

Updating of PRAIRIE™ Databases

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R&D Technical Report P70

Publishing Organisation

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Statement of Use

This report details the modifications made to the PRAIRIE™ (Pollution Risk from Accidental Influxes to Rivers and Estuaries) databases relating to physico-chemical properties and toxicity of substances. The report will be of limited general use but provides a statement of the rationale behind the changes and a definitive statement of the position in March 1997.

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This document was produced under R&D Project No 707 by:

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EXECUTIVE SUMMARY

This report summarises work conducted by AEA Technology for the PRAIRIE Development Group to extend the PRAIRIE databases.

The work was conducted under two separate contracts with the Environment Agency: first, extension of the chemical database; and second, revision of the water quality database.

The chemical database has been extended from 89 to 250 entries. The work included: checking of existing entries; database and literature searches for missing entries; and finally, an evaluation of estimation methods to fill-in gaps.

Suggested No Adverse Response Levels for Humans (SNARLs) were revised under a sub-contract with the National Centre for Environmental Toxicology and included in PRAIRIE substances database.

The report concluded with some recommendations for the PRAIRIE Development Group:

- to periodically check the substances database (say every five years);
- that PRAIRIE users are made aware of aspects of chemical modelling and shown how parameters are related to the final result;
- that depletion mechanisms for priority substances are considered on a case by case basis rather than rely on previous compilations for appropriate data.

1. INTRODUCTION

The early versions of PRAIRIE (eg 2.0, 3.0 and 5.0) contained two physically distinct databases, namely the **chemical** and **water quality** databases. These databases were compiled from two separate sources: one, the chemical database, consisted of priority chemicals nominated by both the NRA and the HMIP; the other, the water quality database, was based largely upon data supplied by WRc under a contract with the NRA. Although both databases were revised and enlarged for the release of PRAIRIE 5.0 it was agreed that there should be no attempt at that stage to match the two databases. With the release of the windows version of PRAIRIE (version 6.01) the two databases were combined.

This report documents the efforts of AEA Technology, under a contract with the Environment Agency, to: (i) match the chemical database with the more extensive water quality database; (ii) to check entries in the chemical database; and (iii) to search for new chemical data to extend the completeness of the database.

Also reported here is work conducted under a separate but related contract by the National Centre for Environmental Toxicology to review the entries in the PRAIRIE 6.01 water quality database. The purpose of this contract was to check that the data entries are appropriate for a risk assessment tool such as PRAIRIE. There was no intention to extend the water quality database to include new chemicals.

2. CHEMICAL DATABASE - LITERATURE SEARCH METHODOLOGY

The PRAIRIE 6.01 database contained 89 records and formed the basis of the work reported here.

Because the database was merged from two individual databases there were names in the chemical database for which there were no corresponding entries in the water quality database and vice versa. The merged list contained a total of 250 chemical names.

The modelling of chemical processes by PRAIRIE imposes a hierarchy of data requirements. Figure 1 schematically shows how PRAIRIE models the fate of organic pollutants (inorganic substances are treated in a similar manner). There are minimum needs if PRAIRIE is to be able to model the uptake of pollutants onto suspended sediments and their depletion in water. The chemical solubility is the minimum requirement - without solubility data it is assumed that a chemical released to the river will be advected and diffused downstream but without adsorption (onto suspended solids) or reaction. For organic pollutants the hierarchy of physico-chemical needs is: (1) solubility data; (2) octanol-water partition coefficient; (3) chemical reactivity data. For inorganic pollutants the hierarchy is simpler, namely solubility data.

The data sheets used to create the earlier chemical databases (eg PRAIRIE 2.0 and 5.0) were first checked against the database entries to ensure that the starting point for this project was sound. A few minor discrepancies and omissions were found and corrected; of most interest was the inclusion of more data for photolysis rates.

Physico-chemical data such as solubilities, vapour pressures, and octanol-water partition coefficients were searched then from a wide variety of sources. The OHMTADS¹ database was used for preference to collect the basic data requirements since its listings were more extensive than the other databases searched. Once the OHMTADS searches were complete a variety of other databases were searched for missing data, including HSDB², RTECS³, CHRIS⁴ and the Merck Index.

