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Paradigm for analysing complex model uncertainty

A general concept for dealing with uncertainties in ecotoxicological models

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Data sheet

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Abstract:	Model calculations have a central place in e.g. the risk assessment of chemicals. More and more sophisticated models have been developed in the last 20 years and the boundary for the possible calculations has been extended dramatically during the years. The quantification and minimisation of uncertainty have become key issues in the attempt to make useful mathematical models for decision support. In this report a systematic approach is described to guide a systematic uncertainty analysis in relation to risk assessment. This report relates the decision support problem to mathematical modelling on a conceptual basis. The focus is risk assessment of chemicals but the relevance is broader and covers decision support based on mathematical models in general. A close evaluation of model uncertainty is in general a rather resource demanding task and in reality the user of a model can easily be brought into a situation where a model have to be used without the possibility for such an evaluation. A possible way to deal with this situation can be to use a kind of tiered approach where more easy screening methods can help to identify model uncertainty in relation to a specific problem. A guideline for such an approach is shown as the conclusion in this report.

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Contents

Summary

Predictive models involving theoretical studies combined with empirical knowledge, i.e. field and laboratory experiments are useful as support for decisions in environmental related problems. These models can help to take action before the actual problems become serious and to evaluate the consequences of different future scenarios formed by different actions taken. Therefore, model calculations have a central place in e.g. the risk assessment of chemicals. More and more sophisticated models have been developed in the last 20 years and the boundary for the possible calculations has been extended dramatically during the years. But a wide gap has open up between what is possible calculations and what is realistic calculations, the later yielding some kind of new information. The quantification and minimisation of uncertainty have become key issues in the attempt to make useful mathematical models for decision support.

Models involving high complexity are often associated with seriously uncertainty. Thus, the use of the models needs to be supported with a careful uncertainty analysis, which is one of the major challenges in model application. Uncertainty analysis is more and more widely used as an integrated part of risk analysis and denoted probabilistic risk assessment. However, even though the basic principle of probabilistic risk assessment is sound, there exist some pitfalls to be aware of. It is important to realise that the uncertainty estimate may be uncertain. An incomplete uncertainty estimate can easily underestimate the true uncertainty and thereby end up with conclusions of false realism.

In this report a systematic approach is described to guide a systematic uncertainty analysis in relation to risk assessment. The problem can in general be formulated as a duality between models which: "Say much about little" and models which "Say little about much". If the goal is to make a detailed prediction ("to say much") by a model then the model needs to be so complex in order to take many processes into account that only a limited system ("about little") can be described. On the other hand, if less detailed predictions are the topic ("Say little") then the model complexity is more limited and it will be possible to say something about a larger system ("about much"). This is the dualism in any prediction and thus also for mathematical models.

This report relates the decision support problem to mathematical modelling on a conceptual basis. The focus is risk assessment of chemicals but the relevance is more broad and covers decision support based on mathematical models in general. Two basically different sources of uncertainty is considered:

1 Input uncertainty and variability, which arises from missing information about actual values and natural variability due to a heterogeneously environment

2 Structural (model) uncertainties arise from the fact that every model is a simplification of reality due to a limited systemic knowledge.

The input uncertainty can in principle be solved in most cases either analytical or more often by using a Monte Carlo type analysis. In practise, however, it can be difficult to get the necessary information about the variability of the input parameters and results from Monte Carlo calculations needs to be interpreted with caution due to this problem. The structure uncertainty, on the other hand, is more problematic to quantify and a complete determination is in principle impossible because this will demand a complete knowledge about the system to be model and thus no need for a model! In this investigation it is shown, however, how the structural uncertainty improvement can be determined for sub-processes in a model. In this way it is possible to answer the question: Are there any sub-processes (sub-models) in the model which is unnecessary and/or harmful for the total uncertainty. It can thus easily be the case that a model having many sub-models does a poorer job compared to a simpler model even if every sub-model is theoretical relevant and well described. Combined uncertainty analyses using the concept of input and structure uncertainty are useful to investigate these problems. In very simple models the necessary input parameters are often available, yielding output values with low uncertainty from the input parameters. On the other hand these models will exhibit high structural uncertainties resulting in low accuracy. With very complex models the reverse trend is seen. High input uncertainties are introduced from a large number of input parameters and furthermore default values have to be applied in several cases. The structural uncertainties will, however, be lower.

Even though the total uncertainty system seems complicated, there will only be a few dominating sources of uncertainty in most cases. A model can be said to be discordant (inharmonious) when some parts of the model operates with a relatively low uncertainty while other parts of the model includes a higher level of uncertainty. In a discordant model minor uncertainty sources have been improved at the expense of major uncertainty sources. However, if all information needed for an existing discordant model is available then the model can be used without consideration as a 'best obtainable knowledge approach'. The problems arise if such a model is used to identify data necessary for the decision making, because resources are wasted on collecting superfluous information. Furthermore, a discordant model can easily produce conclusions of false realism when detailed parameter studies of low uncertainty sources are considered when the emphasis should be on other parts of the model.

It is crucial and often a forgotten issue to integrate the uncertainty analysis with the need for decision support. This is a result of the fact that the uncertainty will increase and thus more complex structures have to be implied for the desire of more detailed information (higher information level). This is very important to realise for a decision-maker that will ask an 'expert' about a prediction to support a decision. If the question is formulated by the decision-maker at a higher information level than strictly necessary for the decision a lot of resources can easily be wasted. This problem has been formulated in the statistical learning theory for problem solution using a restricted amount of information as: *When solving a given problem, try to avoid solving a more general problem as an intermediate step.*

A close evaluation of model uncertainty is in general a rather resource demanding task and in reality the user of a model can easily be brought into a situation where a model has to be used without the possibility for such an evaluation. A possible way to deal with this situation can be to use a kind of tiered approach where more easy screening methods can help to identify model uncertainty in relation to a specific problem. A guideline for such an approach is shown in this report.

This work is a part of a larger project concerning the fate of xenobiotics in a catchment in Denmark (Roskilde). The conclusions from this report will form the paradigm in the modelling performed in the project as such for four specific systems, each one being a part of an overall system describing the flow of xenobiotics in Roskilde municipality and catchment.

Danish summary

Modeller, hvor teoretiske studier er kombineret med empirisk viden kan virke som beslutningsstøtte indenfor miljørelaterede problemer. Disse modeller kan hjælpe med til at lave tiltag før miljøproblemerne bliver for store og til at undersøge konsekvenserne ved forskellige fremtidige scenarier. Modelberegninger har derfor en central plads ved f.eks. risikovurdering af kemiske stoffer. Mere og mere sofistikerede modeller er blevet udviklet til disse formål, især gennem de sidste 20 år, og begrænsningerne for hvad der er muligt at beregne er drastisk forbedret. Men dette har betydet at et stort gab er blevet åbnet op mellem det der er muligt og så det der er realistisk at beregne. Bestemmelse og minimering af usikkerhed er derfor blevet et nøgleområde i forsøget på at lave brugbare matematiske modeller til beslutningsstøtte.

Modeller med stor kompleksitet har typisk en stor usikkerhed. Derfor skal brugen af disse modeller ledsages af grundige usikkerhedsanalyser, hvilket er en af de største udfordringer ved modelbrugen. Usikkerhedsanalyser er derfor i stadigt stigende omfang brugt som en integreret del af risikoanalyser. Men selvom det er fornuftigt at udføre usikkerhedsberegninger, er det vigtigt at være opmærksom på nogle faldgruber. En usikkerhedsanalyse er i sig selv behæftet med en usikkerhed. En ufuldkommen usikkerhedsanalyse kan derfor nemt underestimere den virkelige usikkerhed og dermed bidrage til at modelberegningerne fremstår med en falsk realisme.

Denne rapport beskriver en systematisk fremgangsmåde for usikkerhedsanalyser i relation til risikovurdering. Problemet kan i generelle ord blive beskrevet som et dilemma mellem at "sige meget om lidt" eller "sige lidt om meget". Hvis formålet er at lave detaljerede forudsigelser ("sige meget"), så skal modellen nødvendigvis være kompleks, da mange processer skal inddrages, og der er derfor kun muligt at beskrive er afgrænset system ("om lidt"). Omvendt hvis et en mindre detaljeret forudsigelse er målet ("sige lidt") så kan modelkompleksiteten begrænses og færre processer skal inddrages, hvilket ofte vil muliggøre beskrivelse af et mere omfattende system ("om meget"). Dette er et dilemma for en hvilken som helst forudsigelse, og altså dermed også for enhver matematiske model.

