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The risk evaluation of difficult substances in USES 2.0 and EUSES

A decision tree for data gap filling of Kow, Koc and BCF

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Abstract

This report presents a decision tree for the risk evaluation of the so-called "difficult" substances with the Uniform System for the Evaluation of Substances (USES). The decision tree gives practical guidelines for the regulatory authorities to evaluate notified substances like organometallic compounds, cationic compounds, anionic compounds, surfactants, inorganic compounds, acids, bases and compounds without an available octanol/water partition coefficient (Kow). The decision tree gives reasonable worst case estimates for the Risk Characterisation Ratios of substances of which no Kow value can be estimated or measured. The decision tree only asks for more a detailed analysis of both sorption and bioaccumulation, when the predicted environmental concentrations are sufficiently high to make a difference for the outcome of the risk assessment. The report suggests to use the Kow value of the neutral molecule of acids and bases even when these molecules are present as anions or cations at pH 7. The guidelines and suggestions in this report were based on the evaluation of a large data set with the Kow, soil sorption coefficient (Koc) and bioconcentration factor (BCF) of pesticides. It is argued that these guidelines and suggestions are valid for a wide range of ”difficult” substances. The uncertainties encountered with the estimation of Koc and BCF from Kow for different classes of "difficult" substances were estimated and their influence on the outcome of the risk evaluation with USES 2.0 or EUSES was analysed.

Samenvatting

Dit rapport presenteert een beslisboom voor de risico-evaluatie van de zogenaamde " moeilijke" stoffen met het Uniform Systeem voor de Evaluatie van Stoffen (USES). De beslisboom geeft praktische richtlijnen voor de beoordelende instanties om de aangemelde stoffen (zoals organometaalverbindingen, kationen, anionen, surfactanten, anorganische verbindingen, zuren, basen en stoffen zonder een beschikbare octanol/water partitiecoëfficiënt) te evalueren. De beslisboom geeft redelijk pessimistische schattingen voor de Risico Karakteriserings Ratio van stoffen waarvoor geen octanol/water partitiecoëfficiënt kan worden geschat of gemeten. De beslisboom vraagt alleen om een meer gedetailleerde analyse van zowel sorptie als bio-accumulatie, wanneer de voorspelde milieu-concentraties hoog genoeg zijn om een verschil te maken voor de uitkomst van de risico -evaluatie. Het rapport beveelt aan om de octanol/water partitiecoëfficiënt van het neutrale molecule van zuren en basen te gebruiken zelfs wanneer deze moleculen als anionen of kationen aanwezig zijn bij pH 7. De aanbevelingen en suggesties in dit rapport zijn gebaseerd op de evaluatie van groot gegevensbestand met de octanol/water partitiecoëfficiënt, de bodem sorptie coëfficiënt en de bioconcentratie factor van pesticiden. Er wordt aangegeven dat deze richtlijnen en suggesties geldig zijn voor een groot bereik aan verschillende "moeilijke" verbindingen. De onzekerheden die ontmoet werden bij de schatting van de bodem sorptie coëfficiënt en de bioconcentratie factor vanuit de octanol/water partitiecoëfficiënt werden ingeschat en hun invloed op de uitkomst van de risico evaluatie met USES 2 of EUSES werd geanalyseerd.

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Introduction

The Uniform System for the Evaluation of Substances (USES) has been developed at the RIVM in the Netherlands [8, 9, 16, 32, 36] to evaluate the potential hazards and risks of notified substances on the basis of a specified data set [2]. Based on USES 1.0 and the European Union Technical Guidance Document [4] the European Union System for the Evaluation of Substances (EUSES) has been developed [3, 35]. Recently USES 2.0 and 3.0 were developed as updates of USES 1.0 comprising both EUSES and the risk assessment system for pesticides [22, 22]. This risk assessment system is based on the European Union Uniform Principles and on Dutch legislation on the use of pesticides. These risk assessment systems are available in computerised form. The user has to type in a few properties of the chemical and a few assumptions about the use of the chemical to get a risk assessment of the chemical for both man and environment.
When industries want to utilise a new specific chemical in amounts exceeding 0.1 ton per year they have to notify the regulatory authorities and supply a part of the base set of data on the chemical which can be employed by USES to estimate the risk of the application. In this report the general term USES will be used to refer to shared and identical properties of USES 2.0, 3.0 and EUSES.
The USES program was originally designed for apolar organic substances. For the estimation of sorption to organic material for example, a QSAR is used in USES, which was made for compounds that consist solely of carbon, hydrogen, and halogen atoms [23]. Nowadays many notified substances also contain oxygen or nitrogen atoms and can even have a charge distribution over the molecule. The substances like organic cations, anions, surfactants and inorganic compounds were generally regarded as "difficult" substances for the prediction of their environmental distribution in USES. Problems did occur with the environmental risk assessment of organic non-agricultural pesticides like antifoulings, biocides or wood preservatives [27]. In order to assess the problems with “difficult” substances it is important to know how well USES performs with “normal” substances. The validation status of USES is still limited [22]. In the future probabilistic risk assessment can provide confidence limits to the PEC and the PNEC [11], which can make it possible to falsify the model. The best scientific theories and also the best models make accurate predictions which can be falsified (in other words " shown wrong") by experimental observations [20]. The prediction of the environmental concentrations by the sewage treatment plant part of the model and by the drinking water module were fairly accurate whereas the predicted concentrations in fish, plants and cattle deviated several orders of magnitude from data in the literature [22]. Local sediment concentrations were sometimes up to 7 orders of magnitude higher than the regional concentration calculated by USES [10], because the sediment concentrations were measured at pollution hot spots while USES calculates a regional average concentration [10]. Although the USES program was designed for neutral organic substances it could still predict the zinc concentrations in water, sediment, air and both agricultural and natural soil when the proper partition coefficients were incorporated into the model [10]. The USES 1.0 program was able to predict atmospheric and aquatic anthropogenic background concentrations of

tetrachloroethene present due to the use of this compound in textile dry cleaning [21].
A previous report gave an inventory of the problems which arise when "difficult" substances are evaluated with USES [30]. The notified chemicals were divided into 10 classes based on environmental distribution and toxicity: Inorganic cations, inorganic anions, neutral inorganic compounds, organic cations, organic anions, organic acids, organic bases, organic surfactants (which can be cationic, anionic or neutral), neutral organic compounds with a slightly polar substituent, and neutral organic compounds. The previous report recommended to develop methods to estimate all required partitioning and biocentration factors from a single partition coefficient of a charged molecule and to perform a literature search to derive realistic worst case safety factors and to give information about reasonable worst case estimates when no partitioning on bioaccumulation factors are available.
The present report follows these recommendations and gives a practical guideline for the regulatory authorities to evaluate notified difficult substances by the use of a simple decision tree. The choices made in the decision tree are motivated, tested and evaluated by the use of a test set of difficult substances which consists of organic and organometallic substances. In Chapter 1 of this report a database is constructed using pesticides as a test database for difficult substances. Pesticides were selected because a number of partitioning and bioaccumulation factors are available for these chemicals and because many pesticides belong to different classes of the organic difficult substances which are described above. The report focuses on the octanol/water partition coefficient Kow, the organic matter partition coefficient Koc and the bioconcentration factor BCF because the environmental distribution of these difficult substances is not always accurately predicted by the standard approach of USES. Chapter 2 describes the influence of the uncertainties of the physicochemical properties of these chemicals (the input) on the risk assessment by USES (the output). It also gives a reasonable worst case estimate for the risk assessment of compounds without any information about environmental partitioning.

1. Data analysis

1.1 The construction of a database on the partition coefficients of pesticides

The main sources of information were the illustrated handbook of physical chemical properties and environmental fate for organic chemicals [18], the pesticide manual [29] and a publication on QSAR modelling of soil sorption [23]. Table 1 (in appendix 2) gives an overview of the most relevant data for the estimation of the fate of a chemical by USES. The pesticides were classified as acid, neutral acid, base, cation base, cation, ionic, organometallic, polar and hydrophobic compounds. The pesticides classified as acids are able to release a proton above their pKa and become an anion. The pesticides classified as " neutral acids" have a pKa value above 7 and are normally present as neutral molecules. The pesticides classified as bases are able to pick up a proton and become a cation at pH values below their pKa. The bases with a pKa above 7 like Thiophanate-methyl and Terbacil are normally present as cations. The three organometallic pesticides Metiram, Ziram and Zineb contain covalently bound Zn and are neutral compounds. The acid, neutral acid, base, cation base, cation, ionic, and organometallic pesticides together are classified as “difficult” pesticides in this report. The pesticides classified as hydrophobic pesticides contain only carbon, hydrogen and halogen atoms as described by Sabljic [23]. The polar pesticides are neutral compounds which contain also oxygen, nitrogen, sulfur, or phosphorus. The three classes of pesticides namely hydrophobic, polar and difficult pesticides will be used further in this report.