Database searches were completed by inspection of the CHEMFATE⁵, AQUIRE⁶ and EPA⁷ reference sources. These databases are less extensive than those searched primarily for physico-chemical data but contain data related to chemical reactivity, such as rates of hydrolysis, photolysis, hydrolysis and oxidation (which are not found in the other databases).

Data searches are time consuming exercises which not only require care but also judgement since discrepancies are often found between the various databases. Little or no background information is found in most compilations of data and it is therefore very difficult to identify the more reliable data. In the event of significant discrepancies we attempted to select the value which would give the more pessimistic PRAIRIE predictions (ie high solubilities, low octanol-water partition coefficients).

3. CHEMICAL DATABASE - PROPERTY ESTIMATION METHODS

There were inevitably gaps in the database following completion of the steps outlined in Section 2 (above). The omissions fell into three types: (i) chemicals for which even the most basic solubility information could not be found; (ii) chemicals for which octanol-water and Henry's constants could not be found (important for determining absorption onto suspended solids and volatilisation respectively); and (iii) chemicals for which a complete list of reactivity data could not be found. Only solubility data is needed for the modelling of inorganic substances since the other requirements are hard-wired into the DYNUT dispersion code.

3.1 Solubility And Octanol/Water Partition Coefficients

As discussed above, solubilities (for both organic and inorganic pollutants) and octanol / water partition coefficients (for organic pollutants) are important input parameters if pollutant dispersion and depletion is to be modelled properly. Much effort has been devoted by other researchers to estimating both parameters and it has been demonstrated that there is a linear relationship between S and K_{ow} ⁸. A variety of regression equations have been derived; some are claimed to be representative of a mixed class of chemicals whilst others are most suitable for a narrower range of chemicals. Of the regression equations tabulated in reference [8] the following was thought to have the widest range of applicability to PRAIRIE:

$$\log \frac{1}{S} = -1.12 \log K_{ow} + 7.30 - 0.015t_m \quad (1)$$

where S , K_{ow} and t_m are terms which represent the solubility (units of μ mol/L), octanol-water partition coefficient and melting points (units °C) respectively.

Many of the substances from which the regression equation was obtained are liquid at room temperature. However, the use of such an equation for solid solutes will tend to produce an overestimation of the solubility. For this reason a correction factor for solids has been included which requires a knowledge of the melting point. (A t_m value of 25°C is used for substances which are liquid at room temperature.)

Equation 1 was selected because it gave the best reported correlation ($r^2 = 0.922$) of the many equations tabulated in reference [8].

To test the relationship between S and K_{ow} a linear regression was first performed for S and K_{ow} data entries in the PRAIRIE database which had been taken from the various data sources discussed in Section 2 above. A residual sum of squares of 0.68 was computed (see Figure 1). Although Figure 1 shows an approximately linear relationship between S and K_{ow} the computed r^2 is relatively poor (compared to literature values of between 0.74 and 0.97 and an ideal of 1.0). There are a number of factors which may explain the apparently poor fit:

(i) it is often not clear whether the literature values are from experiment or calculated (CHEMFATE was the only database used during this study which differentiated between experimental and calculated values); calculated values will be estimated by methods similar to those under discussion here and it is possible that errors may be propagated;

(ii) regression equations are sensitive to outliers. Some researchers omitted outliers from their data set and as a consequence improved their fit. No outliers were excluded from the PRAIRIE data set and inspection of Figure 1 shows that there are outliers, especially towards the extremes of S and K_{ow} - these will contribute to the “poor” r^2 value. Regression equations typically are accompanied by ranges of S and K_{ow} values for which the equations are applicable. Equation 1 is applicable for S between 10^{-4} and 10^6 mg l⁻¹ and K_{ow} between 10^{-3} and 10^6 .

(iii) the plot of PRAIRIE database entries of S against K_{ow} made no account for t_m . However, as mentioned above, regression equations can overestimate the solubility for solid solutes unless a correction factor is applied.

Reference [8] tabulates, as a percentage, the errors between measured and observed solubilities for a wide range a substances. The percentage errors range from a few percent to overestimates of more than 10^6 . It is clear that a significant number of K_{ow} values found in the literature are estimated although rarely do the compilers indicate that large uncertainties may be associated with the selected values. This provides further evidence that even database compilations should be treated with care and that the user should take every opportunity to confirm independently the validity of parameters used for simulations.