Rapporten relatere behovet for beslutningsstøtte til modelforudsigelser på et konceptuelt plan. Der er fokus på risikoanalyse af kemikalier, men konklusionerne er også relevant på et langt mere generelt plan. To grundlæggende forskellige kilder til usikkerhed bliver behandlet:

1 Usikkerhed som resultat af at inputparametre er behæftet med usikkerhed (input-usikkerhed), enten p. g. a. manglende viden eller fordi der hersker en naturlig variabilitet

2 Strukturel (model) usikkerhed, der opstår som resultat af de forudsætninger, der ligger til grund for modellen.

Input-usikkerheden kan i princippet bestemmes ved forskellige metoder så som f.eks. Monte Carlo simuleringer. Ofte kan det dog være svært at få de nødvendige information omkring input-parametrenes variabilitet. Så resultatet fra selv omfattende Monte Carlo analyser skal tolkes med varsomhed. Strukturel usikkerhed er på den anden side principel umulig helt at kvantificere, fordi det ville kræve en komplet og reel uopnåelig viden om systemet. I det omfang der hersker en komplet viden er der ikke brug for nogen model ! Så modellens berettigelse medfører at det ikke er muligt at udføre en komplet analyse for strukturel usikkerhed. I denne rapport er det dog vist hvordan forbedringer (mindskning) af den strukturelle usikkerhed kan beregnes for delbeskrivelser i en model. Udfra dette er det muligt at svare på følgende spørgsmål: Er der nogen delproces (delmodel) i modellen, der synes at være unødvendig og ødelæggende for den samlede usikkerhed. Det kan nemlig let ske at en model, der består af mange delmodeller (meget kompleks) give resultater, der er mere usikre end sammenlignet med en mere simple model (mindre kompleks) med færre delmodeller selvom der måske er klare teoretiske argumenter bag alle delmodellerne i den komplekse model. En samlet usikkerhedsanalyse, der bestemmer både input-usikkerheden og dele af den strukturelle usikkerhed, er yderst brugbar til at undersøge sådanne forhold omkring modelkompleksitet.

Meget simple modeller vil typisk kun behøve viden om relativt få og let tilgængelige inputsparametre, hvilket betyder at input-usikkerheden blive begrænset. På den anden side vil disse simple modeller typisk lide under en betydelig strukturel usikkerhed fordi en lang række restriktive forudsætninger er nødvendige for at opnå den simple formulering af modellen. En model er for simpel (underkompleks) hvis den strukturelle usikkerhed overskygger gevinsten ved den begrænsede input-usikkerhed.

De omvendte forhold kan gælde for komplekse modeller. Her vil input-usikkerheden typisk være betydelig fordi de en lang række detaljerede inputsparametre skal fødes ind i den komplekse model. Nogle af disse parametre vil måske oven i købte blive fastlagt som "default" værdier i en erkendelse af at deres aktuelle værdi er svær at fremskaffe. Den strukturelle usikkerhed vil derimod være mere begrænset sammenlignet med en simpel model, da flere processer er inkluderet i modellen, hvilket igen betyder at det ikke har været nødvendigt at bruge så mange restriktive forudsætninger. En model er overkompleks, hvis input-usikkerheden overskygger gevinsten ved den detaljerede beskrivelse og deraf følgende lave strukturelle usikkerhed.

I det omfang det er muligt at vurdere modellers kompleksitet, som ovenfor beskrevet, skulle det være muligt at bestemme den optimale kompleksitet så modellen hverken er under- eller overkompleks.

Det er meget vigtigt, men desværre ofte forsømt, at integrere usikkerhedsanalyse med behovet for beslutningsstøtte. Dette skyldes at usikkerheden vil vokse når mere specifik information (højere informations niveau) ønskes fremskaffet, som et resultat af at mere komplekse modeller er nødvendige. Det er meget vigtigt for en beslutningstager at være klar over dette forhold når et spørgsmål formuleres. Hvis et spørgsmål blive fremsat af en beslutningstager på et højere informations niveau end strengt nødvendigt så kan det medføre et stort spild af ressourcer i et for-

søg på at kommer med en besvarelse uden for stor usikkerhed. Dette forhold er blevet formuleret som en slags læresætning inden for den statiske læringsteori: *Når et problem skal løses under mangelfuld viden så prøv at undgå en løsning af et mere generelt problem* (større informations niveau, red.) *som en del af løsningen.*

En grundig bestemmelse af model usikkerhed er ofte ret ressourcekrævende og en bruger af modeller bliver let bragt i en situation, hvor det ganske simpelt ikke er muligt at foretage en sådan bestemmelse. En mulig løsning af dette problem er en slags prioriteret tilgang hvor mere simple screeningsmetoder kan hjælpe til med at fastlægge usikkerheden i forbindelse med en konkret modelberegning. Denne rapport fremsætter en sådan metode.

Dette arbejde er en del af et større projekt, der behandler skæbnen af miljøfremmede stoffer i et opland i Danmark (Roskilde). Konklusionen fra denne rapport danner baggrund for paradigmet bag den matematiske modellering, der vil blive udført under dette projekt for fire forskellige systemer.

1 Introduction

It is important to raise the scientific insight on emissions, fate and effects of xenobiotics in the environment. This can be done using predictive models as an integrated approach involving theoretical studies combined with empirical knowledge, i.e. field and laboratory experiments.

Such mathematical models are useful as support for making decisions in environmentally related problems, as they can help to take action before problems become serious and to evaluate consequences of different future scenarios formed by different actions taken. Therefore, model calculations have a central place in the risk assessment of chemicals as e.g. formulated in the European Union System for the Evaluation of Substances (EUSES) as described in EUSES (1997).

A complete multimedia fate model system for organic compounds should describe the cycle of the substances in the environment and a set of main investigation areas can be formulated according to the following list.

- Sources.
- Primary emissions to air, (waste) water and soil.
- Secondary emissions from wastewater treatment plant (WWTP) discharges (effluent water and sludge) to air, water and soil.
- Transport and degradation in the environmental compartments and WWTP (sorption, degradation).
- (Bio) availability
- Ecotoxicity.
- Human toxicity.

Each area could be formulated as a model comprising a set of processes. If a process is to be included in the model assessment it must be both meaningful and informative. A process is meaningful if it relates to a subject of concern and affects the outcome of the model calculations. A process is informative if the knowledge with respect to this process is sufficient, so that the analysis based on this process actually narrows the uncertainty of the outcome and hence is able to provide understanding that was not apparent prior to the analysis (*Hertwich et al., 2000*).

A compartment model will often involve a high level of complexity, which tends to be associated with a high degree of uncertainty. Thus, the use of the models needs to be supported with a careful uncertainty analysis, which is one of the major challenges in model application. Uncertainty analysis is more and more widely used as an integrated part of risk analysis and denoted probabilistic risk assessment. However, even though the basic principle of probabilistic risk assessment is sound, there exist some pitfalls to be aware of. It is important to realise that the uncertainty estimate is uncertain. An incomplete uncertainty estimate can easily underestimate the true uncertainty and thereby end up with conclusions of false realism. In this report a systematic approach is described to guide an uncertainty analysis avoiding false realism of the results.

The problem of a systematic uncertainty analysis has been investigated by several authors as *Costanza and Sklar (1985), Jørgensen (1994), Håkanson (1995)* and *Payne (1999)*. All these references focuses on ecosystem modelling. A systematic approach for uncertainty is given by *Hertvich et al. 2000* having focus on fate and exposure models. In case of more integrated policy models an approach for uncertainty analysis is made by e.g. *Kann and Weyant (2000)*. The problem all of these references address can in general terms be formulated as a duality between models which "Say much about little" and models which "Say little about much" (*Costanza and Sklar, 1985*). If the goal is to make a detailed prediction ("to say much") by a model then the model needs to be so complex in order to take many processes into account that only a limited system ("about little") can be described. On the other hand, if less detailed predictions are the topic ("Say little") then the model complexity is more limited and it will be possible to say something about a larger system ("about much"). This is the dualism in any prediction and thus also for mathematical models. This report will relate the decision support problem to mathematical modelling on a conceptual basis. The focus will be risk assessment of chemicals but the relevance will be broader and covers decision support based on mathematical models in general.

As a conclusion of the report guidelines for model evaluation will be given in the end using more or less resource demanding methods.

2 Uncertainties in modelling

2.1 Two types of uncertainty

Morgan et al. (1990) (cited by *Hertwich et al., 2000*) distinguish between the uncertainty in empirical quantities, defined constants, decision variables, value parameters, model domain parameters and outcome criteria arising from random error, statistical variation, systematic error, subjective judgement, linguistic imprecision, variability, true randomness and disagreement between experts. A simpler framework developed by *Finkel (1990)* distinguishes between decision rule uncertainty, model uncertainty and uncertainty and variability of input parameters. Decision rules specify the goals and methods of the analysis and decision rule uncertainty arises whenever there is ambiguity about how to choose an appropriate measure to quantify or compare social objectives, i.e. what methods to use to evaluate specific impacts.