1.2 The selection of the octanol/water partition coefficient as input parameter for USES

Three different values of the logarithmically transformed octanol/water partition coefficient (log Kow) are presented in table 1 (in appendix 2). The first column of the three log Kow columns represents the best estimate of the log Kow according to expert judgement by Mackay [18] based on different experimental and estimated values, while the second and third columns were measured at pH values above or below the pKa value. The acids will be converted into anions above their pKa value which often lowers the log Kow considerably. Anions have more affinity to the water phase and less affinity to the octanol phase compared to the neutral molecule. For Mecoprop and pentachlorophenol the Kow of the neutral acid form is more than one thousand times higher than the Kow of the anionic form of the molecule (see table 1). The selection of the best estimate for the log Kow is not a trivial task since there often is a wide range of data available. For a neutral apolar substance like for example Aldrin, the log Kow varies between 3.01 and 7.4. This is probably caused by the low

solubility of Aldrin and its high hydrophobicity which results in a very low concentration in the water phase during the octanol/water partitioning experiments. This very low concentration can give analytical problems. The use of the shake flask method for the determination of higher Kow values can cause experimental artefacts and therefore the slow stirring method or an HPLC method often give better results [25]. For a more soluble compound like for example Aldicarb, the log Kow varies between 0.5 and 1.57 [18]. With Aldicarb the concentration in the water phase during the octanol/water partitioning experiments is much higher than for Aldrin, which makes the Aldicarb concentration more easy to determine and less prone to experimental artefacts.

1.3 The estimation of the organic carbon sorption coefficient from the octanol/water partition coefficient

The reported log Koc values are the experimentally determined logarithmically transformed sorption coefficients which are normalised for the percentage of organic carbon in soil, sediment or in a sewage treatment plant. The first column presents the best estimate of the log Koc according to expert judgement from different experimental and estimated values by Mackay [18] whereas the following two columns present the lowest and the highest experimentally determined log Koc values reported [18]. Table 1 shows that there is a large variation in the reported log Koc values, especially at the higher values.The QSAR which is used in USES to estimate the organic carbon sorption coefficient (Koc) from the octanol/water partition coefficient (Kow) is derived for hydrophobic chemicals which contain only carbon and halogen atoms [23]. This QSAR is also suited to estimate log Koc for polar compounds with a log Kow above 3 but it is definitely erroneous for polar compounds with a log Kow below 2 [23] . Fig. 1 compares the experimental log Koc values with the estimated log Koc values which are derived using the QSAR from USES 2.0 equation 24.

Y=estimated log Koc -experimental log Koc = (log (1.26) +0.81*log Kow) -log Koc {1}

The "best estimates" are used for log Kow at the x-axis and for log Koc. Koc is expressed in liter/kg. The round data points are from the polar substances while the diamond data points are from the hydrophobic substances. The square data points are from the pesticides classified as "difficult" substances which are not classified as polar or hydrophobic substances as described above. The Y value represents the spread of residuals on a logarithmic scale. That means that a Y value of 2 represents an overestimation of Koc by a factor of 100 by USES. The Y values of the difficult and polar pesticides in Fig. 1 range from –2 to 1.8 which is much larger than the range from –0.5 to 0.5 of the Y values of the hydrophobic chemicals with a log Kow from 1 to 4 as reported in the original publication from which the QSAR in equation 1 was derived [23]. At log Kow values between 3 and 4, the Y values scatter around 0 within a range from –1.2 to 1.6 indicating that Koc is correctly predicted within a factor of 40. At log Kow values above 3, Koc is slightly underestimated (on average with a factor 1.6 up to a factor 4 for a-BHC) for the hydrophobic substances but it is overestimated (on

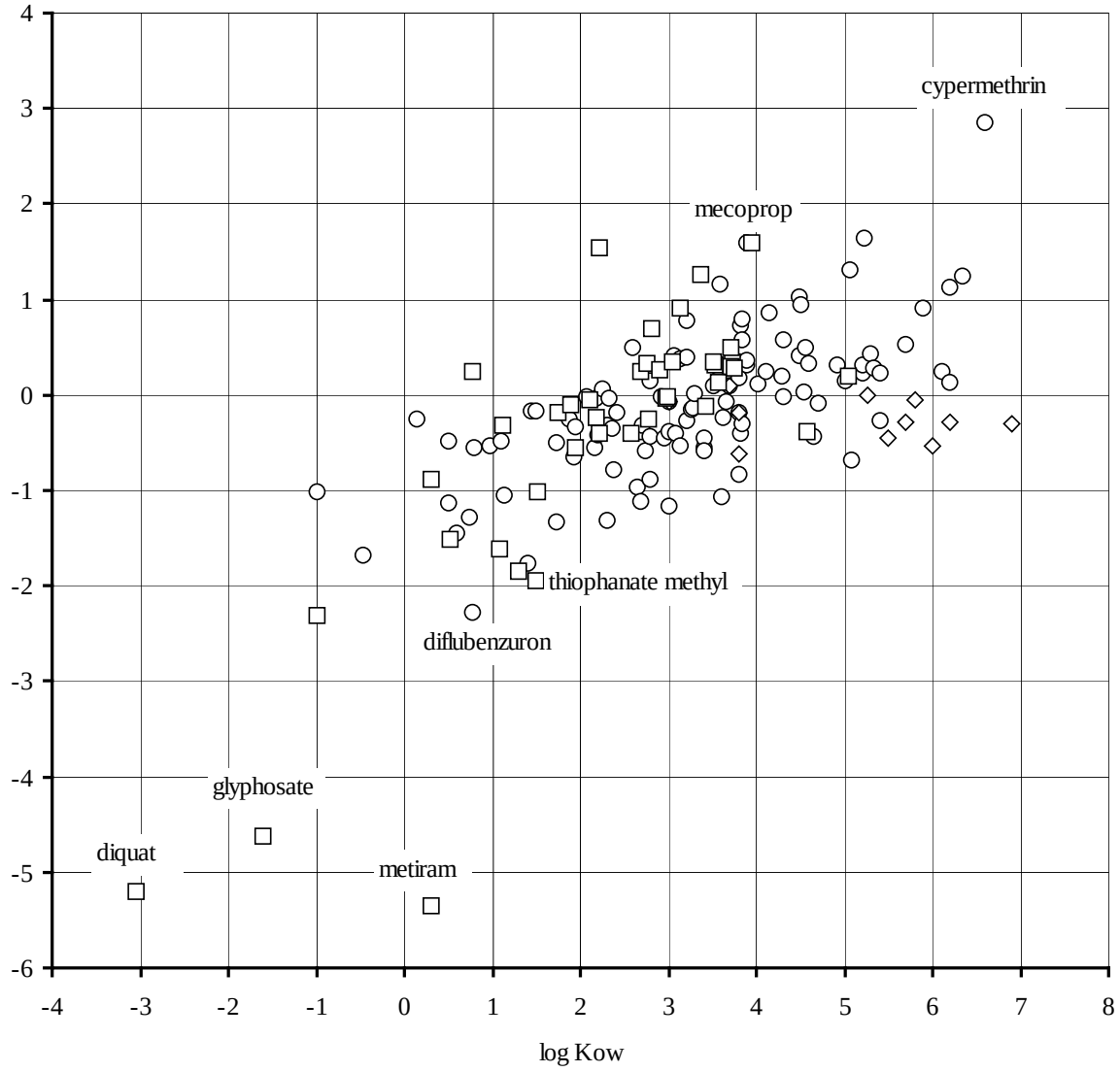

Figure 1 The residual errors of the estimation of log Koc from log Kow by USES calculated using equation 1. The square points represent "difficult" substances, the circles represent polar substances and the diamonds represent hydrophobic substances as defined in paragraph 1.1.

average with a factor 7 up to a factor 44 for Diallate) for the polar substances. Only the Koc of Cypermethrin is largely overestimated. The log Kow of Cypermethrin is 6.6 whereas the experimental log Koc is only 2.59 which gives$Y = 5.45-2.59 = 2.86$ according to equation 1. This gives an overestimation factor of $10^{2.86} = 724$. This outlier might be caused by the selection of the "best" values by Mackay [18] since a log Kow of 4.47 and a log Koc of 4.53 were also reported [18]. These latter two values would give a $Y = -0.81$ which corresponds with an underestimation with a factor 6. This example clearly indicates the importance of selecting the right input data for the notified chemical by the regulatory authorities. Fig. 1

also shows that the Koc values estimated from a log Kow below 3 are highly underestimated. In table 1 there are no pesticides classified as hydrophobic pesticides consisting solely of carbon, hydrogen and halogen atoms, with a log Kow below 3 which means that there are only polar or difficult substances with low Kow values. For the polar pesticides with a log Kow below 3, the Koc is underestimated with an average factor of 5.5 with a maximum factor of 190 for Diflubenzuron.