Solubility and K_{ow} values were estimated for entries in the partially complete PRAIRIE database for which either S or K_{ow} values (but not both) were known. The estimated values are shown in Table 1. It is stressed, for reasons explained above, that these database entries should be treated with caution. An overestimate of S should help to produce a pessimistic PRAIRIE simulation. However, an overestimate of K_{ow} could, when combined with fast depletion mechanisms, overestimate the loss of a pollutant from the river and therefore underestimate the consequences to humans and the aqueous environment.

Table 1: Estimated values for S and K_{ow}

Substance name	Database Solubility (mg l ⁻¹)	Database log K_{ow}	Estimated Solubility (mg l ⁻¹)	Estimated log K_{ow}
4,4-DIAMINO DIPHENOL SULPHONE (DAPSONE)	0	0.97	689604.4	-
ACETIC ANHYDRIDE	120000		-	0.12
CHLORFENVINPHOS	145		-	3.91
CRESYLIC ACID		1.94	56519.72	-

Substance name	Database Solubility (mg l ⁻¹)	Database log K _{ow}	Estimated Solubility (mg l ⁻¹)	Estimated log K _{ow}
(CRESOL)				
CYANOGEN CHLORIDE	2500		-	2.32
CYFLUTHRIN	0.002		-	8.60
DI-ISOBUTYL KETONE	200		-	3.71
DICHLOROPHENOL-2,6		2.64	9293.943	-
DIETHYLAMINE	1000000		-	-0.37
ETHYLENE CHLOROHYDRIN	1000000		-	0.18
ETHYLENE DIAMINE TETRACETIC ACID (EDTA)	500		-	6.58
IOXYNIL	50		-	7.42
MALEIC ANHYDRIDE	1000000		-	0.26
PARAQUAT	1000000		-	0.51
PERMETHRIN	1800		-	3.25
PHOSPHONOMETHYL (GLYCINE N) (GLYPHOSPHATE)	12000		-	2.19
SULPHUR OXYCHLORIDE	1000000		-	0.34
TETRAETHYL LEAD	0.29		-	6.56
TETRAMETHYL LEAD	0.828		-	5.84
TRIOXANE(S) 2,4,6 TRIMETHYL	55555		-	1.50

It is therefore concluded that whilst estimation methods are claimed to have generally wide applicability for the estimation of S and K_{ow} the uncertainties associated with these estimates can be appreciable. Whilst estimates can be useful (and have been used in the compilation of the PRAIRIE database) it is preferable to use measured values.

3.2 Rate Of Hydrolysis

Hydrolysis is a chemical transformation process in which an organic molecule reacts with water, forming a new oxygen-carbon bond and cleaving a carbon-X bond in the original molecule (most commonly by replacement of X by OH). This process should be distinguished from several other possible reactions between organic chemicals and water such as: (i) acid-base reactions (dissociation); (ii) addition to carbon-carbon bonds; and (iii) elimination.

The rate equation employed by PRAIRIE takes the form:

$$-d[RX]/dt = kH[H^+][RX] + k_o[RX] + k_{OH}[OH^-][RX] \quad (2)$$

which recognises that the reaction may proceed under neutral conditions, or may be either acid- or base-catalysed. Within the PRAIRIE database there are entries (if the information is available) for k_{IH} , k_O and k_{OH} .

Four steps are required for the experimental measurement of the hydrolysis rate:

1. determination of the form of the rate law;
2. measurement of the magnitude of k_H , k_O and k_{OH} ;
3. determination of the products of reaction; and
4. determination of the temperature dependence.

Database information regarding hydrolysis rates are patchy, probably reflecting the difficulty of properly characterising the nature of the hydrolysis reaction. Moreover, the reaction medium is also believed to influence the reaction by affecting changes in the solvating power of the reaction medium. Both changes in ionic strength and the presence of organic solvents can affect the solvating power and thus alter the hydrolysis rate. Specific medium effects due to general acid/base and trace-metal catalysis are also possible. (Unfortunately, many old experiments were conducted in mixed organic-aqueous solvents (to achieve solubility of RX); the influence of solvent composition on organic reactivity is only poorly understood in theory.)