In this project two basically different sources of uncertainty will be considered *(Costanza and Sklar (1985), Jørgensen (1994), Håkanson (1995) and Payne (1999))*:

1 *Input uncertainty.* Uncertainty of input parameter values which arises from missing information about actual values, and results in low precision. This is partly a consequence of estimation error and partly a consequence of the variability, or stochastic uncertainty arising from statistical variance that again derives from random factors or natural heterogeneity in the model input parameters.

2 *Structural (model) uncertainties* arise from the fact that every model is a simplification of reality and the mathematical expressions are approximations for real systems due to a limited systemic knowledge.

Simplifications such as a reduced number of removal mechanisms, e.g. volatilisation is considered negligible compared to bio-degradation, or assumptions such as uniform mixing, constant emissions in time or steady-state conditions will act to increase the structural uncertainties. To evaluate the influence of model structure, different model set-ups must be developed for the same application. In some cases when optimum model structures are sought the increase in structural uncertainty will be justifiable if the input uncertainties are reduced.

Figure 1 illustrates the uncertainty relationships in a complete environmental modelling system for risk assessment of organic contaminants. Both structural and input uncertainties are introduced on all levels. The input uncertainties are accumulated from one model to the other while the structural uncertainties act individually at each modelling level.
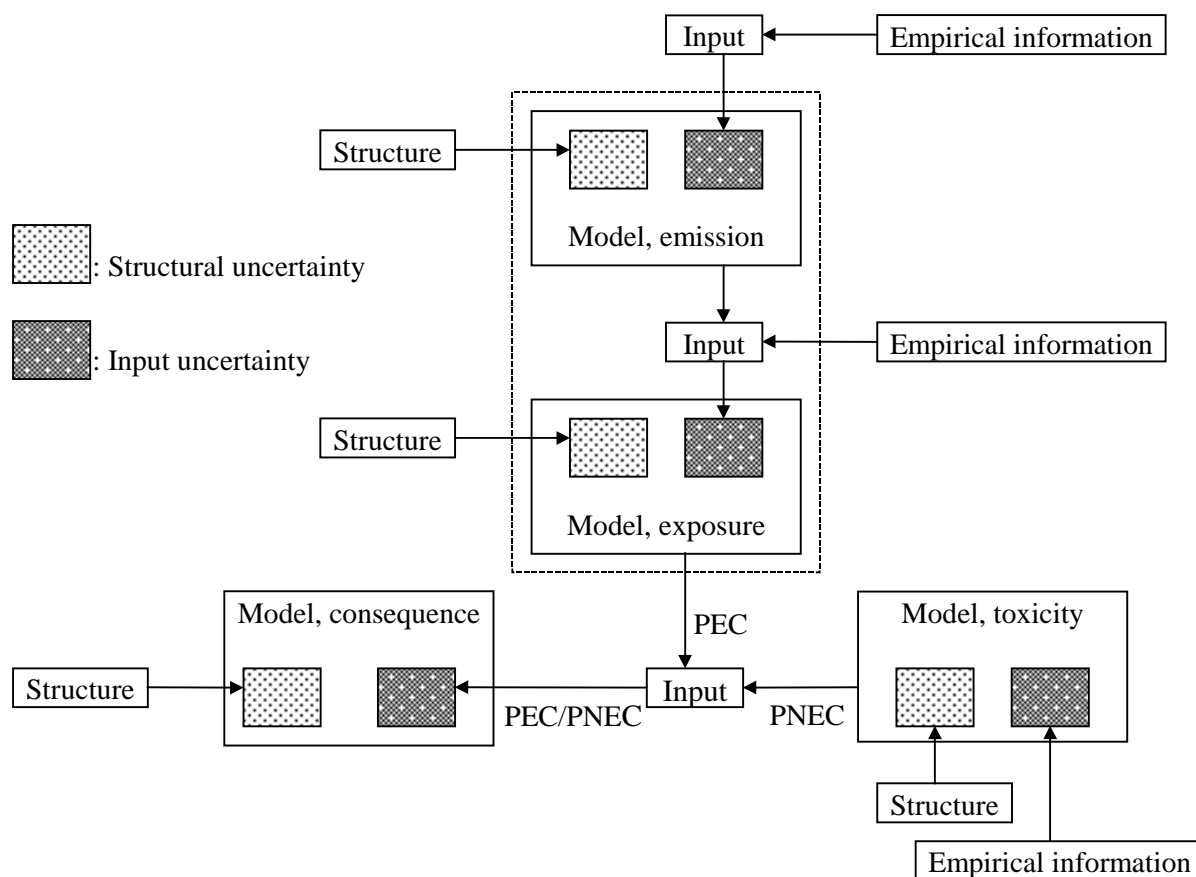
Figure 1. Uncertainty relationships in a complete environmental modelling system for organic contaminants. The dashed line box is the area of more detailed analysis in the investigation of Fauser, P. (2000), Sørensen, P.B. (2000a), Sørensen, P.B. (2000b) and Vikelsøe, J. (2000).

The input uncertainty can in principle be solved in most cases either analytical or more often by using a Monte Carlo type analysis as done by *Hertwich et al. (1999)* for exposure models. In practise, however, it can be difficult to get the necessary information about the variability of the input parameters and results from Monte Carlo calculations needs to be interpreted with caution due to this problem.

The structure uncertainty is more problematic to quantify. *Payne (1999)* applies theory from the statistical learning theory as developed by *Vapnik (1995)*. This theory sets up the upper bounds on the amount of uncertainty, including the structure uncertainty. However, the methodology is only applicable for specific types of models and thus not directly useful in a general form. *Costanza and Sklar (1985)* developed a more applicable method, which is more pragmatic and thus not so mathematical well defined. The model articulation level is defined in *Costanza and Sklar (1985)* based on several key properties for model complexity, where high articulation level is associated with high complexity level. The way the articulation level is calculated relays on more or less subjective judgements and there is no general and objective way for calculating a unique number for articulation level.

2.2 Uncertainty bottle neck

Even though the total uncertainty system seems complicated, there will typically only be a few dominating sources of uncertainty. The law of uncertainty accumulation can identify these

$$\Delta^2_{total} = \Delta^2_1 + \Delta^2_2 + \Delta^2_3.....$$ **(1)**

where Δ_{total} is the total or resulting uncertainty and Δ_1 , Δ_2 and Δ_3 are the uncertainty contributions from different sources. Δ_{total} can be defined for a single model or a set of sub-models, and Δ_n can be uncertainties connected to input parameters or to individual sub-models. If all uncertainty sources are known the values can be ranked according to: $\Delta_1 > \Delta_2 > \Delta_3 >...$ and equation **1** rewritten as

$$\Delta_{total} = \Delta_1 \cdot \sqrt{1 + \left(\frac{\Delta_2}{\Delta_1}\right)^2 + \left(\frac{\Delta_3}{\Delta_1}\right)^2 + ...}$$ **(2)**

This equation shows that the sources associated to the largest uncertainty values will tend to dominate more than their actual values indicate. Lets consider a numerical example where there are totally 11 sources of uncertainty having the values of:

Δ_1:   0,1
Δ_2-Δ_{11}:   0,025

So in this case one source of uncertainty induces a variation of 0,1 and 10 other sources induce a variation of 0,025 each. Intuitively, it should be expected that the 10 smaller contributions of uncertainty do have a rather large influence on the total uncertainty because their values are not very much smaller than Δ_1. However, using Eq. 2 the total uncertainty is calculated to be Δ_{total}=0.13, which only differs from the single uncertainty source Δ_1, by 30 %. If the uncertainty should be improved in this system by removing one or more of the uncertainty sources two alternatives can be considered: (1) removing of only Δ_1 or (2) removing of all the uncertainty sources Δ_2-Δ_{11}. The first alternative will reduce the uncertainty from 0.13 to 0.08, while the second alternative will reduce the uncertainty from 0,13 to 0,1. So the elimination of only Δ_1 will improve the uncertainty nearly double so much as an elimination of all the uncertainty sources Δ_2-Δ_{11}. Hence, according to equation **2**, 'uncertainty bottle neck' will often exist in the model system, which will account for most of the total uncertainty.

The example indicates that great care must be taken where to allocate resources to improve the model structure. A model can be said to be discordant (inharmonious) when some parts of the model operates with a relatively low uncertainty while other parts of the model includes a higher level of uncertainty. In a discordant model minor uncertainty sources have been improved at the expense of major uncertainty sources. However, if all information needed for an existing discordant model is available then the model can be used without consideration as a 'best

obtainable knowledge approach'. The problems arise if such a model is used to identify data necessary for the decision making, because resources are wasted on collecting superfluous information. Furthermore, a discordant model can easily produce conclusions of false realism when detailed parameter studies of low uncertainty sources are considered when the emphasis should be on other parts of the model.

