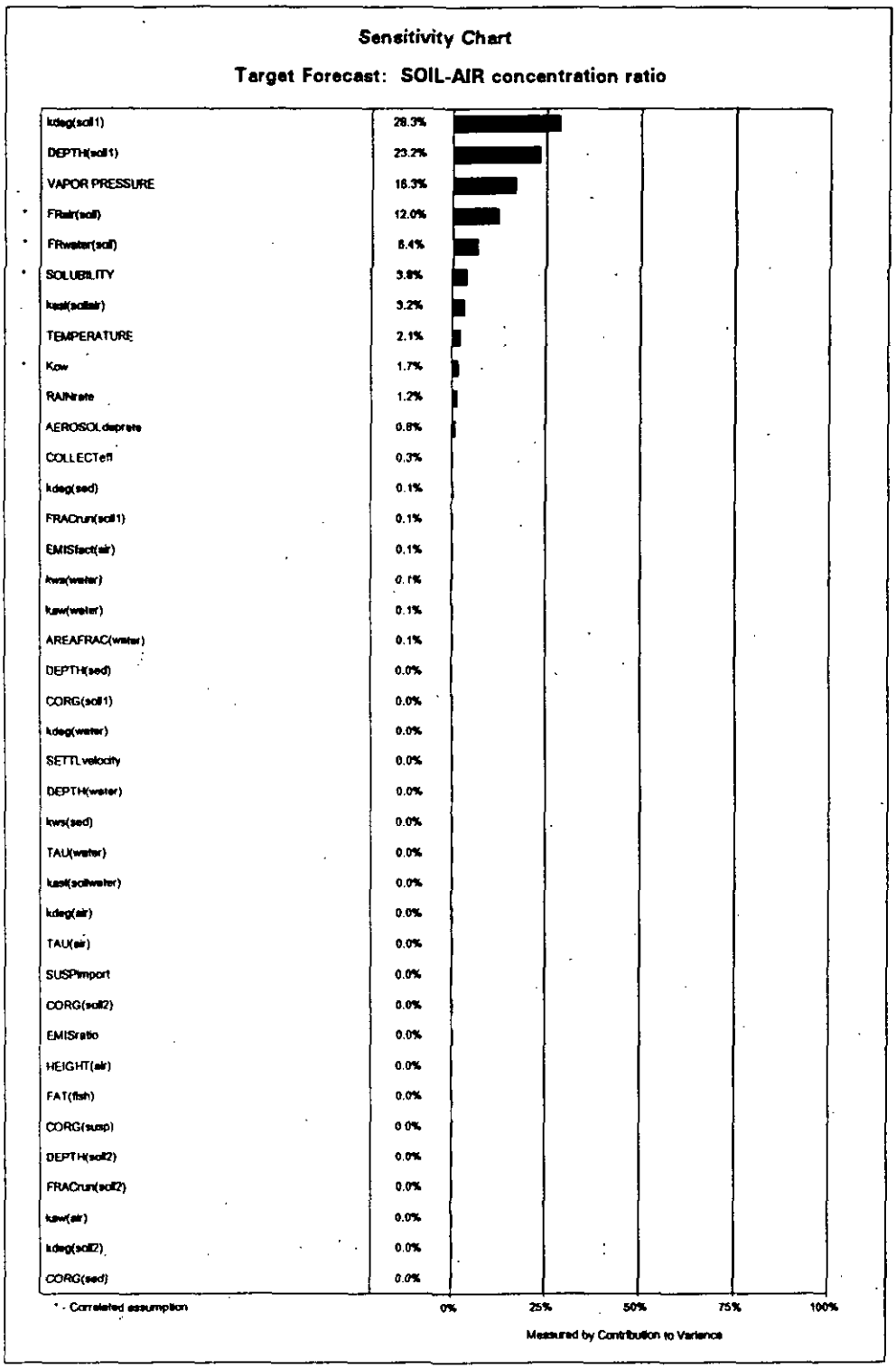
Statistics:	Value
Trials	2000
Mean	3.75E+01
Median (approx.)	2.67E+01
Mode (approx.)	1.34E+01
Standard Deviation	3.46E+01
Variance	1.20E+03
Skewness	3.00
Kurtosis	18.35
Coeff. of Variability	0.92
Range Minimum	2.64E+00
Range Maximum	4.31E+02
Range Width	4.28E+02
Mean Std. Error	7.74E-01