Estimation of k_H , k_O and k_{OH} is discussed in reference [8]. However, the methods are applicable for a very limited range of materials, such as benzyl and dimethyl benzyl halides and benzyl tosylates. This list is much more restricted than the requirements for PRAIRIE.

It is therefore concluded that estimation of hydrolysis rates for the range of substances within the PRAIRIE database is not feasible. Estimation techniques might be suitable on a substance by substance basis.

3.3 Rate Of Photolysis

Photolysis may help to determine the fate of organic pollutants in the aqueous environment, either by (i) direct photolysis in which the pollutant directly absorbs solar radiation or (ii) sensitised photolysis, in which energy is transferred from some other species in the aquatic environment to the pollutant.

The rates of these processes in a river would depend on the properties of the aquatic environment (intensity and spectrum of solar radiation, presence or absence of sensitisers, quenchers, etc.) and on the properties of the organic pollutant.

Models exist for the determination of direct photolysis by estimating the net rate at which the aqueous solution plus pollutant absorb light. The equation takes the form:

$$-\frac{d[P]}{dt} = \Phi_{solar} [P] \frac{2.303}{j} \sum_{\lambda} I_{\lambda} \epsilon_{\lambda} \quad (3)$$

where:

Φ_{solar} = quantum yield

I_{λ} = the flux of solar energy of wavelength λ incident on the chemical

ϵ_{λ} = is the molar absorptivity of the chemical at wavelength λ

j is a conversion constant numerically equal to 6.023×10^{20} .

The chemical groups which absorb light are called chromophores and the models depend upon a knowledge of the compound's molar absorptivities. Determination of the photolysis rate is dependent upon: (i) knowledge of whether the compound contains a chromophore (for which lists are available); and (ii) information of the compound's molar absorptivity (for which limited lists are available, eg reference [8]). Attempting to work through the PRAIRIE database for missing photolysis rates and then applying the above equation would be an involved exercise and beyond the scope of this project. Moreover, such approaches only allow for an estimation of direct photolysis (therefore ignoring indirect photolysis).

It is therefore concluded that man's understanding of photochemical reaction mechanisms is insufficient to allow for robust estimation of photochemical rate constants and that estimation of photolysis rates for the range of substances within the PRAIRIE database is not feasible.

3.4 Rate Of Oxidation

PRAIRIE models the chemical oxidation of pollutants in natural waters as a second-order rate equation:

$$\frac{dc}{dt} = -K.Ox.C \quad (4)$$

where:

K is the second-order rate constant;

Ox is the concentration of oxidant; and

C is the concentration of pollutant.

This model is different to PRAIRIE's other chemical sink models because it treats the reaction as a second order process (ie it is dependent upon two concentrations, namely pollutant and oxidant) rather than as a first order process where the rate is dependent upon just the pollutant.

Strict oxidation may occur with dissolved oxygen as a reactant or, more commonly, with atomic oxygen $O(1D)$ or free radicals such as OH^\bullet , or ROO^\bullet . Typically, the free radicals are themselves generated by photochemical reactions or redox reactions involving hydrogen peroxide, singlet oxygen or ozone.

In the absence of information relating to the river under consideration it is difficult to predict in advance the exact requirements of the PRAIRIE user. For example, the rate selected will be dependent upon the type of oxidant found within the river. The database entries within PRAIRIE should therefore be used as a point for departure rather than as definitive rate constants relevant to the situation under consideration. The oxidation rates found within PRAIRIE have been selected from two databases^{5,7}; where possible the database entry is for atomic oxygen ($O(1D)$) but entries for $O(3P)$ have been included if the $O(1D)$ values could not be found. (Literature values for ozone, hydrogen peroxide, organic peroxides and hydroxyl free radicals were not selected.) In general, the rates for $O(1D)$ are faster than $O(3P)$ and the priority used for the database selection should ensure that the modelling errs towards making conservative estimates.