1.4 The estimation of the organic carbon sorption coefficient from the octanol/water partition coefficient of bases and cations

For the pesticides classified as "difficult" substances the prediction of the log Koc seems to work reasonably well for substances with a log Kow above 0.5 (see Fig. 1). On average the Koc is very slightly underestimated with a factor of 1.07 while the maximum overestimation factor is 39 for Mecoprop and the maximum underestimation factor is 87 for Thiophanate methyl (see table 1 for the classification, the log Kow, log Koc and the estimated log Koc). The QSAR from USES can be a factor 1000 off since most pesticides in Fig. 1 have a Y value between –3 and 3 but the Koc of a cationic pesticide like Diquat, a zwitterion like Glyphosate or an organometallic pesticide like Metiram is underestimated with a factor between 10,000 and 100,000 (see Fig. 1). Hydrophobic interaction with soil organic material is probably not the major sorption mechanism for Glyphosate or Metiram. For Diquat the interaction of the positively charged molecule with negatively charged clay particles is the main mechanism for its strong sorption to soil [15]. Note that the sorption is also underestimated for the other positively charged pesticides e.g. Thiophanate methyl and Terbacil. For the pesticides classified as base in table 1 the pKa is below 7 which means that these compounds are normally present as neutral molecules which can be compared with polar substances with a corresponding log Kow. The average difference between the experimentally determined log Koc and the log Koc predicted by USES is -0.62 for the bases and -0.39 for the polar substances in the same range of log Kow (between 0.5 and 3.75). The standard deviation of this difference is 1.27 for the bases and only 0.59 for the polar substances in the same range of log Kow.
This indicates that USES is better at predicting soil sorption for polar substances than for bases. On average the soil sorption of the bases is underestimated with a factor of 4. There is also a large uncertainty in this estimation.

1.5 The estimation of soil sorption from the octanol/water partition coefficient and the pKa of acids

All the acids except Bromacil and Oryzalin have a pKa below 7 and are therefore present as anions in neutral environments. Normally the log Kow of the neutral molecule is measured at relatively high concentrations in an octanol/water partition experiment. For weak and

moderately strong organic acids, this means that the pH in the water phase is lowered unintentionally below the pKa value of the acid. Therefore the log Kow measured below their pKa corresponds quite well with the best estimate of the log Kow of the neutral molecule. In order to measure the log Kow at an environmentally relevant pH value, the acid molecule has to be neutralised with sodium or potassium hydroxide to obtain a sodium or potassium salt of the pesticide. For MCPA, Dinoseb, Mecoprop and pentachlorophenol table 1 shows information about the log Kow measured above and below their pKa. In addition there is information about the log Kow above the pKa (that is the log Kow of the anion) for the acid pesticides Dichlorprop P, Dicamba and Diclofop methyl. Since anions have a relatively high affinity for water, it is obvious that the log Kow of the anion is much lower than the log Kow of the neutral form of the acid molecule. In table 1 the best value of the log Kow of the neutral form of the acid pesticide is used to estimate log Koc with equation {1}. The difference between the experimentally determined log Koc and the predicted log Koc is only 0.22 on average for the acid pesticides with a log Kow above 0.5 in table 1. This indicates that the indiscriminate use of the log Koc of the neutral molecule for dissociating acids in USES gives on average an overestimation of the soil sorption with only a factor 1.66. The standard deviation of this difference is 0.04. The difference between the experimentally determined log Koc and the predicted log Koc from the Kow of the corresponding anion is -2.59 which indicates an underestimation of the soil sorption with a factor of 389. This indicates that the log Kow of the neutral acid is a better predictor for the soil sorption at pH values above the pKa, than the log Kow of the corresponding anion which is present at these pH values. For pentachlorophenol for example the log Kow of the neutral molecule is 4.84 while the log Kow of pentachlorophenolate is only 1.3 (see table 1). This large difference (a factor of 3467) is not found between the log Koc values of different soils which range from 3.49 to 5.71 (a factor of 166) in table 1. The sorption of pentachlorophenol is about 15 to 60 times stronger than the sorption of pentachlorophenolate in soils [13],[14],[24]. This might be due to the interaction of the pentachlorophenolate anion with cations like calcium or potassium which causes an increased sorption of pentachlorophenolate [14]. Alternatively, the sorption of pentachlorophenolate to clay minerals can also play a role [6].
Therefore it is advisable to use the log Kow of the neutral acid form of a molecule in USES to predict soil sorption even when the pKa of the acid indicates that the molecule is in the deprotonated anionic form.

1.6 The estimation of the log bioconcentration factor in fish from the octanol/water partition coefficient of pesticides

The octanol/water partition coefficient is used in USES to estimate the bioconcentration factors in fish, earthworms, plant leaves, plant roots, meat and milk. The bioconcentration factors in fish and earthworms are used to calculate the ecological risks for predators which feed on earthworms or fish. In addition, the bioconcentration factors for fish, plant leaves, plant roots, meat and milk are used together with the concentrations in drinking water and air to calculate the daily intake of the substance in humans. The bioconcentration factor in fish is

calculated with equation 86 in USES 2.0 for substances with a log Kow from 1 to 6 which was derived by Veith [34]. Although this equation was derived for 55 compounds on a single fish species 20 years ago, it was shown to be valid for a much larger array of fish species and organic chemicals [1]. Fig. 2 compares the experimental log BCF for a number of pesticides from Mackay [18] with the estimated log BCF calculated using equation 2.

Y = estimated log BCF -experimental log BCF = (0.85 log Kow -0.70) -log BCF {2}

The best estimate of log Kow from Mackay [18] was used as input parameter. In contrast with the data in Fig. 1 there is much more variation in the BCF compared to the Koc. Therefore each chemical is indicated at its log Kow value as a bar with the bottom showing the minimal log BCF and the top the maximal log BCF. Fig. 2 a shows the Y values of the neutral substances and the Y values of the difficult substances which are listed in table 1. For the neutral compounds there also is a large spread in the data, with a maximal overestimation of 2.83 for Mirex (a factor of 676) and an underestimation of -3.29 for Aldrin (an underestimation factor of almost 2 000). For the neutral compounds the estimated log BCF falls within the wide range of experimental log BCF values except for the log BCF of Aldrin which is systematically underestimated (see also table 1). The underestimation of the log BCF of Aldrin might be attributed to the low log Kow which was selected. The selected log Kow was 3.01 while the rest of the Kow values ranged from 5.48 to 7.5 [18]. For the bioconcentration factors of difficult substances less information was available and therefore the log BCF of many of these substances is indicated as a single point in Fig. 2 because only a single log BCF was available. The maximal underestimation was -1.94 (a factor of 87) for Picloram while the maximal overestimation was 6.69 (a factor of 5 000 000) for 2,4-Dichlorophenoxyacetic acid (2,4-D). This large overestimation is probably caused by biological variation, differences in environmental conditions and by errors in the experimental determination of the bioconcentration factors of 2,4-D which range from an extremely low value of log BCF = -5 to 1.94 (see table 1). With a log Kow = 2.81 an estimated log BCF of 1.69 was calculated in table 1 for 2,4-D. A possible overestimation of an already low log BCF is of little consequence for the risk evaluation since it does not matter whether the risk is low or extremely low. Most of the difficult substances have a log Kow below 4 and show log BCF values below 2.5. Fig. 2b shows the Y values of the polar substances, the neutral substances and the difficult substances. Apparently, the log BCF for the polar compounds with the log Kow above 3 is slightly overestimated. From the figures 2a and 2b it can be concluded that the bioconcentration factor for fish is not predicted with great accuracy by USES 2.0 since the measured values can be a factor 1000 higher or lower than the predicted values. The figures 2a and 2b also indicate that the predicted bioconcentration factors for difficult substances seem to fall within this range. For example the BCF of PCP was reported to be 584 at pH 6 when 5% of the PCP is in the pentachlorophenol form, while the BCF was 8.9 at pH 10 when the percentage in the neutral pentachlorophenol form was 10,000 times lower [12]. The difference between 584 and 8.9 is only a factor of 66 which is relatively small compared to a factor of 1000.

This indicates that for acid pesticides, the log Kow value of the neutral molecule can be used in equation 2 since it gives a better prediction of the bioconcentration factor compared to log Kow value of the corresponding anion of the acid pesticide.