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	2.64E+00
2.5%	6.48E+00
5.0%	8.51E+00
50.0%	2.67E+01
95.0%	1.04E+02
97.5%	1.40E+02
100.0%	4.31E+02

Crystal Ball Report
Simulation started on 95/1/25 at 0:22:19
Simulation stopped on 95/1/25 at 0:42:23

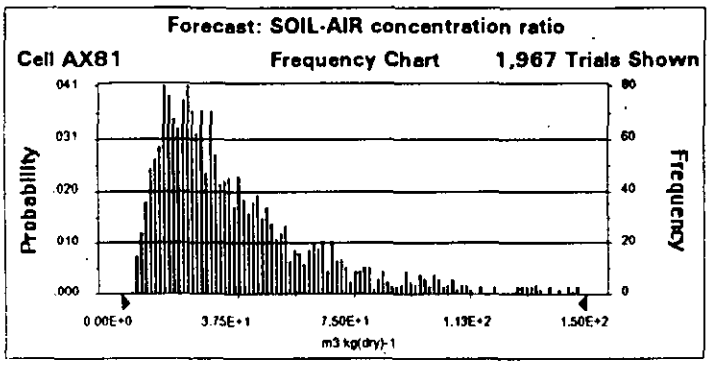


Hexachlorobenzene

Summary:

Display Range is from 0.00E+0 to 1.50E+2 m3.kg(dry)-1
Entire Range is from 3.32E+0 to 3.32E+2 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 7.64E-1

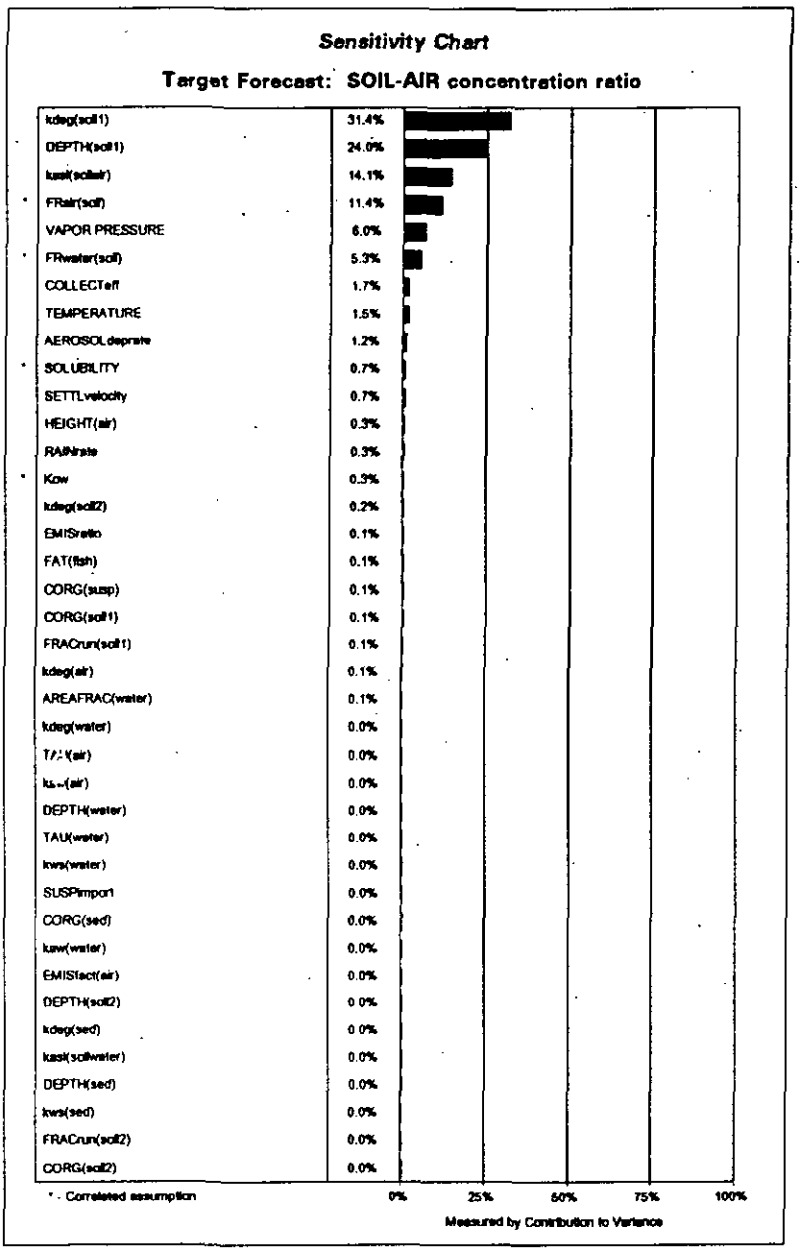
Statistics:	Value
Trials	2000
Mean	4.03E+01
Median (approx.)	3.00E+01
Mode (approx.)	1.48E+01
Standard Deviation	3.42E+01
Variance	1.17E+03
Skewness	2.78
Kurtosis	14.76
Coeff. of Variability	0.85
Range Minimum	3.32E+00
Range Maximum	3.32E+02
Range Width	3.29E+02
Mean Std. Error	7.64E-01