The case of methanol usefully illustrates the care that should be exercised when modelling oxidation reactions. The CHEMFATE database lists a variety of rate constants; these are summarised below:

oxidant	second order rate constant (cc/molecule/s)
OH	$6.1 \times 10^{-11} - 7.7 \times 10^{-13}$
O(1D)	6.1×10^{-10}
O(3P)	5.8×10^{-15}

The value for oxidation of methanol in the PRAIRIE database, selected from the CHEMFATE compilation, is $1.32 \times 10^{15} \text{ l mole}^{-1} \text{ hr}^{-1}$ and assumes that the oxidant is present as O(1D). (To convert from units of cc/molecule/s to $\text{mole l}^{-1} \text{ hr}^{-1}$: (i) multiply by 6×10^{23} (convert from molecules to moles); (ii) multiply by 3600 (convert from seconds to hours); and (iii) divide by 1000 (convert from cubic centimetres to litres).) The PRAIRIE help screen suggests a starting molar oxidant concentration of 10^{-9} M . Assuming a pollutant concentration of 10 mg l^{-1} the initial depletion rate may be estimated:

$$K = 1.32 \times 10^{15} \text{ l mole}^{-1} \text{ hr}^{-1}$$

$$O_x = 10^{-9} \text{ mole}$$

$$C = 10 \text{ mg l}^{-1}$$

then

$$dc/dt = -1.32 \times 10^8 \text{ mg l}^{-1} \text{ hr}^{-1}.$$

If the oxidant were O(3P) then for the same values of O_x and C the initial depletion rate would be $-1.25 \times 10^3 \text{ mg l}^{-1} \text{ hr}^{-1}$.

This illustrates that the depletion rate can be highly dependent upon assumptions made regarding the nature and concentration of the oxidant. With the assumptions made above the pollutant would be very quickly depleted if the oxidant were O(1D) and the user could run the risk of making an optimistic prediction.

It should be noted that the molar oxidant concentration is not depleted during the modelling of chemical oxidation. In this respect the reaction is treated as a pseudo-first order reaction although the form of the PRAIRIE implementation might suggest otherwise. This again will tend to make PRAIRIE predictions err towards the optimistic when oxidation reactions are enabled.

Efforts to find estimation methods for oxidation reactions were unsuccessful.

4. THE WATER QUALITY DATABASE

PRAIRIE's chemical and water quality databases have historically evolved in isolation. The human SNARLSs (suggested no adverse response levels) that are one of the key entries in the water quality database were derived by WRc under a research contract that was independent of the PRAIRIE development. The entries in the chemical database were nominated by the NRA and the HSE. It is worth remembering, however, that SNARLS and risk assessment methodologies formed an important part of the technical argument presented by the NRA when applying for permission to set-up a Water Protection Zone on the River Dee and their combined effectiveness is greater than the parts.

The water quality database supplied with earlier versions of PRAIRIE (2.0 to 6.01) contained SNARL data which had been supplied to the NRA by WRc. WRc expressed some concern that the data that they had given to the NRA had not been prepared with the intention of inclusion into a risk assessment tool such as PRAIRIE. To ensure that the best possible data is provided with PRAIRIE a contract was therefore placed with the National Centre for Environmental Toxicology (which is part of WRc) to:

- (i) check SNARL values which had been provided with previous versions of PRAIRIE;
- (ii) to search for missing SNARL data (ie to fill in gaps where there were values for chemical data but no corresponding SNARL data).

In addition to this, NCET also provided confidence ratings to the data they supplied. The confidence ratings range from 1 (highest confidence) to 5 and are based on the underlying information from which the values were derived:

Confidence 1 - for SNARL data which was derived from a standard or guideline derived by any recognised international body. (These include UK/European standards, US standards and guidelines, WHO guidelines, FAO ADIs);

Confidence 2 - (i) for SNARLS which were based on NOAEL or LOAEL for which sufficient background information was available; or (ii) for SNARLS which were based on a taste or odour value which was measured in a WRc test);

Confidence 3 - (i) for any SNARLS which were based on NOAEL or LOAEL for which limited background information was available; or (ii) for SNARLS which were based on a taste or odour (or other aesthetic) value for which background information was available;

Confidence 4 - for any SNARL which was based on one for a compound of similar structure, or was based on one component of a salt or mixture;

Confidence 5 - (i) for any SNARL which was based on an LD₅₀ or occupational exposure standard; or (ii) for any SNARL based on a taste odour (or other aesthetic) value derived from published collections of values.