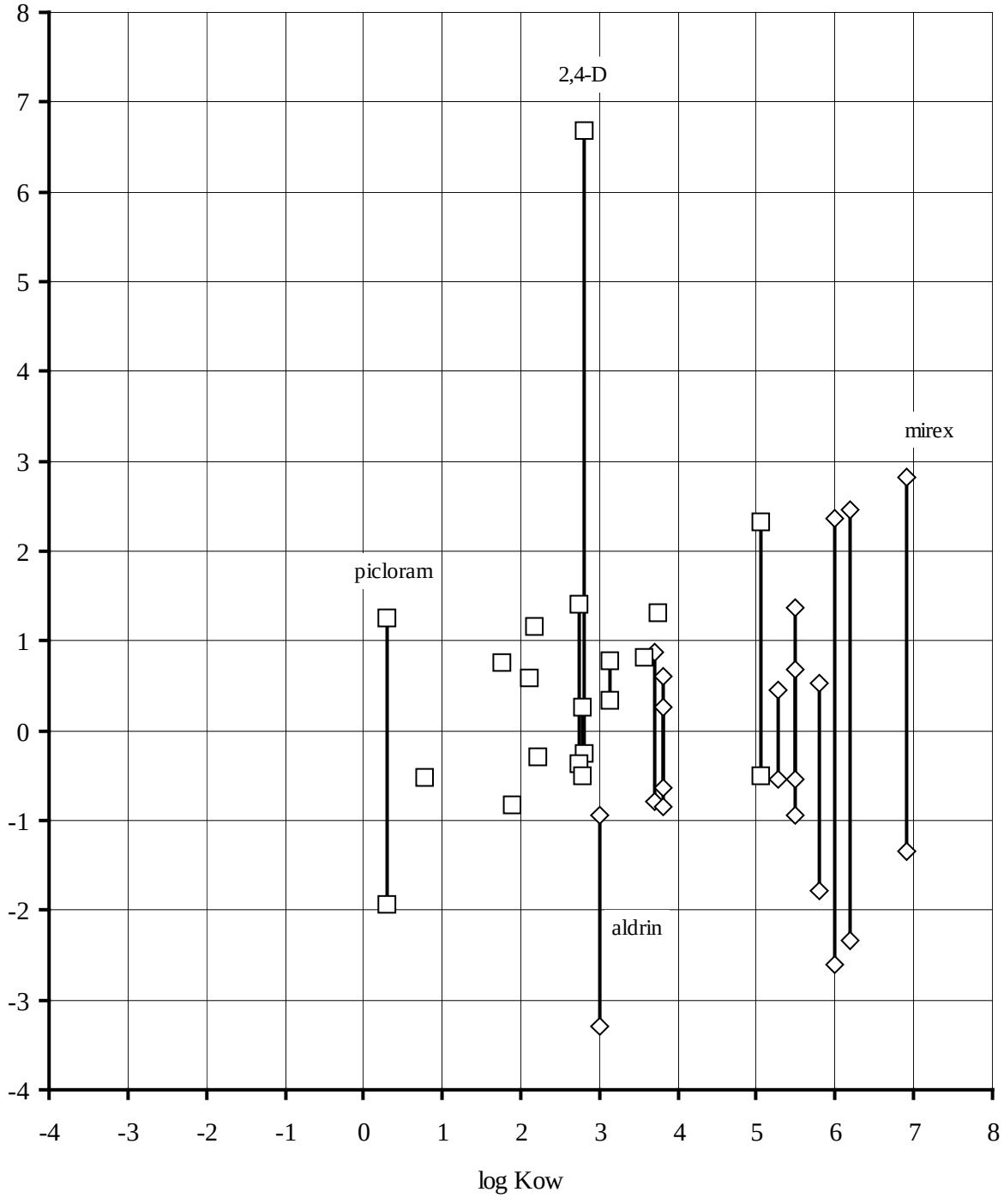

Fig. 2a. The residual errors of the estimation of log BCF by USES calculated using equation 2. The bars represent the range of experimental log BCF values of a single substance. The square points represent "difficult" substances and the diamonds represent hydrophobic substances.

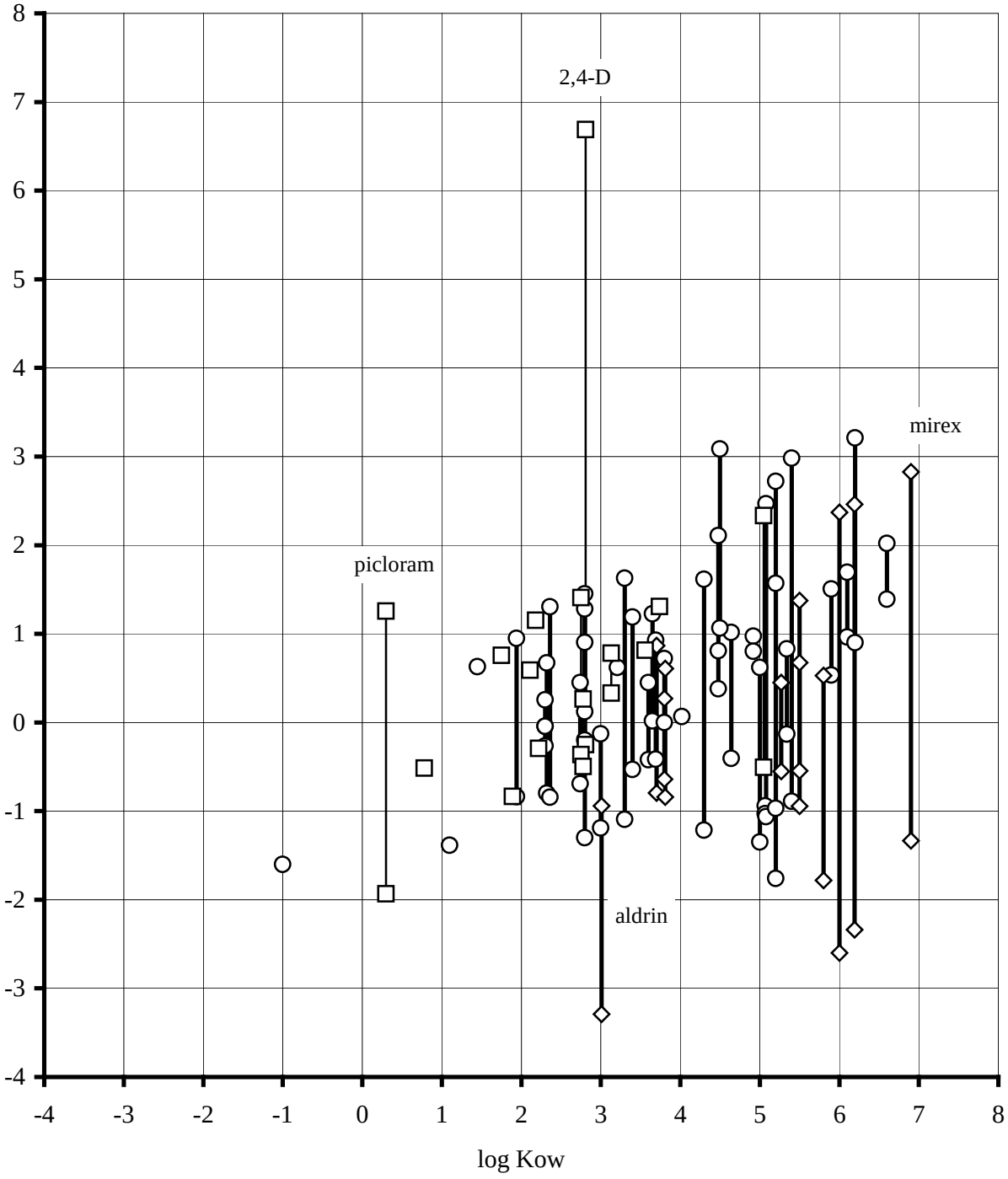

Fig. 2b. The residual errors of the estimation of log BCF by USES calculated using equation 2. As in Fig. 2a the bars represent the rates of experimental log BCF values of a single substance but here also the hydrophobic substances are shown. The square points represent "difficult" substances, the circles represent polar substances and the diamonds represent hydrophobic substances.