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	3.32E+00
2.5%	8.03E+00
5.0%	9.69E+00
50.0%	3.00E+01
95.0%	1.03E+02
97.5%	1.33E+02
100.0%	3.32E+02

Crystal Ball Report
Simulation started on 1/25/95 at 9:29:47
Simulation stopped on 1/25/95 at 9:54:59

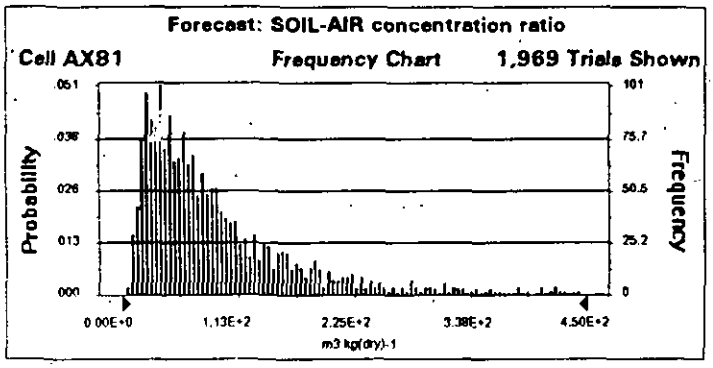


Pentachlorobenzene

Summary:

Display Range is from 0.00E+0 to 4.50E+2 m3.kg(dry)-1
Entire Range is from 5.29E+0 to 1.81E+3 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 2.65E+0

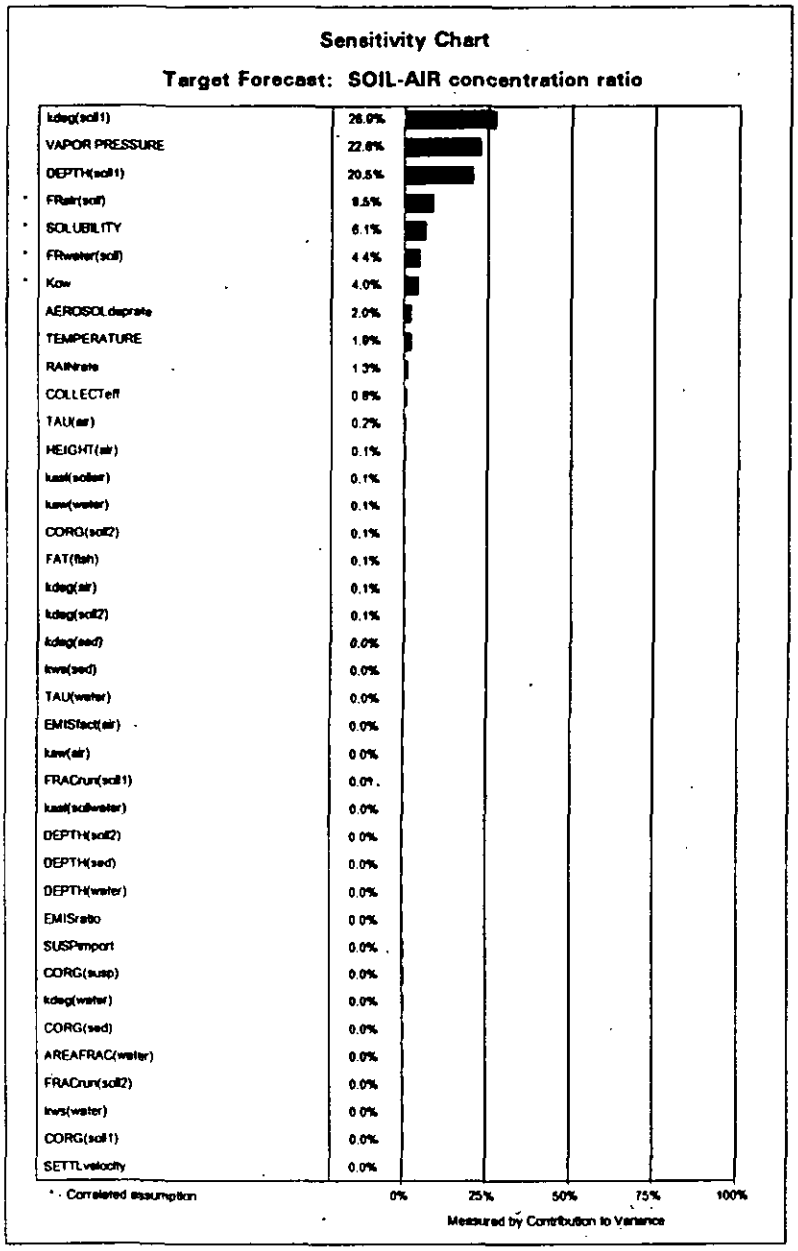
Statistics:	Value
Trials	2000
Mean	1.04E+02
Median (approx.)	7.04E+01
Mode (approx.)	3.24E+01
Standard Deviation	1.18E+02
Variance	1.40E+04
Skewness	5.22
Kurtosis	50.93
Coeff. of Variability	1.14
Range Minimum	5.29E+00
Range Maximum	1.81E+03
Range Width	1.81E+03
Mean Std. Error	2.65E+00