2.3 Ranking of completity level

The missing unique scale for quantifying complexity articulation level of mathematical models is a general problem in a systematic uncertainty analysis. In some cases it is possible to rank the complexity level for a series of models and thus avoid the need for an absolute complexity scale. An example of a complexity ranking is shown in Fig. 2 using a polynomial type of model. In general: If **model 2** can be considered as a sub set of **model 1**. Then **model 1** has a higher complexity than **model 2**. E.g. in Fig. 2 **model 4** is a sub set of **model 3** which again is a sub set of **model 2** and **model 2** is a sub set of **model 1**. Thus, it is possible to order the models as done in Fig. 2.
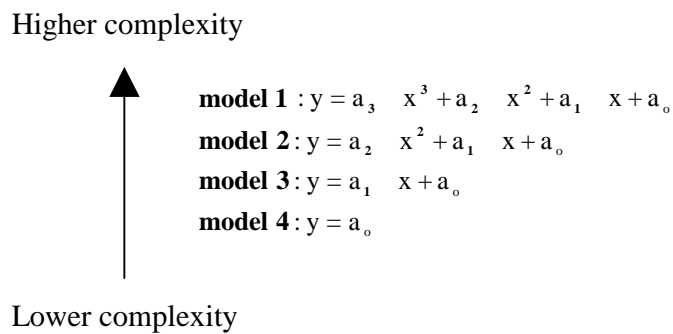
Higher complexity

$$\text{\textbf{model 1}} : y = a_3 \; x^3 + a_2 \; x^2 + a_1 \; x + a_0$$
$$\text{\textbf{model 2}} : y = a_2 \; x^2 + a_1 \; x + a_0$$
$$\text{\textbf{model 3}} : y = a_1 \; x + a_0$$
$$\text{\textbf{model 4}} : y = a_0$$

Lower complexity

Figure 2. *An example of ranking models in relation to the complexity level.*

The needed knowledge in Fig 2 about input parameter values becomes more resource demanding as the complexity increases because the number of coefficients increases. It is a general tendency for mathematical models that increasing complexity yields an increasing demand of a priori knowledge. In fact no knowledge is completely certain. Thus, any increase in the demand of a priori knowledge will include additional input uncertainty.

The ranking with respect to complexity is illustrated in the following using the model analysis in *Sørensen et al., (2001a)* for the water/sediment concentration in a lake/marine area. The focus is the removal processes other than hydrodynamic removal (convection) and removal by evaporation. Three possible removal processes are leaved in form of: (1) degradation (*degr*), (2) Deposition to the sediment surface (*dep*), and (3) Diffusion into the sediment (*diff*). Furthermore in relation to EUSES the diffusion is described using a so-called thin film (layer) diffusion (*diff$_{film}$*) approximation in order to simplify the model equations. Obviously, *diff$_{film}$* is a special case of the more general phenomenon *diff*, which is shown in *Sørensen et al., (2001a)*. Thus, it involves a higher complexity level to describe *diff* compared to *diff$_{film}$*. The processes can be combined

to form a serious of models and these models will have different complexity levels depending on the processes included. The model using *degr + diff* will in this way be ranked above the model using only *diff*. It is then possible to make a partial ranking of the models with respect to the complexity levels as shown in Fig.3.

Model complexity level	Included terms
4	$degr + dep + diff$
3a	$degr + dep + diff_{film}$
3b	$degr + diff$
3c	$dep + diff$
2a	$degr + dep$
2b	$degr + diff_{film}$
2c	$dep + diff_{film}$
2d	$diff$
1 a	$degr$
1 b	dep
1 c	$diff_{film}$

Higher complexity
Higher input uncertainty
Lower structural uncertainty

Hasse diagram:

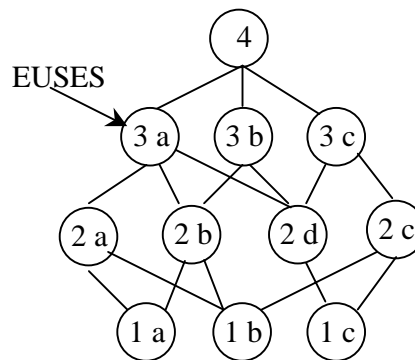*Figure 3. Ranking of the model to calculate water concentration in marine areas or lakes focussing on the removal processes: (1) Degradation (degr), (2) Deposition on the sediment surface (dep), and (3) Diffusion into the sediment (diff or diff$_{film}$). The ranking criteria are described in the text. The Hasse diagram shows all the possible rankings between the different models as lines, where upwards means high rank (high complexity) and downwards means low rank (low complexity). Thus 4 is above 3a and 4 is above 2a because 4>3a and 3a>2a, but 3a is NOT compared with 3b.*

In EUSES the removal is described using the relationship: *degr + dep + diff$_{film}$*(model 3a) and this model is seen to be ranked below the model 4 because the diffusion is described as a thin film diffusion process. The structural uncertainty is increased for every step downward along a line so model 3b will have higher structural uncertainty compared to model 4.

On the other hand step downward will in general yield lower input-uncertainty and a model, which is less, complicated to handle mathematically. This is the argument for selecting model 3b instead of model 4.

The conclusion in *Sørensen et al., (2001a)* is that the diffusion process is not well described by the thin layer diffusion approximation. It is also shown that often the removal by diffusion (*diff*) can be neglected compared to the removal by deposition (*dep*). Thus, a step downward in the Hasse diagram in Fig. 3 from 3a to 2a is beneficial because it will reduce the complexity and thereby reduce both the input uncertainty and the resources demand for the model to be used without increasing the structural uncertainty remarkable.

3 The concept of obtimal complexity

Some complexity is needed for any prediction and an increase in complexity enhance the opportunities for a closer and thus more certain description of reality (decreased structure-uncertainty). So there seems to be a dilemma between the demand of low input uncertainty (low complicity) and a low structural uncertainty (high complexity). The optimal model structure based on the actual a priori knowledge is a compromise between these two sources of uncertainty. The model structure can be optimised through a mutual evaluation of the input and structural uncertainties. The problem is to quantify the uncertainties, where especially the structural uncertainty can form a problem as discussed above. However, by using the concept of relative complexity it may under some circumstances be possible to identify the optimal model complexity as exemplified below.

The principle is illustrated in the following, where three different models are mutually ranked with respect to complexity as illustrated above. The example of uncertainty analysis is based on the work of *Vikelsøe et al., (2001)* and the details is shown in Appendix A. The problem in the example is to calculate the dissolved water concentration at a specific depth below the sediment surface. The depth is chosen to be 1 cm and only steady state conditions are considered. Three different models having three different complexity levels is formulated for the same problem and uncertainty is calculated for each model. However, as pointed out earlier the structural uncertainty is difficult to quantify so the relative structural uncertainty (relative to the most complex model) is calculated instead. The calculation of the relative structural uncertainty is described in the Appendix and illustrated in Fig. 3A in appendix.

The results of the analysis is shown in Fig. 4, where the two types of uncertainty is shown for the three models, which are ranked in relation to the level of complexity. The simplest model (model 3) does not include any processes and thus simply assumes the water concentration in the sediment to equalise the water concentration in the water column. The input uncertainty is therefore equal zero under these circumstances. The best model is seen to be model 2, which includes deposition and degradation but neglects diffusion.

Complexity

Absolute structural uncertainty
for Model 1

Model 1:
$$0 = \frac{D}{R} \cdot \frac{d^2C}{dz^2} - S \cdot \frac{dC}{dz} - \frac{k_1}{R} \cdot C$$

0.13

Additional structural uncertainty:
Model 1 – Model 2=0.02

Model 2:
$$0 = S \cdot \frac{dC}{dz} - \frac{k_1}{R} \cdot C$$

0.07

Additional structural uncertainty:
Model 1 – Model 3=0.24

Model 3:
$$0 = S \cdot \frac{dC}{dz}$$

Uncertainty: (absolute structural) +(absolute input)

Uncertainty: (Additional structural) + (absolute input)

Signature:

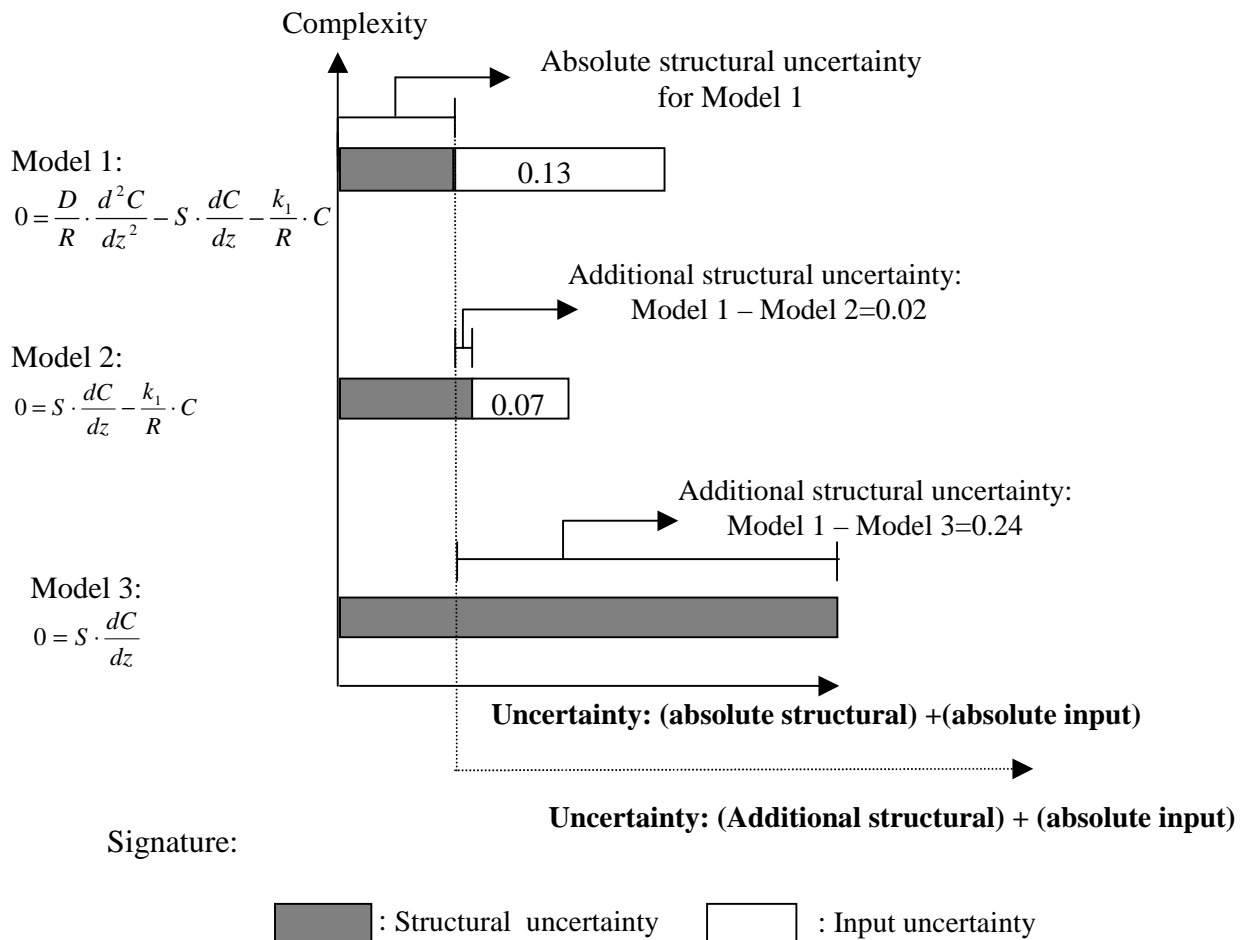: Structural uncertainty   : Input uncertainty

Figure 4. This is a Illustration of complexity ranking, where a series of models are identified as subsets of each other. It is not possible to quantify the absolute structural uncertainty for model 1. But, it is possible to determinate the increase in structural uncertainty (additional structural uncertainty) between the different models as illustrated by the dashed line. For the optimal model the sum of the additional structural uncertainty and the input uncertainty is minimal (model 2 in this case).

However, in praxis the principle is difficult to use in real uncertainty calculations due to difficulties in quantifying the complexity. The problem of quantifying complexity is solved in the example above by ranking the model complexity as described in Fig. 4, where different number of terms are added in the governing differential equations. In this way it is only possible to place the different models on the complexity level axis in Fig. 5 relative to each other. However, it will still be possible to keep the concept of a continuously scale for complexity in order to develop a method which can help to select the "best" model from possible alternatives having the lowest total uncertainty.

The structure uncertainty is difficult to quantify completely, but it is not necessary to make a complete quantification in order to find the optimal model complexity. In the example above only the differences in structure uncertainty values are calculated as the value difference between the most complex model (Model 1, having the lowest structural uncertainty) and the other models (Models 2 and 3). In this way the quantified part of the structure uncertainty for the Models 2 and 3 is the addition in structure uncertainty when either Model 2 or 3 replaces Model 1. By using

this principle, the total uncertainty, as illustrated in Fig. 5, will be re-placed by the fraction of the total uncertainty formed by adding the input uncertainty to the differences in structural uncertainty between Model 1 and Model 2, and between Model 1 and Model 3, respectively. The re-duced total uncertainty will become equal to the input uncertainty for Model 1 simply because the reduced structure uncertainty is zero in this case.

Payne (1999) discusses the relationship between uncertainty and com-plexity level in general terms as illustrated in the example above. The problem is illustrated graphically in Fig. 5.
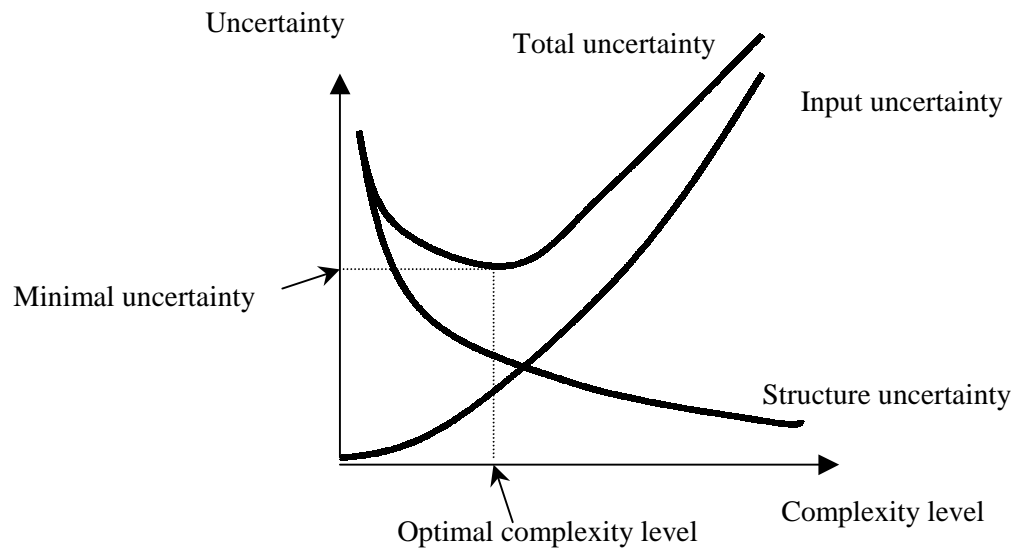

Figure 5. *The relationship between the structural uncertainty and the input uncertainty. Vapnik (1995) shows similar relationships.*

Fig. 5 is a principal figure, which summarises the conclusion, in this chapter. The input uncertainty is claimed to increase and the structure uncertainty is claimed to decrease as the model complexity is increased. Obviously, the resulting total uncertainty will tend to have a minimum value at the optimal complexity level yielding the lowest total uncer-tainty. This figure represents a systematic paradigm for model evaluation and will form the basis in the tiered approach for uncertainty analysis in a coming chapter.