1.7 The estimation of the log bioconcentration factor in fish from the octanol/water partition coefficient of difficult compounds which are not pesticides

The selected data set of pesticides shown in table 1 gives only limited information about the bioconcentration factors for difficult substances. Therefore more information was gathered from a few recent reviews on the bioconcentration of compounds which were obtained by a literature search from 1996 to November 1999. These reviews contained information on the bioconcentration of a few classes of difficult substances like phenols, anilines, surfactants, organometallic compounds and metals.
For a large data set of 68 phenols and 56 anilines with a log Kow below 4 a log BCF value of 0.5 was estimated regardless of pKa and log Kow [19]. Even for the few phenols or anilines with a log Kow above 4 a relatively low log BCF below 2 was estimated [19]. The computer program “BCFwin” [19] can be used to calculate the bioconcentration factor for fish in a more detailed way for a wider range of compounds than is available in USES. The bioconcentration of ionizable organic compounds in fish cannot be accurately predicted by the partitioning between water and octanol or phospholipids because the pH and ionic composition of the water layer on the gills will be different from the exposure medium [33]. Triphenyltin and tributyltin can be converted to cationic forms at pH 5 which have a log BCF value of 2.7 and 2.2 while the neutral forms at pH 8 have a slightly higher log BCF value of 2.8 and 2.5 respectively [17]. For tributyltin with a pKa value of 6.25, the log Kow is 4.1 at pH 8 and 2.9 at pH 5 [17]. Apparently the log Kow value of the neutral molecule is a better predictor of the log BCF than the log Kow value of the cation of these organotin compounds. Surfactants reduce surface tension of water in a concentration dependent manner until the point of self association is reached. They are subdivided into anionic, cationic, amphoteric and nonionic surfactants. The bioconcentration factors range between 2.4 for octyltrimethylammonium chloride and 1960 for tallow trimethylammonium chloride [28] and tend to increase with Kow and the length of the alkyl side chain.
The bioaccumulation of difficult substances in the preceding paragraphs was studied by searching biodegradation data for difficult substances. The bioaccumulation problem can also be approached from a different side and by gathering data from the compounds which are known to bioaccumulate. Among the 25 compounds which were selected by the author as compounds with a potential for secondary poisoning only methyl mercury and pentachlorophenol could be classified as difficult organic substances[31]. Cadmium, copper, and mercury are metals with a high potential for secondary poisoning while the remaining 20 compounds were pesticides with a high bioaccumulation factor [31]. Methyl mercury is a difficult substance because it is a monovalent cation which can form stable complexes with sulphur compounds and with anions like chloride, carbonate of sulphate [26]. These complexes can bioaccumulate in fish [7]. Methyl mercury has a log Kow of 1.5 at pH 5 and 0.2 at pH 9 [5], the average log BCF is 4.1 and the maximal value is 4.5 [31]. For tin and mercury compounds, the log BCF for fish can be calculated from the log Kow using the

equation of Veith [34] which is the default in USES when 1.4 is added to the estimated log BCF [19].
In conclusion it is clear that for organic acids and bases the log Kow value of the neutral molecule is a better predictor of the log BCF than the log Kow value of the corresponding anion or cation. Even for metal compounds and surfactants a high log Kow value is associated with an increased risk of bioconcentration.

1.8 Conclusion on the estimation of sorption and bioconcentration by USES

Difficult substances like acids, bases, cations, anions, amphoteric molecules or surfactants show a more complex environmental behaviour than neutral substances. These difficult substances often show strong interactions with other cations, anions or complexing agents and their sorption to soil and their bioaccumulation, are often dependent on the pH and other environmental conditions. The partition of surfactants, cations, anions, organometallic compounds, and inorganic compounds can not be predicted from the octanol/water partition coefficient by USES. The octanol/water partition coefficient of the neutral form of many acids or bases can be used to predict soil sorption and bioaccumulation. This Kow of the neutral form can even give a better prediction of sorption to organic matter at pH values where the acid is mainly in the anionic form or the base is mainly in the cationic form because many cations and anions can form neutral complexes under environmental conditions. The prediction of the sorption coefficient by USES from the octanol/water partition coefficient of polar compounds including acids and bases can be a factor 1000 to high or to low. Whereas most difficult substances show a relatively low bioaccumulation there are some exceptions which show strong bioaccumulation up to a log BCF of 4.5. The uncertainties in the estimation of the log BCF for difficult substances are not significantly larger than the already large uncertainties for hydrophobic substances. Table 2 presents the different approaches to estimate the sorption and bioaccumulation factors from the octanol/water partition coefficient.

Table 2 The application of different approaches for the risk assessment of various classes of difficult compounds by USES.

Classes of compounds	Log Kow available?	Default USES?	Default USES with factor 1000?	Class specific QSAR available?
Inorganic cations	No	No	No	No
Inorganic anions	No	No	No	No
Neutral inorganic compounds	No	No	No	No
Organic cations	Yes	No	No	?
Organic anions	Yes	No	No	?
Organic acids	Yes	No	Yes	Yes
Organic bases	Yes	No	Yes	Yes
Organic surfactants	Yes	No		Yes
Polar organic compounds	Yes	No	Yes	Yes
Hydrophobic organic compounds	Yes	Yes	Not necessary	In USES

2. The influence of uncertainties in the log Kow value on the risk assessment performed by USES

The previous section of this report indicated that for different classes of difficult substances the default approach of USES can be applied with different levels of confidence. For some classes of difficult compounds the use of a Kow value as input for USES clearly gives erroneous estimations of the sorption and the bioconcentration factors. For other classes however the estimations deviated up to a factor 1000 from measured sorption or bioconcentration factors. These large uncertainties surely have an impact on the outcome of the calculations performed by USES. This impact was estimated by running USES a number of times with a hypothetical compound which is nonbiodegradable and nonvolatile with different log Kow values.Table 2 shows the outcome of the calculations by USES 2.0 for a hypothetical compound which has a production volume in EU of 1 ton per year, a molecular weight of 100 gram/mol, the melting point of 400 ºC, a boiling point of 500 ºC, a vapor pressure of 1 µPa and a water solubility of 100 gram/litre. The solubility is set at an extremely high level to avoid the estimation of a high Henry coefficient according to equation 22 at p. III-21 in the USES 2.0 documentation. Normally, high log Kow values are associated with low solubilities but the unrealistically high solubility gives no problem in the USES calculations as long as the evaporation is negligible. Many difficult substances have a very low vapor pressure [30]. The compound is assumed to be non-biodegradable and all default assumptions of USES are used to calculate the environmental concentrations due to processing at the local scale. The default assumptions lead to a local emission to waste water of 73.3 kg in one day. The input concentration in untreated waste water is 36.7 mg/litre and the treated waste water is diluted 10 times with river water.

Table 3. The outcome of USES calculations with different log Kow values for a hypothetical compound.

			surface water	sediment	soil	ground water	fish	worms	humans
log Kow	log Koc	log BCF	mg/liter	mg/kg	mg/kg	µg/liter	mg/kg	Mg/kg	mg/kg/day
-1	-0.71	0.15	3.67	3	0.003	12	0.01	0.002	0.001
0	0.10	0.15	3.66	3	0.019	73	0.01	0.015	0.008
1	0.91	0.15	3.66	4	0.149	395	0.01	0.079	0.10
2	1.72	1.00	3.64	7	2	1930	0.05	4	0.60
3	2.53	1.85	3.51	29	39	6250	0.34	125	1.49
4	3.34	2.70	2.88	139	271	6980	1.98	1400	3.95
5	4.15	3.55	1.41	435	819	3280	6.87	6560	14.60
6	4.96	4.40	0.48	946	1160	720	16.40	14400	28.40
7	5.77	4.66	0.18	2270	1240	119	11.10	7530	41.90

2.1 Soil sorption and bioconcentration

For compounds with a log Kow of -1 virtually all the emission ends up in surface water, while for compounds with a log Kow of 7 most of the emission is bound to sludge and eventually spread out on agricultural soil. For the local environmental distribution of substances with a very low volatility and a high log Kow the main emission route in USES goes via the sewage treatment plant to agricultural soil and subsequently to groundwater and bioaccumulation in worms, plants, meat and milk. The bioaccumulation in plants, meat, milk and fish together with drinking water pollution and air pollution is used to calculate the total exposure of humans. As this report focuses on substances which have a "difficult" environmental distribution, only the predicted environmental concentrations are shown in table 3 and not the Risk Characterisation Ratios. These RCRs are obtained by dividing the predicted environmental concentration from the distribution module, by the predicted no effect concentration from the effect module. The previous section of this report indicated that for most classes of difficult compounds the Koc value estimated from the log Kow can be a factor 1000 higher or lower than the measured Koc value. This indicates that the predicted sewage sludge concentration and as a result the predicted soil concentration might be a factor 1000 too low. Therefore only an RCR below 0.001 can be considered as safe. With RCR values above 0.001 it is worthwhile to look for more accurate estimates of the Koc value. This is indicated in the decision tree in the appendix. The RCR value for human exposure is calculated from the daily uptake divided by the lowest observed adverse effect level, which are both in kg compound per kg body weight per day.

2.2 The risk assessment for aquatic ecosystems

Fig. 1 shows that the sorption to sludge (expressed as log Koc) is underestimated with a factor of about 100 000 for the pesticides Diquat, Glyphosate and Metiram when the very low log Kow values of these compounds are used. For the risk assessment for aquatic ecosystems this underestimation does not have large consequences since the measured log Koc values are below 5.7. Table 2 shows that the surface water concentration drops from 3.67 mg/litre to 0.18 when the log Koc rises from -0.71 to 5.77. The difference between 3.67 and 0.18 (a factor 20) is relatively minor compared to the large uncertainties which are encountered in these risk assessment procedures. Moreover an overestimation of the predicted environmental concentration in water with a factor 20 leads to an overestimation of RCRs with a factor 20 for difficult substances which might be quite acceptable for most of the notified difficult substances.