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	5.29E+00
2.5%	1.52E+01
5.0%	1.92E+01
50.0%	7.04E+01
95.0%	3.01E+02
97.5%	4.05E+02
100.0%	1.81E+03

Crystal Ball Report
Simulation started on 1/25/95 at 10:02:48
Simulation stopped on 1/25/95 at 10:28:29

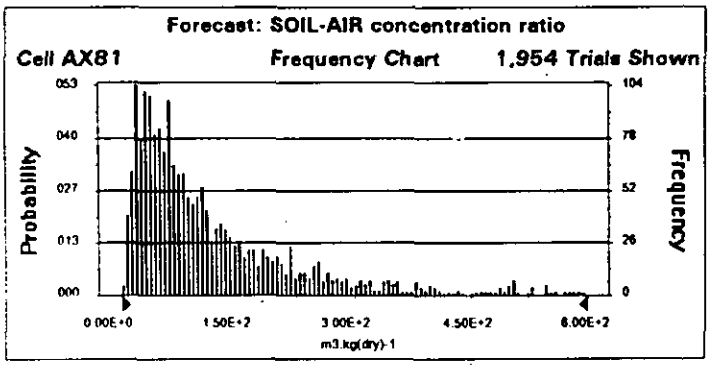


Pentachlorophenol

Summary:

Display Range is from 0.00E+0 to 6.00E+2 m3.kg(dry)-1
Entire Range is from 3.86E+0 to 2.61E+3 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 3.93E+0