The use of complexity rank and reduced structure uncertainty is illus-trated in Fig. 6, where the three Models 1, 2, and 3 are shown for illus-tration. The actual placements of the three models on the complexity scale are unknown. However, due to the complexity level rank as Model 1 > Model 2 > Model 3 it must be true that the position of Model 3 is at a lower complexity level than the optimal level and Model 1 needs to be placed at a higher complexity level than the optimal level. This is true because the total reduced uncertainty for Model 2 is lower than for the two other models.
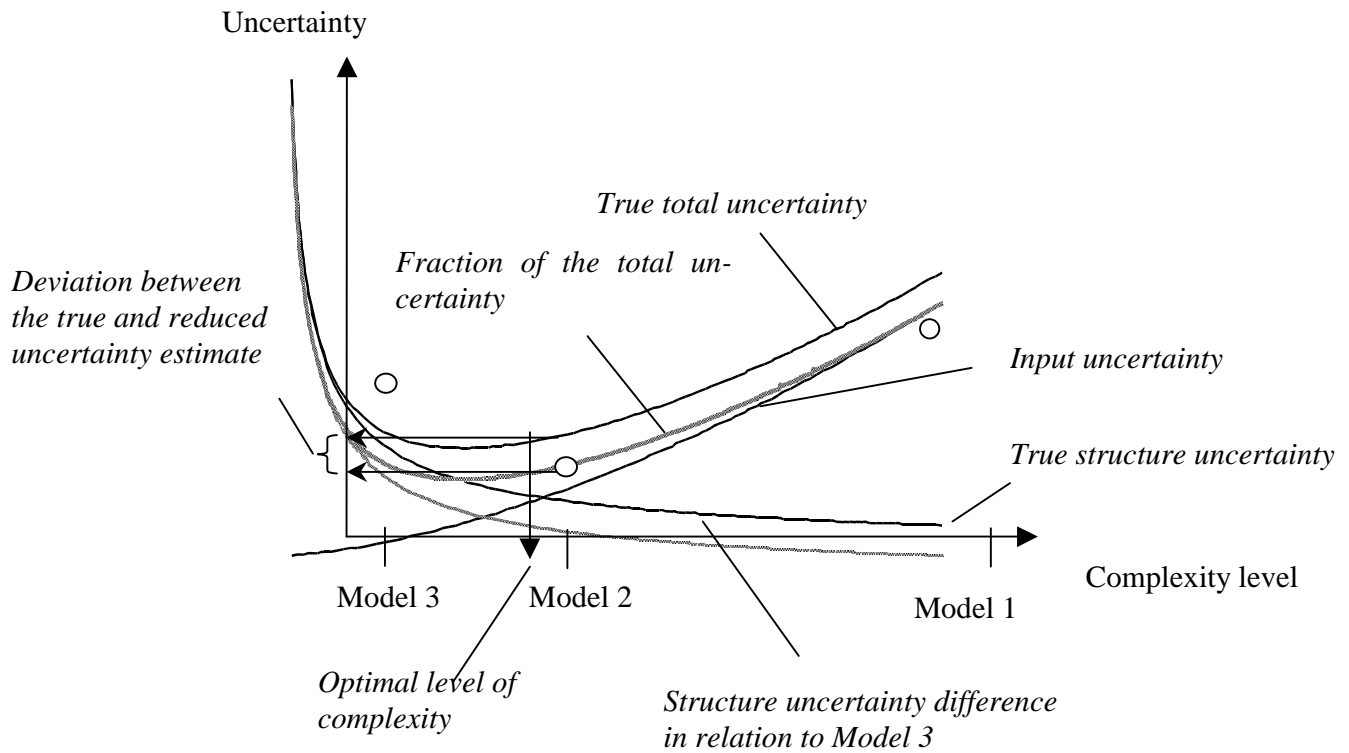
Figure 6. The interpretation of the results in Fig. 4, where three model complexity levels are analysed using the principle shown in Fig. 5 including the concept of complexity level ranking and additional structure uncertainty. The actual position of the Models 1, 2 and 3 are arbitrary, but the Models 1 and 3 are placed respectively above and below the optimal complexity level and Model 2 represents the best choice of complexity level among the three models.

It may not be obvious that the minimum value of the true total uncertainty and the fraction of the total uncertainty relates to the same optimal level of complexity. However, this will always be true because the deviation between the true and the fraction of the total uncertainty is constant for all levels of complexities.

4 The relation ship between information's level of model result and uncertainty

The model structure uncertainty depends on the choice of the outcome, i.e. what question needs to be answered and thus the amount of information (knowledge) that is required from the model. In the shown example the question was about the steady-state concentration at a depth of 1 cm in the sediment and it was not the most complex model that had the smallest total uncertainty. If the demand of information increases in the question to comprise the concentration change in time in the depth of 1 cm, the diffusion will play an important role and model 1 will probably be needed. In the immediate upstart of the system, i.e. for t = 0, the concentration gradient will be large at the sediment surface and the substrate flux to the sediment will be governed by diffusion and not by sedimentation. After a number of days the amount of substrate originating from sedimentation will dominate. In *Sørensen et al. (2001a)* the change in process kinetics is described.

The input uncertainty curve is identical to the one with a lower information level, whereas the uncertainty curve for the model structure has increased caused by the need of more complex structures to answer for the desire of more detailed information (higher information level). This is very importance to realise for a decision-maker that asks an 'expert' about a prediction to support a decision. If the question is formulated to the expert at a higher information level than strictly necessary for the decision then a lot of resources can easily be wasted. This problem is illustrated in Fig. 7 and has been formulated in the statistical learning theory for problem solution using a restricted amount of information as: *When solving a given problem, try to avoid solving a more general problem as an intermediate step (Vapnik, 1995).*
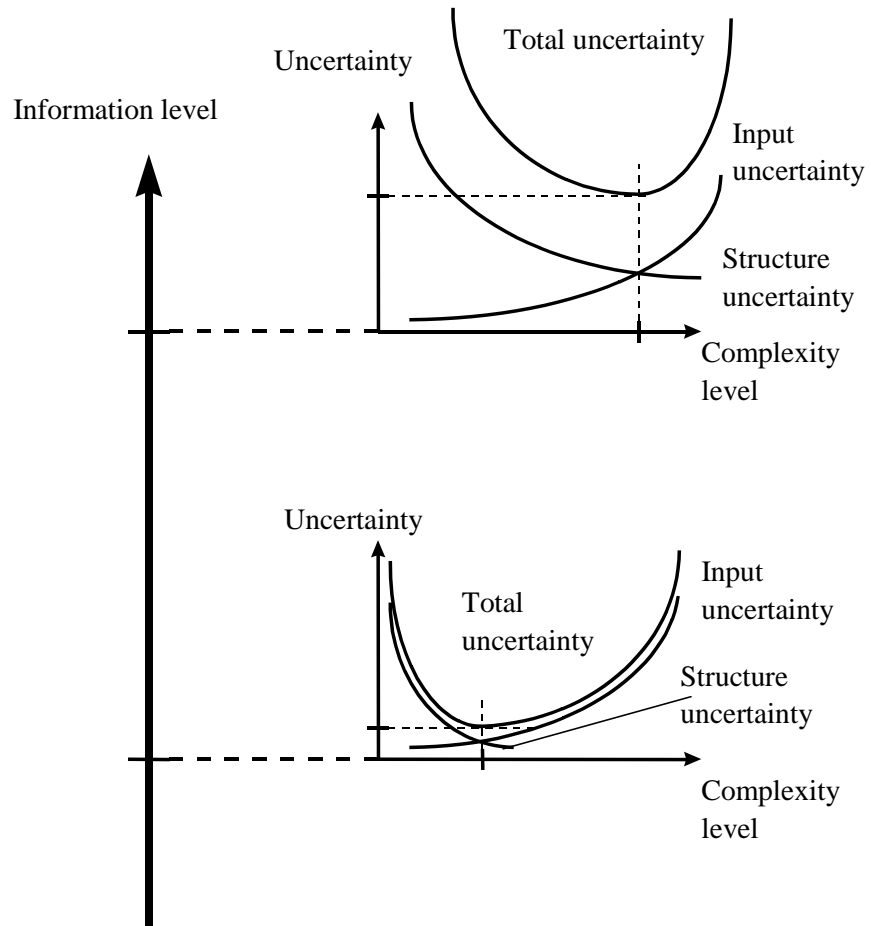
Figure 7. *Influence of level of information on the optimum model structure complexity. Similar relationships are discussed by Vapnik, (1995).*

When mathematical models are needed to support decision-making it is critical to be aware of this close relationship between the needed information level of the result and the uncertainty of the prediction. A dialog is important between the model designer/developer and the model user. Unfortunately, in the process of model development the model user (decision maker) sets up the goal (question to be answered at a given information level) and then subsequently the model designer tries to fulfil the goals as good as possible without any dialog with the model user. It can easily happen that the model results turns out to be very uncertain, but a slight reduction in the information level of the results (less ambitious model answer) may improve the result certainty dramatically.

5 Tiered approach for uncertainty analysis

A close evaluation of model uncertainty is in general a rather resource demanding task and in reality the user of a model can easily be brought into a situation where a model have to be used without the possibility for such an evaluation. A possible way to deal with this situation can be to use a kind of tiered approach where more easy screening methods can help to identify model uncertainty in relation to a specific problem. A guideline for such an approach is shown in Figure 8 and will be explained in the following.

Step 1. The formulation of the problem to be solved in terms of a question to answer is crucial for the following choice and evaluation of the model. It is therefore important to make a precise formulation of the question.

Step 2. The model is selected based on expert judgement, which again is based on reported validation results and an evaluation of critical assumptions. The magnitude of the structural uncertainty needs to be quantified so much as possible. The structural uncertainty is difficult to quantify however, some kind of judgement is necessary and in most cases possible.

Step 3. As a first approach a few model calculations are done using relatively few different combination of realistic input parameters. There will often exist an a priori knowledge, about which of the input parameters that are the most important for the model and about an interval of variation, which is smaller than the true variability. If the variation of input parameter values in this analysis yields results of unacceptable high uncertainty then is possible to reject the model as a candidate for valid calculations.

Step 4. If the model uncertainty was acceptable in *step 3*, the next step will be to over estimate the input-uncertainty, where unrealistic variations is applied to the input. More effort is needed in this step compared to *step 3* but in many cases it will be a rather easy task to set up an over estimation of the variability intervals. If the input-uncertainty is acceptable then the model prediction will be valid otherwise more detailed and thus also much more resource demanding uncertainty analysis needs to be applied.