2.3 The risk assessment for soils, groundwater and sediments

While the surface water concentration drops a factor of 20 when the log Kow is increased from -1 to 7, the soil concentration increases from 0.003 to 1240 mg/kg (a factor of 413000) in the calculations of USES. When a log Kow of 0.3 is entered in USES for Metiram a log Koc of 0.34 is calculated, while measurements have indicated that a log Koc of 5.7 is more appropriate (see table 1). Table 2 illustrates the large differences between the calculated environmental concentrations with an estimated log Koc of 0.34 or with the measured log Koc of 5.7. While the water concentration is overestimated with a factor 18, the sediment concentration is underestimated with a factor 700 and the soil concentration is underestimated with a factor 36000. The groundwater concentration happened to be estimated quite accurately in this example, but this is a coincidence because the estimated groundwater concentration rises from 0.012 mg/litre at a log Kow of -1 to 6.98 at the log Kow of 4 and then drops again to 0.119 and a log Kow of 7 (see table 2). In conclusion it is clear that the estimated concentrations in soils, groundwater and sediments are very sensitive for errors in the estimation of log Koc. In the decision tree presented in the appendix 1 a more refined estimation of log Koc is only required when the RCR of the terrestrial environment in the preliminary risk assessment is above 0.001 because in that case an underestimation of the Koc with a factor 1000 might lead to an actual RCR above 1.

2.4 The risk assessment for humans and predators

For most difficult compounds in table 1 the prediction of the bioconcentration factor for fish is a factor 1/100 to 100 from the experimental value. This uncertainty in the estimation is not significantly larger for than the uncertainty in the estimation of the bioconcentration factor for fish of the simple apolar compounds that USES was made for. The bioconcentration factor for the difficult compounds in table 1 was also relatively low compared to the corresponding factor for neutral compounds. Therefore it seems that no special measures are

needed when the bioconcentration factor of difficult substances is estimated with USES. The estimation method of the bioconcentration factor from the log Kow in USES is relatively crude and more refined methods have recently become available. For compounds for which a SMILES notation is available it can be recommended to use a commercially available computer program to calculate the bioconcentration factor for fish in a more detailed way [19]. This program calculates the bioconcentration factor for different classes of chemicals in different ways and was validated with experimental data.

2.5 A practical solution for the risk assessment of difficult compounds when information about the environmental partitioning is absent

Table 2 shows the variation in the environmental partitioning behaviour which occurs for compounds with a log Kow of -1 to 7. This actually is the uncertainty which is present for difficult compounds where no information about environmental partitioning is available. This large uncertainty can be circumvented by taking a hypothetical log Kow of 6 for these difficult compounds together with a more cautious interpretation of the so-called Risk Characterisation Ratios. Table 2 shows that USES calculates at log Kow of 6 a surface water concentration which is more than 10% of the maximal value, a sediment concentration which is 50% of the maximal value, and a soil concentration which is roughly equal to the maximal value. When a log Kow of 6 is inserted in USES for compounds for which there is no information about environmental partitioning available, theRCRs for the aquatic environment should stay below 0.1, for the sediment compartment below 0.5, and for the terrestrial compartment below 1.0. Table 2 also shows that a log Kow of 6 gives the maximal concentration in fish and worms and a concentration in humans which is 68% of the maximal value. This indicates that the RCRs for humans should be below 0.68, while it should be below 1.0 for fish eating predators and worm eating predators. This approach should only be followed in the absence of any data about the environmental partitioning. It is only suitable as an indicator whether information about the environmental partitioning is needed or not.

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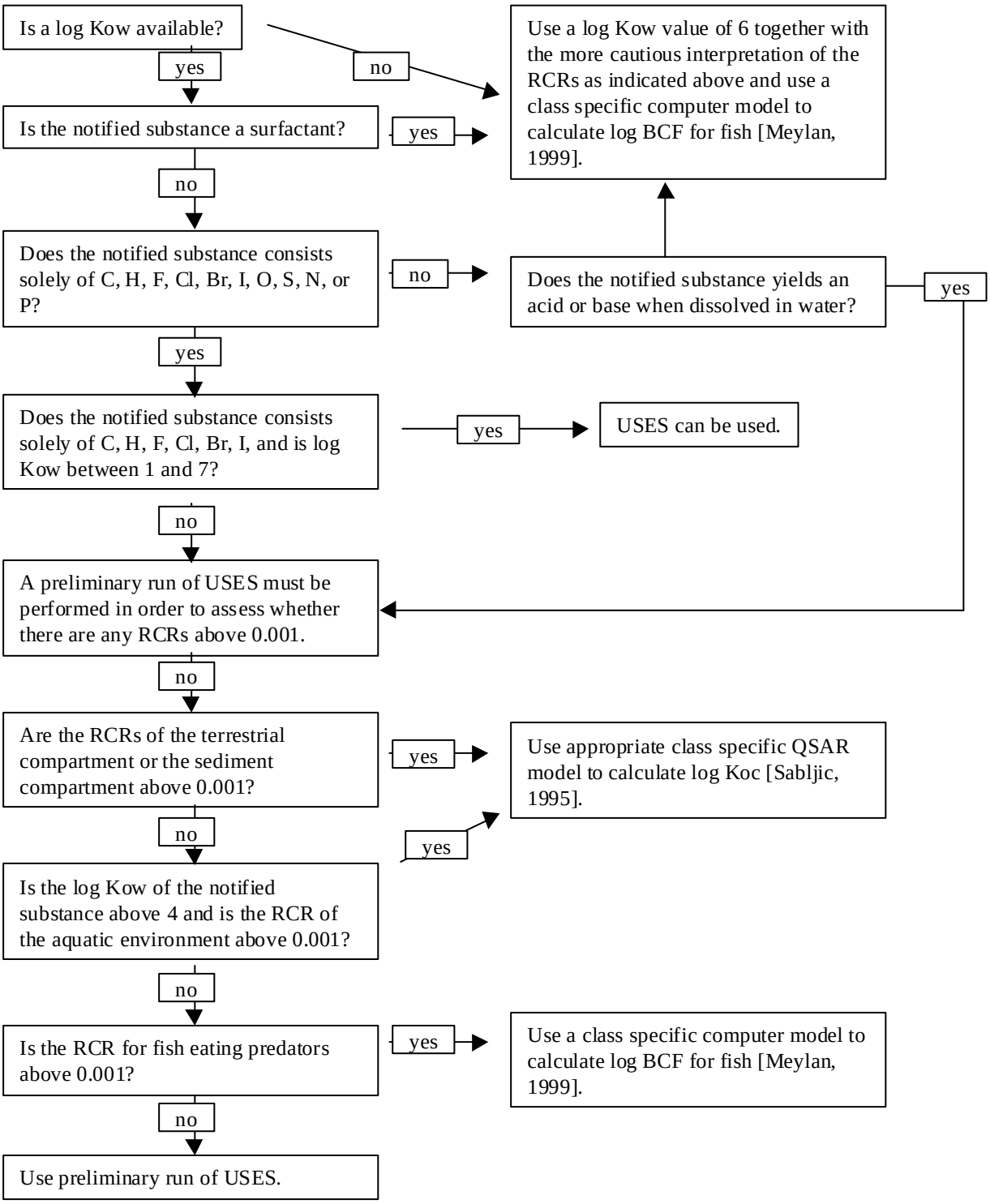
Appendix 1

A flow chart for the introduction of difficult substances in USES



A guide for the use of the decision tree.

The decision tree starts at the upper left with the question if an octanol/water partition coefficient for the notified substance is available. The decision tree has five different endpoints which require a run of the USES computer program which can lead to either the acceptance of the notified substance or a question for more information for a proper risk assessment.

Notified surfactants can often be recognised since data on the effects of these compounds on the surface tension of water are required in the base set for notification. The question whether the notified substance yields a cation or an anion when dissolved in water requires detailed chemical knowledge. When the pKa of an anion is available it is considered to be an acid. When the pKa of the cation is available it is considered to be a base. For acids and bases a preliminary run of USES must be performed in order to assess if there are any RCRs above 0.001.