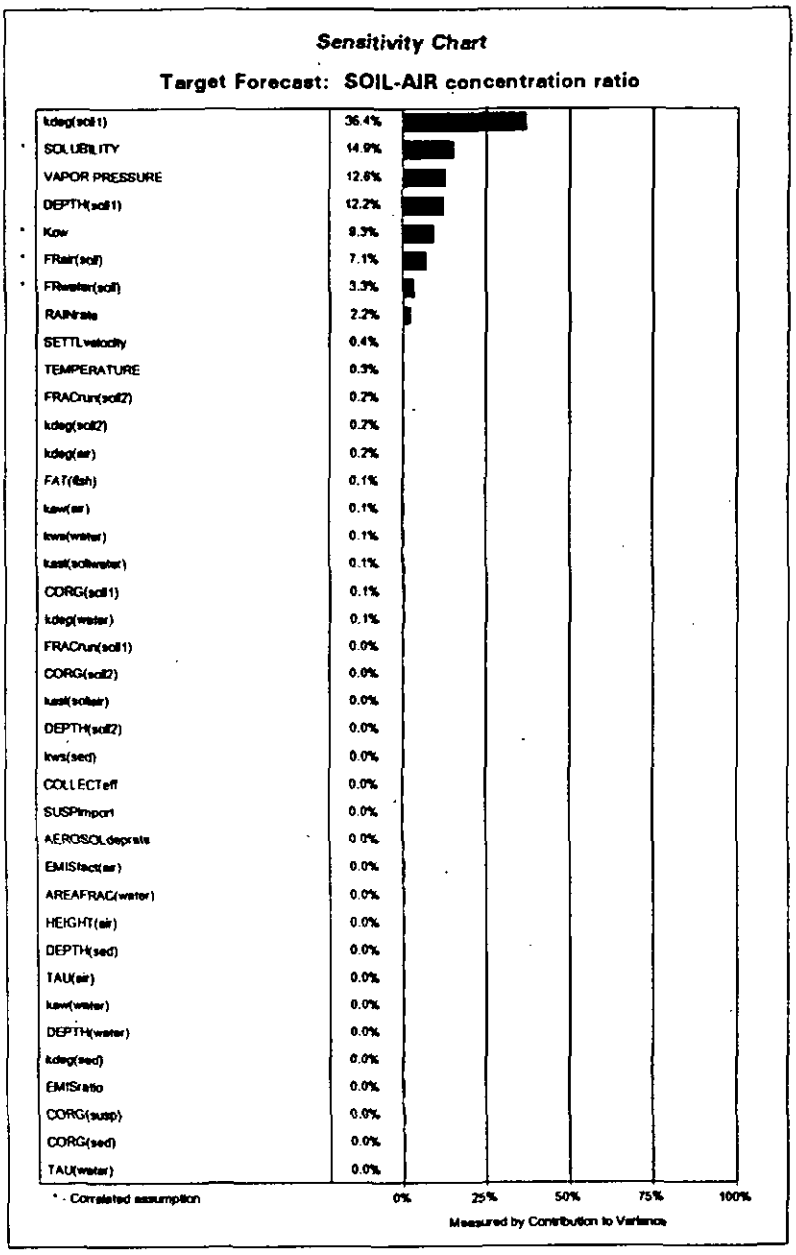
Statistics:	Value
Trials	2000
Mean	1.38E+02
Median (approx.)	8.34E+01
Mode (approx.)	4.29E+01
Standard Deviation	1.76E+02
Variance	3.09E+04
Skewness	4.77
Kurtosis	42.63
Coeff. of Variability	1.27
Range Minimum	3.86E+00
Range Maximum	2.61E+03
Range Width	2.61E+03
Mean Std. Error	3.93E+00



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	3.86E+00
2.5%	1.21E+01
5.0%	1.64E+01
50.0%	8.34E+01
95.0%	4.38E+02
97.5%	5.86E+02
100.0%	2.61E+03

Crystal Ball Report
Simulation started on 1/25/95 at 11:10:23
Simulation stopped on 1/25/95 at 11:30:41

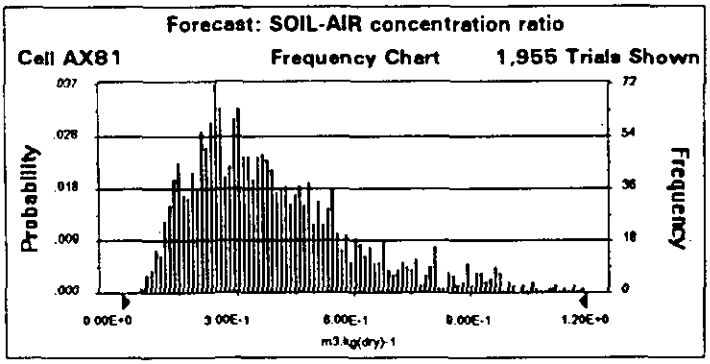


Quintozene

Summary:

Display Range is from 0.00E+0 to 1.20E+0 m3.kg(dry)-1
Entire Range is from 5.54E-2 to 2.72E+0 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 6.24E-3

Statistics:	Value
Trials	2000
Mean	4.23E-01
Median (approx.)	3.55E-01
Mode (approx.)	2.55E-01
Standard Deviation	2.79E-01
Variance	7.80E-02
Skewness	2.29
Kurtosis	11.91
Coeff. of Variability	0.66
Range Minimum	5.54E-02
Range Maximum	2.72E+00
Range Width	2.67E+00
Mean Std. Error	6.24E-03