Step 5 a. The model is acceptable and can be used to answer the question. There may exist a more complex model which can make an answer at a higher information level than the actual question.

Step 5 b. A detailed uncertainty analysis is made for input-uncertainty. The information needed is knowledge about the distribution function for input-parameter variability, which can be used in a Monte Carlo simulation. In some cases a sensitivity analysis can be used before the Monte-Carlo analysis to identify the parameters for which the model is most

sensitive. Such a sensitivity analysis can help to focus the MonteCarlo analysis and thus minimise the resources needed.
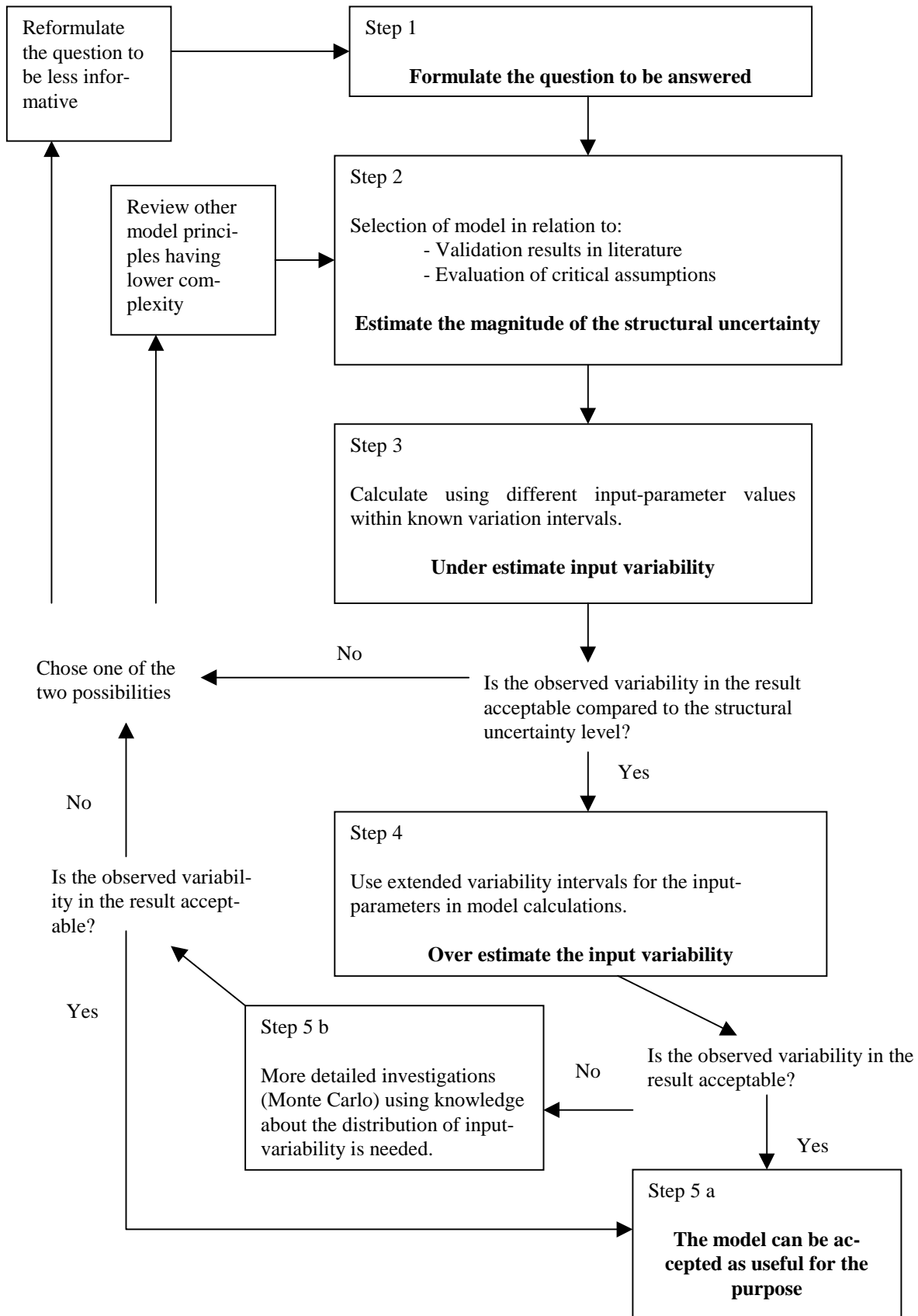

Figure 8. The guideline for a tiered approach in the model evaluation.

6 Perspective in relation to a specific xenobiotic fate analysis

This report is a part of a project where models are evaluated for four specific systems, each one being a part of an overall system describing the flow of xenobiotics in Roskilde municipality and catchment area (see figure 7). The models is discussed in relation to their harmony (Same level of uncertainty in all parts of the model) and their Input/structure uncertaintyes (The input uncertainty is related to the structure uncertainty). The results is summerised in *Carlsen et al. (2001).*

Survey   Sources and emissions of the xenobiotics in question.
Model 1   Fate of substances in Roskilde WWTP *(Fauser et al. 2001).*
Model 2   Fate of substances in Roskilde Fjord (water and sediment) *(Vikelsøe et al. 2001 and Sørensen et al. 2001).*
Model 3   Fate of substances in sewage sludge amended soil.
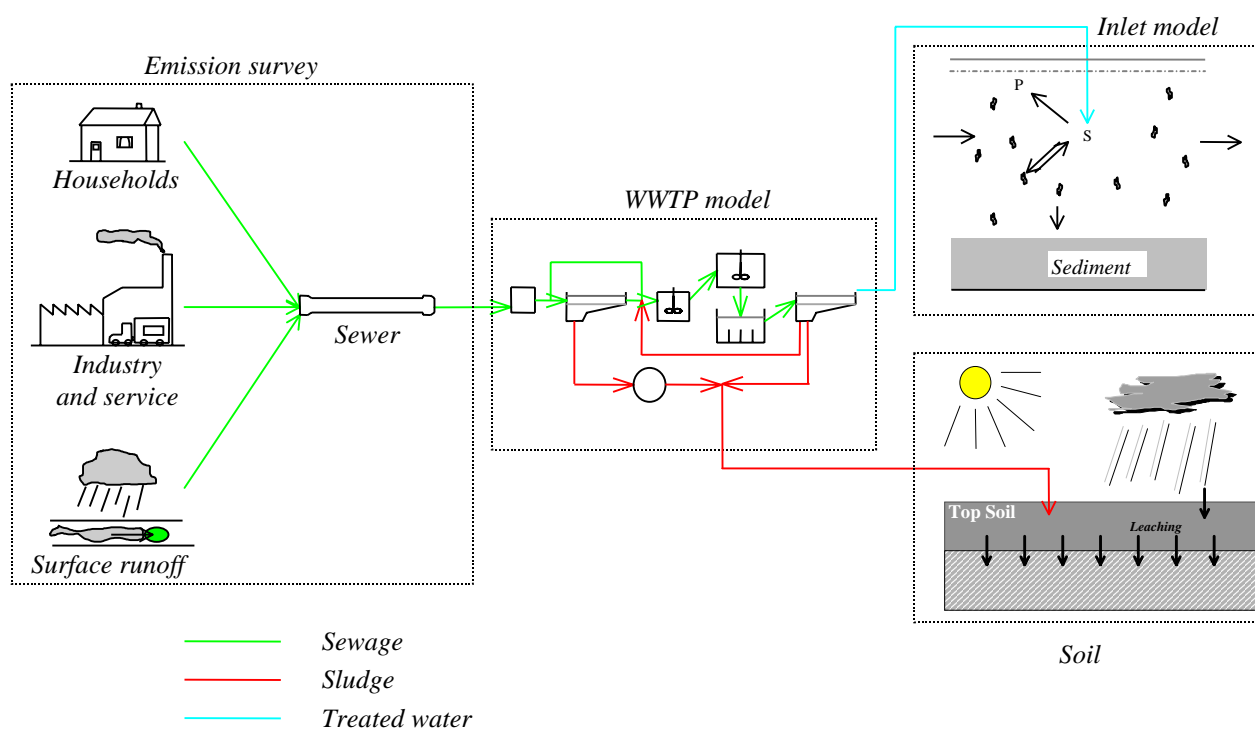

Figure 7. Schematic overview of modelling system.

These four models can be used separately; however, the combined approach permits an integrated uncertainty analysis of the total emission/fate modelling system. The emission survey gives input concentrations to the WWTP, the effluent water and digested sludge from the WWTP provide input data to Roskilde inlet and the field plough layer respectively.