In addition to providing confidence levels NCET also derived SNARLS for old entries based on LD₅₀s and checked for new data to help fill any missing gaps in their previous surveys. Some SNARLS were changed following the discovery of new data, eg:

ammonia (changed from 30 mg l⁻¹ to 0.5 mg l⁻¹);

calcium sulphate (changed from 400 mg l⁻¹ to 0.5 mg l⁻¹);

formaldehyde (changed from 0.45 mg l⁻¹ to 4.5 mg l⁻¹).

The checked and corrected data form the basis of the updated waterquality database.

In a few cases there were entries in the old database for which no revised data was provided by NCET. In these circumstances the old data was kept rather than replacing them with null (-1) entries.

5. DISCUSSION AND RECOMMENDATIONS

The PRAIRIE chemical database has been significantly extended from 89 to 250 entries. A reduced dataset (consisting of solubilities and octanol-water partition coefficients) has been compiled for the majority of entries. Extensive database searches were then conducted to fill in the gaps concerning rate data (for hydrolysis, photolysis and oxidation depletion mechanisms); although many additional entries were found there remain gaps for more than half the chemicals in the database. There is no way of telling whether an absence of a literature value reflects no reactivity for a particular chemical or whether, the more likely explanation, the reviewers could find no relevant information.

The literature was also reviewed to see how the gaps might be estimated. The most useful reference was that compiled for the US EPA on estimating chemical properties for organic materials [8]. The empirical equations for solubility, octanol-water partition coefficients and vapour pressure were identified as having sufficiently wide applicability for use within the context of PRAIRIE (see Section 3 above). The estimation methods for hydrolysis and photolysis (also discussed in Section 3 above) were identified as both (i) too restricted in their range of applicability; and (ii) too involved to be undertaken during this project. No estimation methods were identified for oxidation.

The entries in the Water Quality database were checked by the National Centre for Environmental Toxicology and revised values incorporated into the database.

On the basis of the work reported here we would suggest that the PRAIRIE Development Group consider the following issues:

perform periodic reviews of data: man's scientific knowledge and understanding does not remain constant but instead evolves with time as new facts and interpretations emerge. This is reflected by the revisions made to some of the SNARL data. It is important that a risk assessor uses reliable and up-to-date data. We therefore recommend that periodically (say once every five years) the PRAIRIE database is reviewed to ensure: (i) that current entries are up-to-date; and (ii) that any new data is incorporated into the database.

provide advice to users: every effort has been made to ensure that the database entries are free from errors. However, as discussed above, the reliability of selected entries it is not always clear from the literature. In many instances it is likely that PRAIRIE users will be interested in just a few substances, and quite possibly have access to data that was not included in our literature searches (eg in-house Materials and Safety Data Sheets). We would therefore recommend that: (i) all PRAIRIE users are properly trained in its use, especially regarding how parameters are inter-related and the dangers in making overly optimistic predictions; and (ii) that users are encouraged to view the chemical data as a starting point, and to question the applicability of the data to their own needs - errors or omissions in the database should be reported in the usual way.

consider the importance of various depletion mechanisms: although the chemical database has been extensively extended there remain many gaps concerning rate data. (As discussed above it is not certain whether this is due an absence of data or lack of reactivity.) Whilst there are dangers in making overly optimistic predictions there are difficulties in making pessimistic predictions - too many substances might be identified

as presenting an unacceptable risk and therefore deserving of additional (and unwarranted) attention. It is therefore suggested that further efforts are made to fill the gaps. Reliance cannot be placed upon database compilations and we would suggest that future studies; (i) go back to original references; and (ii) contact directly experts in depletion reactions. This would be a time consuming exercise, and should therefore be concentrated on priority chemicals (selected by the Development Group) in the first instance.

6. REFERENCES

- 1 OHMTADS, "Oil and Hazardous Materials technical Assistance Data System", US Environmental Protection Agency.
- 2 HSDB, "Hazardous Substances Data Bank", US National Library of Medicine.
- 3 RTECS, "Registry of Toxic Effects of Chemical Substances", US National Institute for Occupational Safety and Health.
- 4 CHRIS, "Chemical Hazards Response Information", US Coast Guard.
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- 7 Schnoor, J.L. et. al., "Processes, coefficients, and models for simulating toxic organics and heavy metals in surface waters", EPA/600/3-87/015, 1987.
- 8 Leyman, W.J, Reehl, W.F., and Rosenblatt, D.H., eds., "Handbook of chemical property estimation methods", American Chemical society, 1990.