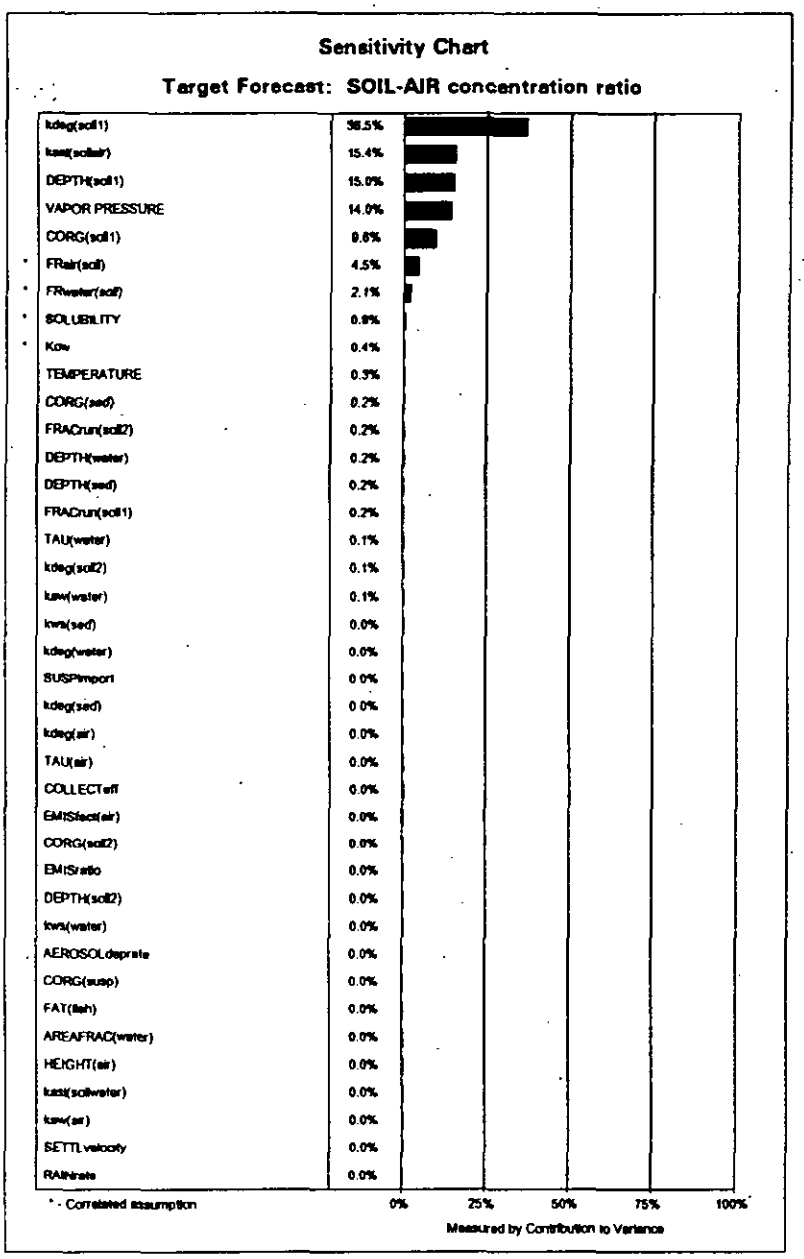
Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	5.54E-02
2.5%	1.10E-01
5.0%	1.31E-01
50.0%	3.55E-01
95.0%	9.49E-01
97.5%	1.16E+00
100.0%	2.72E+00

Crystal Ball Report

Simulation started on 1/25/95 at 11:41:09

Simulation stopped on 1/25/95 at 12:01:19

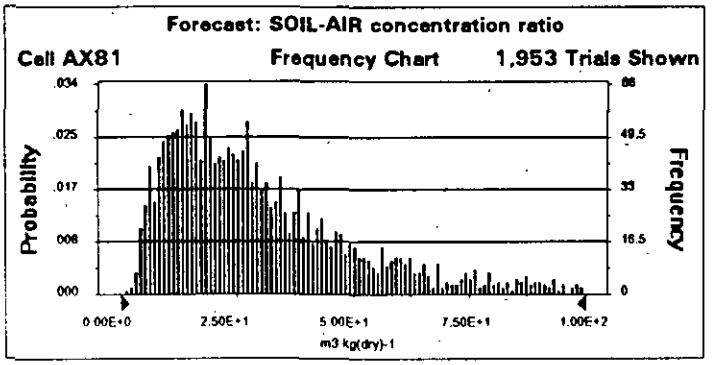


Thiram

Summary:

Display Range is from 0.00E+0 to 1.00E+2 m3.kg(dry)-1
Entire Range is from 1.94E+0 to 2.42E+2 m3.kg(dry)-1
After 2,000 Trials, the Std. Error of the Mean is 5.69E-1

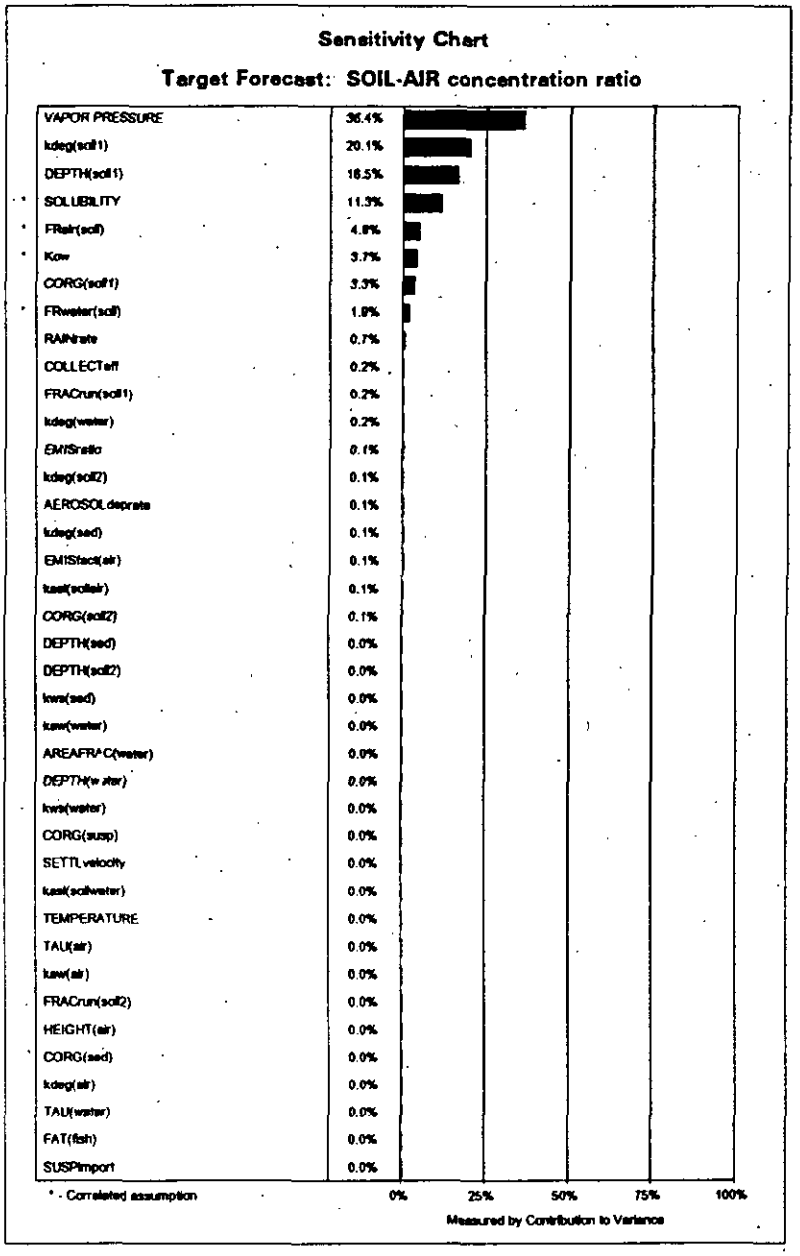
Statistics:	Value
Trials	2000
Mean	3.25E+01
Median (approx.)	2.58E+01
Mode (approx.)	1.28E+01
Standard Deviation	2.55E+01
Variance	6.48E+02
Skewness	2.21
Kurtosis	10.70
Coeff. of Variability	0.78
Range Minimum	1.94E+00
Range Maximum	2.42E+02
Range Width	2.40E+02
Mean Std. Error	5.69E-01



Percentiles:

Percentile	m3.kg(dry)-1 (approx.)
0.0%	1.94E+00
2.5%	5.68E+00
5.0%	7.14E+00
50.0%	2.58E+01
95.0%	8.24E+01
97.5%	9.88E+01
100.0%	2.42E+02

Crystal Ball Report
Simulation started on 1/25/95 at 12:19:19
Simulation stopped on 1/25/95 at 12:39:34



APPENDIX 8: Quasi-dynamic model output for Thiram