The question whether the notified substance yields and acid or base when dissolved in water is relatively complicated and requires detailed chemical knowledge. Many metals salts dissolve into a metal cation and an organic anion in water. When this organic anion picks up a proton from the water a neutral organic acid can be formed which consists only of C, H, O, S, N, P, F, Cl, Br, or I. When the pKa and the log Kow value of this organic acid can be estimated a more detailed analysis by USES is possible. One has to be reasonably sure however that the toxicity can be attributed to the organic moiety and not to the metal part of the notified substance. In general the toxicity of metals like Na, K, Ca, Mg, and Fe is relatively low while many heavy metals are relatively toxic. In organometallic compounds the metal atom is directly attached to a carbon atom. This metal carbon bond can be so strong that it is stable in water. The Na and K atoms are generally present as cations in salts and do not form organometallic compounds. For example, $NaCl_3CCO_2$ is not an organometallic compound and it will split into the cation Na^+ and the anion $Cl_3CCO_2^-$ when dissolved in water. This also means that the risk assessment of $Ca(Cl_3CCO_2)_2$ is very similar to that of $NaCl_3CCO_2$ since the anion $Cl_3CCO_2^-$determines the environmental risk while the Na^+ and Ca^{2+} cations are relatively harmless.

For the upper right endpoint of decision tree a default log Kow = 6 is used and the RCRs for water should stay below 0.1, for sediment below 0.5, for soil below 1.0, for predators below 1.0 and for humans below 0.68 as mentioned in paragraph 2.5.

For the other four endpoints of the decision tree, the RCRs should stay below 1.0 as is normally the case in USES. The RCRs above 0.001 are only used to indicate when more effort is needed for a more detailed risk assessment.

Appendix 2

Table 1. The estimation of log Koc and log BCF from log Kow.

Name		pKa*	log Kow			log Koc			log BCF		log Koc	log BCF
			best	above	below	best	lowest	highest	lowest	highest	calculated	calculated
Chlorsulfuron	acid	**3.6**	-1	**-1.34**		1.6	1.02	1.6			-0.71	-1.55
Picloram	acid	2.3	0.3			1.23	-0.222	2.2	-1.7	1.49	0.34	-0.45
Dalapon	acid	1.79	0.78			0.48	0	2.13	0.477		0.73	-0.04
Chloramben	acid	**3.4**	1.11			1.32	1.32	2.28			1.00	0.24
Dichlorprop-P	acid	3.67	1.95	-0.25		2.23					1.68	0.96
Dicamba	acid	1.97	2.21	-0.15		0.342	-1	2.67			1.89	1.18
MCPA	acid	3.07	2.69	0.46	2.75	2.03	-0.57	3.25			2.28	1.59
2,4-D	acid	2.73	2.81		2.7	1.68	1	2.73	-5	1.94	2.38	1.69
2,4,5-T	acid	**2.8**	3.13			1.72	1.72	2.63	1.18	1.63	2.64	1.96
Dichloroprop	acid	3	3.43			3	1.08	1.6			2.88	2.22
2,4-DB	acid	4.8	3.53			2.64	1.3	2.64			2.96	2.30
Dinoseb	acid	**4.62**	3.56	**3**	**3.57**	2.85	1.48	3.82	1.51		2.98	2.33
Mecoprop	acid	3.78	3.94	0.1004	3.2	**1.705**	1.3	2.11			3.29	2.65
Diclofop-methyl	acid	3.43	4.58	1.61		4.2	4.15	4.39			3.81	3.19
Pentachlorophenol	acid	4.71	5.05	1.3	4.84	4	3.49	5.71	1.26	4.1	4.19	3.59
Bromacil	acid -neutral	9.27	2.11		1.88	1.86	1.34	3.13	0.505		1.81	1.09
Oryzalin	acid -neutral	9.4	3.73		3.73	2.78	2.78	3.04			3.12	2.47
Amitrole	base	4.2	0.52			2.04	1.73	2.31			0.52	-0.26
Carbendazim	base	4.2	1.52	1.51		2.35	2.3	2.69			1.33	0.59
Metalaxyl	base	0	1.75			1.7	1.7	3.22	0.03		1.52	0.79

Name		pKa*	log Kow			log Koc			log BCF		log Koc	log BCF
			best	above	below	best	lowest	highest	lowest	highest	calculated	calculated
Simazine	base	1.62	2.18	2.1		2.11	1.43	3.34	0		1.87	1.15
Cyanazine	base	0.63	2.22			2.3	0.48	2.63	1.48		1.90	1.19
Ametryn	base	4.1	2.58			2.59	2.23	2.59			2.19	1.49
Atrazine	base	1.7	2.75			2	0.7	4.13	0.23	2	2.33	1.64
Diuron	base	**-1**	2.78			2.6	1.97	3.03	1.4	2.16	2.35	1.66
Propazine	base	1.7	2.9			2.19	1.69	2.56			2.45	1.77
Fluridone	base	**1.7**	2.98	1.87		2.544	1.6	3.81			2.51	1.83
Prometon	base	4.3	2.99			2.54	1.92	3.93			2.52	1.84
Terbuthylazine	base	2	3.04	3.21		2.21					2.56	1.88
Etridiazole	base	2.77	3.37			**1.5745**	0.149	3			2.83	2.16
Prometryn	base	4.1	3.51	3.1		2.6	2.28	2.92			2.94	2.28
Propiconazole	base	1.09	3.72	3.72		2.82					3.11	2.46
Penconazole	base	1.51	3.72	3.72		2.62					3.11	2.46
Terbutryne	base	4.3	3.74	3.65		2.85	2.85	4.07	1.17		3.13	2.48
Thiophanate-methyl	base-cation	7.28	1.5			3.26	0.079	3.26			1.32	0.58
Terbacil	base-cation	**9**	1.89			1.74	1.62	1.98	1.74		1.63	0.91
Diquat	cation	4	-3.05			**2.84**	2.84				-2.37	-3.29
Glyphosate	ionic	3	-1.6			3.43	-0.43	3.69			-1.20	-2.06
Metiram	organometallic		0.3			5.7					0.34	-0.45
Ziram	organometallic		1.086			2.6					0.98	0.22
Zineb	organometallic		1.3			3					1.15	0.41
Acephate	polar		-1			0.301	0.3	0.48	0.053		-0.71	-1.55
Oxamyl	polar		-0.47			1.4	-0.7	1.84			-0.28	-1.10
Dazomet	polar		0.15			0.48					0.22	-0.57
Mevinphos	polar		0.5			1.64					0.51	-0.28

Name		pKa*	log Kow			log Koc			log BCF		log Koc	log BCF
			best	above	below	best	lowest	highest	lowest	highest	calculated	calculated
Trichlorfon	polar		0.51			1	0.99	1.9			0.51	-0.27
Methomyl	polar		0.6			2.03	1.86	2.2			0.59	-0.19
Oxycarboxin	polar		0.74			1.98					0.70	-0.07
Diflubenzuron	polar		0.78			3.01					0.73	-0.04
Dimethoate	polar		0.8			1.3	0.72	1.56			0.75	-0.02
Fenuron	polar		0.98			1.43	0.88	1.43			0.89	0.13
Aldicarb	polar		1.1			1.48	0.85	1.67	1.62		0.99	0.24
Pyrazon (chloridazon)	polar		1.14			2.08	1.95	2.53			1.02	0.27
Tricyclazole	polar		1.4			3					1.23	0.49
Dichlorvos	polar		1.45			1.45			-0.097		1.27	0.53
Propoxur	polar		1.5			1.48	0.48	1.97			1.32	0.58
Aminocarb	polar		1.73			2					1.50	0.77
Thirain	polar		1.73			2.83	2.82	3.39			1.50	0.77
Dicrotophos	polar		1.88			1.88	1.04	2.27			1.62	0.90
Diphenamid	polar		1.92			2.31					1.66	0.93
Monuron	polar		1.94			2	1.46	2.36	0	1.786	1.67	0.95
Chloropicrin	polar		2.07			1.79	1.79	1.91			1.78	1.06
Carboxin	polar		2.17			2.41	2.41	0.57			1.86	1.14
Propachlor	polar		2.18			1.9	1.9	2.42			1.87	1.15
Triforine	polar		2.2			2.3					1.88	1.17
Crotoxyphos	polar		2.23			2.23	2	2.23			1.91	1.20
Isoproturon	polar		2.25			1.86					1.92	1.21
Monolinuron	polar		2.3			2.3	1.6	2.7	1.3	1.52	1.96	1.26
Benomyl	polar		2.3			3.28					1.96	1.26
Captan	polar		2.3			2.29	2.06	2.3	1	1.3	1.96	1.26