Figure 1 Schematic representation of the fate of organic pollutants

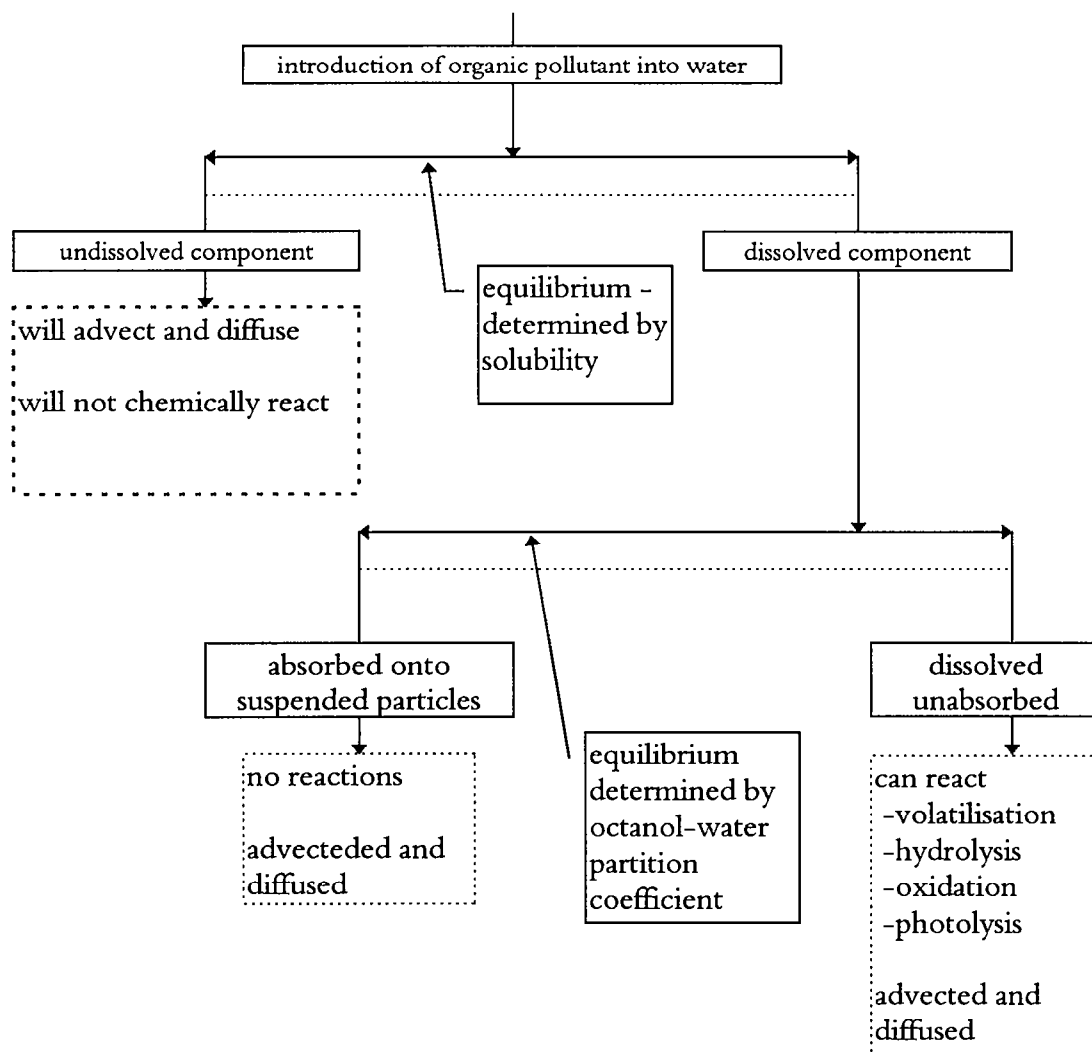


Figure 2 Relationship between S and K_{ow}