Name		pKa*	log Kow			log Koc			log BCF		log Koc	log BCF
			best	above	below	best	lowest	highest	lowest	highest	calculated	calculated
Carbofuran	polar		2.32			2.02	1	2.7	0.6	2.07	1.98	1.27
Carbaryl	polar		2.36			2.36	1.78	2.59	0	2.15	2.01	1.31
Chlortoluron	polar		2.38			2.81	1.78	2.81			2.03	1.32
Fluometuron	polar		2.42			2.24	1.46	2.57			2.06	1.36
Propham	polar		2.6			1.71	1.71	2.3			2.21	1.51
Chlorothalonil	polar		2.64			3.2	2.76	4.15			2.24	1.54
Barban	polar		2.68			2.66					2.27	1.58
Thiabendazole	polar		2.69			3.4					2.28	1.59
Azinphos-methyl	polar		2.7			2.61	1.3	3.53			2.29	1.60
Dichlobenil	polar		2.74			2.91	2.08	2.96	1.18	2.32	2.32	1.63
Alachlor	polar		2.8			2.23	1.63	2.53	0.778	1.88	2.37	1.68
Malathion	polar		2.8			3.26	0.903	3.26	0.4	2.98	2.37	1.68
Phosmet	polar		2.8			2.8			0.23	1.56	2.37	1.68
Methiocarb	polar		2.92			2.48	2.08	2.32			2.47	1.78
Thiobencarb	polar		2.95			2.95					2.49	1.81
Linuron	polar		3			2.91	2.19	2.93			2.53	1.85
Parathion- methyl	polar		3			3.7	1.699	3.99	1.98	3.04	2.53	1.85
Vinclozolin	polar		3			2.6	2	2.87			2.53	1.85
Propanil	polar		3.07			2.17	2.17	2.9			2.59	1.91
Triadimenol	polar		3.08			3					2.60	1.92
Metolachlor	polar		3.13			2.26	2	2.49			2.64	1.96
Procymidone	polar		3.14			3.18					2.64	1.97
EPTC	polar		3.2			2.3	2.23	2.45			2.69	2.02
Warfarin	polar		3.2			2.96					2.69	2.02
Molinate	polar		3.21			1.92	1.92	2.28	1.41		2.70	2.03

Name		pKa*	log Kow			log Koc			log BCF		log Koc	log BCF
			best	above	below	best	lowest	highest	lowest	highest	calculated	calculated
Pronamide	polar		3.26			2.9	2.3	2.9			2.74	2.07
Propyzamide	polar		3.28			2.9					2.76	2.09
Diazinon	polar		3.3			2.76	2.12	3.27	0.477	3.2	2.77	2.11
a-Endosulfan	polar		3.4			3.4					2.85	2.19
Fenitrothion	polar		3.4			3.3	2.63	3.3	1	2.72	2.85	2.19
Benalaxyl	polar		3.4			3.44	3.44	3.86			2.85	2.19
Chlorpropham	polar		3.51			2.85	2.6	2.91			2.94	2.28
Phorate	polar		3.56			2.82	2.32	3.6			2.98	2.33
Ethoprophos	polar		3.59			1.85					3.01	2.35
Endosulfan	polar		3.6			4.09	3.11	4.3	1.91	2.78	3.02	2.36
Folpet	polar		3.63			3.27					3.04	2.39
Fluorodifen	polar		3.65			3.13			1.178	2.386	3.06	2.40
Phenthoate	polar		3.69			3			1.51	2.85	3.09	2.44
Fenarimol	polar		3.69			2.78	0.176	2.78			3.09	2.44
Neburon	polar		3.8			3.36	3.36	3.49			3.18	2.53
Parathion	polar		3.8			4.02	2.26	4.2	1.81	2.53	3.18	2.53
Anilazine	polar		3.8			3					3.18	2.53
Chlorfenvinphos	polar		3.82			2.47	2.23	2.47			3.19	2.55
Imazalil	polar		3.82			3.6	1.83	3.6			3.19	2.55
P-Endosulfan	polar		3.83			3.5					3.20	2.56
Pebulate	polar		3.84			2.63	2.63	2.8			3.21	2.56
Vernolate	polar		3.84			2.414					3.21	2.56
Fonofos	polar		3.9			2.94	1.18	2.94			3.26	2.62
Buprirmate	polar		3.9			2.9					3.26	2.62
Tolylfluanid	polar		3.9			1.66					3.26	2.62

Name		pKa*	log Kow			log Koc			log BCF		log Koc	log BCF
			best	above	below	best	lowest	highest	lowest	highest	calculated	calculated
Disulfoton	polar		4.02			3.25	2.67	3.72	2.65		3.36	2.72
Fenthion	polar		4.1			3.18					3.42	2.79
Butylate	polar		4.15			2.6	2.73	4.09			3.46	2.83
Triallate	polar		4.29			3.38	3.34	3.56			3.58	2.95
Dinitramine	polar		4.3			3.6					3.58	2.96
Fenoxycarb	polar		4.3			3	0.89	3.18	1.34	4.17	3.58	2.96
Bifenox	polar		4.48			**3.315**	2.24	4.39	2.3		3.73	3.11
Terbufos	polar		4.48			2.7	2.46	3.03	1	2.73	3.73	3.11
Butachlor	polar		4.5			2.8	2.85		0.041	2.06	3.75	3.13
Butralin	polar		4.54			3.75	3.91				3.78	3.16
Tolclofos-methyl	polar		4.56			3.3					3.79	3.18
Fluchloralin	polar		4.6			3.5	3.56	3.6			3.83	3.21
Quintozene	polar		4.64			4.3	3.38	4.3	2.23	3.65	3.86	3.24
Isopropalin	polar		4.71			4	4	4.88			3.92	3.30
Chlorpyrifos	polar		4.92			3.78	1.61	4.37	2.51	2.68	4.09	3.48
Heptachlor Epoxide	polar		5			4			2.93	4.9	4.15	3.55
Ronnel	polar		5.07			2.9			4.55	4.64	4.21	3.61
Methoxychlor	polar		5.08			4.9	2.79	5	1.15	4.68	4.22	3.62
Dieldrin	polar		5.2			4.08	3.36	4.55	1	5.48	4.31	3.72
Endrin	polar		5.2			4			2.15	4.69	4.31	3.72
Diallate	polar		5.23			2.7	2.28	3.52			4.34	3.75
Benefin	polar		5.29			3.95	3.95	3.95			4.39	3.80
Trifluralin	polar		5.34			4.14	2.7	4.49	3.01	3.97	4.43	3.84
Bromoxynil octanoate	polar		5.4			4.25					4.47	3.89
Kepone	polar		5.4			4.74			0.91	4.78	4.47	3.89

Name		pKa*	log Kow			log Koc			log BCF		log Koc	log BCF
			best	above	below	best	lowest	highest	lowest	highest	calculated	calculated
Ethion	polar		5.7			4.19	3.54	4.34			4.72	4.15
Leptophos	polar		5.9			3.97	3.97	4.45	2.81	3.78	4.88	4.32
Permethrin	polar		6.1			4.8	1.32	5	2.79	3.52	5.04	4.49
Fenvalerate	polar		6.2			4	1.3	3.72	1.36	3.67	5.12	4.57
Flucythrinate	polar		6.2			5					5.12	4.57
Profluralin	polar		6.34			4	3.83	4.26			5.24	4.69
Cypermethrin	polar		6.6			2.59	2.36	4.53	2.89	3.52	5.45	4.91
Aldrin	hydrophobic		3.01			2.61	2.61	4.69	2.8	5.15	2.54	1.86
Lindane	hydrophobic		3.7			3	1.18	3.52	1.58	3.24	3.10	2.45
b-BHC	hydrophobic		3.8			3.36			2.26	3.17	3.18	2.53
a-BHC	hydrophobic		3.81			3.81			1.93	3.38	3.19	2.54
Heptachlor	hydrophobic		5.27			4.38	3.81	4.38	3.33	4.33	4.37	3.78
DDD-p,p’	hydrophobic		5.5			5			3.3	4.92	4.56	3.98
Toxaphene	hydrophobic		5.5			5	4.99	5.32	2.6	4.52	4.56	3.98
DDE-p,p’	hydrophobic		5.7			5					4.72	4.15
DDE-o,p’	hydrophobic		5.8			4.85	3.7	6	3.7	6.01	4.80	4.23
cis-Chlordane	hydrophobic		6			5.5	4.3	5.57	2.03	7	4.96	4.40
trans-Chlordane	hydrophobic		6			5.5					4.96	4.40
DDT-o,p’	hydrophobic		6.19			5.4	3.93	6.3	2.1	6.9	5.11	4.56
Mirex	hydrophobic		6.9			6	5.56	7.38	2.34	6.5	5.69	5.17

The data are from Mackay [18] except for the bold values which are from Tomlin [29]. For some acids and bases also a log Kow value above and/or below the pKa is given. The "best" value of log Kow and log Koc were selected by Mackay [18]. For the log Koc and also for the log BCF the lowest and the highest experimentally determined value a shown. The calculated log Koc and log BCF were derived from the "best" log Kow using equation 1 and equation to respectively. *For the bases the pKa of the protonated form is given. The “best” log Kow value was derived from the neutral form of the acids and bases.