The product will be risk assessment models designed to estimate Predicted Environmental Concentrations (PEC) of LAS, 6 different phthalates, nonylphenol and nonylphenol diethoxylate in the water and soil compartments. Experimental data, generated from laboratory experi-

ments and in-situ monitoring studies provide data for calibration and verification of the models. They act as a tool to estimate the Predicted No-effect Concentrations (PNEC) and in this way help to decide whether or not a substance presents a risk to the environment.

7 References

Carlsen,L., Sørensen, P.B., Vikelsøe,J., Fauser,P. and Thomsen, M. (2001): On the fate of Xenobiotics. The Roskilde region as case story, NERI report (in press)

Costanza, R. and F. H. Sklar, (1985): Ariculation, Accuracy and Effectiveness of Mathematical Models: A Review of Freshwater Wetland Applications, Ecological Modelling, 27, pp. 45-68.

"EUSES, the European Union System for the Evaluation of Substances" EUSES 1.00 User Manual. February 1997, TSA Group Delft by, European Commission - JRC, Existing Chemicals T. P. 280, 1-21020 Ispra (VA), Italy

Fauser,P., Sørensen,P.B., Vikelsøe,J., and L. Carlsen (2001): Phthalates, Nonylphenols and LAS in Roskilde Wastewater Treatment Plant - Fate Modelling Based on Measured Concentrations in Wastewater and Sludge. NERI report (in press)

Hertwich. E. G., T. E. McKone and W. S. Pease (1999): Parameter Uncertainty and Variability In Evaluative Fate and Exposure Models, Risk Analysis, Vol. 19, No. 6.

Hertwich E. G., T. E. Mckone and W. S. Pease (2000): A Systematic Uncertainty Analysis of an Evaluative Fate and Exposure Model, Risk Analysis, Vol. 20, No. 4.

Håkanson, L., (1995): Optimal Size of Predictive Models, Ecological Modelling, 78, pp. 195-204.

Jørgensen, S. E., (1994): Fundamentals of Ecological Modelling (2nd Edition), Elsevier Science B. V.

Kann, A. and J. P. Weyant, (2000): Approaches for performing uncertainty analysis in larger-scale energy/economic policy models, Environmental Modelling and Assessment, 5, pp. 29-46.

Payne, K., (1999): The VC dimension and ecological modelling, Ecological Modelling, 118, pp. 249-259.

Sørensen, P.B., P. Fauser, L. Carlsen and J. Vikelsøe, (2001a): Theoretical evaluation of the sediment/water exchange description in generic compartment models (SimpleBox). NERI report (in press)

Sørensen,P. B., L. Carlsen, J. Vikelsøe and A. G. Rasmussen (2001b): Modelling analysis of sewage sludge amended soil. NERI report (in press)

Vapnik, V. N., (1995): The Nature of Statistical Learning Theory, Springer-Verlag New York, Inc.

Vikelsøe, J., P. Fauser, P. B. Sørensen, L. Carlsen (2001): Phthalates and Nonylphenols in Roskilde Fjord - A Field Study and Mathematical Modelling of Transport and Fate in Water and Sediment. NERI report (in press)

Appendix A: Example of quantifying uncertainty

As an illustrative example, the optimum model structure is sought for in a scenario involving transport and degradation of a hydrophobic, slowly degradable substrate in the sediment compartment in a water-sediment system corresponding to the Fjord model described in *Vikelsøe et al. (2000)*.

Three different models having three different complexity levels will be formulated for the same problem. So the analysis will be based on ranked complexity as illustrated in Fig. 4. This example will show how the input- and the structural uncertainty, respectively, interacts in relation to the total model uncertainty.

The following assumption are made

- Steady-state. i.e. $\dfrac{\partial C}{\partial t} = 0$. A detailed analysis of this simplification can be found in *Sørensen et al. (2000)*.

- 1st order degradation of dissolved substrate (k_1).

- Equilibrium between adsorbed and dissolved substrate, described through the equilibrium partition coefficient K_d.

- Constant pore water volume, θ, and thus concentration of particulate matter, X, in sediment. The retention factor, $R = \theta + X \cdot K_d$, will therefore also be constant throughout the sediment profile.

- Vertical molecular diffusive flow (D).

- Constant sedimentation (solids deposition) rate at the sediment surface (S).

The structural, input and total uncertainties related to the steady-state dissolved concentration at a depth of 1 cm will be calculated for the three models.

Each input parameter is associated with an (input) uncertainty expressed as a standard deviation

Adsorption: $R = 10600 \pm 1000$
Degradation: $k_1 = 2 \cdot 10^{-5} \pm 5 \cdot 10^{-6}$ sec^{-1}
Diffusion: $D = 10^{-10} \pm 5 \cdot 10^{-11}$ m$^2 \cdot$ sec^{-1}
Sedimentation: $S = 2.5 \pm 0.5$ mm $\cdot$ year^{-1}

The dissolved pore water concentration in the surface layer is $C_0 = 1$ µg $\cdot$ liter^{-1}.

Model 1: The more complex model. So, the relative structural uncertainty is calculated based on this model (like model 1 in Fig. 4). The model comprises adsorption (R), degradation (k_1), diffusion (D) and sedimentation (S).

The concentration profile is expressed through the linear, one dimensional and homogeneous 2nd order equation

$$\frac{\partial C}{\partial t} = 0 = \frac{D}{R} \cdot \frac{d^2 C}{dz^2} - S \cdot \frac{dC}{dz} - \frac{k_1}{R} \cdot C \tag{3}$$

the solution being (*Vikelsøe et al., 2000*)

$$C_{\text{model 1}}(z) = C_0 \cdot e^{\left(\frac{S \cdot R}{D \cdot 2} - \sqrt{\left(\frac{S \cdot R}{D \cdot 2}\right)^2 + \frac{k_1}{D}} \right) \cdot z} \tag{4}$$

The mean concentration, $C_{\text{mean,model 1}}$, which is equal to the exact concentration, C_{exact}, is found from n = 2000 random Monte Carlo type selections of the normally distributed input values and insertion in Equation **4**.

$$C_{\text{mean,model 1}} = C_{\text{exact}} = \frac{1}{n} \cdot \sum_{i=1}^{n} C_{i,\text{model 1}} = 0.7667 \frac{\mu g}{\text{liter}}$$

Model 2: Includes adsorption (R), degradation (k_1) and sedimentation (S). The diffusion process is omitted in relation to Model 1.

The concentration profile is now defined by

$$\frac{\partial C}{\partial t} = 0 = - S \cdot \frac{dC}{dz} - \frac{k_1}{R} \cdot C \tag{5}$$

with the solution

$$C_{\text{model 2}}(z) = C_0 \cdot e^{\frac{- k_1 \cdot z}{S \cdot R}} \tag{6}$$
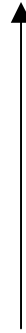
and a mean concentration

$$C_{\text{mean,model 2}} = \frac{1}{n} \cdot \sum_{i=1}^{n} C_{i,\text{model 2}} = 0.7810 \frac{\mu g}{\text{liter}}$$

Model 3: The most simple model. Only adsorption (R) and sedimentation (S) are considered and the steady-state concentration profile will therefore be constant and equal to C_0.

$$C_{\text{mean,model 3}} = 1 \frac{\mu g}{\text{liter}}$$

The three models can be ranked in relation to the complexity level as illustrated in Fig. 5

Higher complexity

$$0 = \frac{D}{R}\frac{d^2C}{dz^2} - S \cdot \frac{dC}{dz} - \frac{k_1}{R} \cdot C$$

$$0 = S \cdot \frac{dC}{dz} - \frac{k_1}{R} \cdot C$$

$$0 = S \cdot \frac{dC}{dz}$$

Lower complexity

Figure 1A. Ranking of the three models in relation to their complexity.

The structural uncertainty is the difference between the exact concentration and the mean concentration of model 1, 2 and 3 respectively

$$\Delta_{structure} = C_{exact} - C_{mean, model} \tag{7}$$

The input uncertainty is the standard deviation of the random concentrations compared to the mean concentration of model 1, 2 and 3 respectively

$$\Delta_{input} = \sqrt{\frac{1}{n-1} \cdot \sum_{i=1}^{n}\left(C_{mean,model} - C_{i,model}\right)^2} \tag{8}$$

The total uncertainty can be calculated according to the law of uncertainty accumulation, cf. Equation **1**. It can also be expressed as the standard deviation of the random concentrations compared to the exact concentration

$$\Delta_{total} = \sqrt{\frac{1}{n-1} \cdot \sum_{i=1}^{n}\left(C_{exact} - C_{i,model}\right)^2} \tag{9}$$

In Table **1** and Figure 6 the uncertainties are compiled for each of the three models.

Table 1 Structural, input and total uncertainties for 3 different models of varying complexities. The models calculate the steady-state concentration at a depth of 1 cm in the sediment. Units in $\mu g \cdot liter^{-1}$.

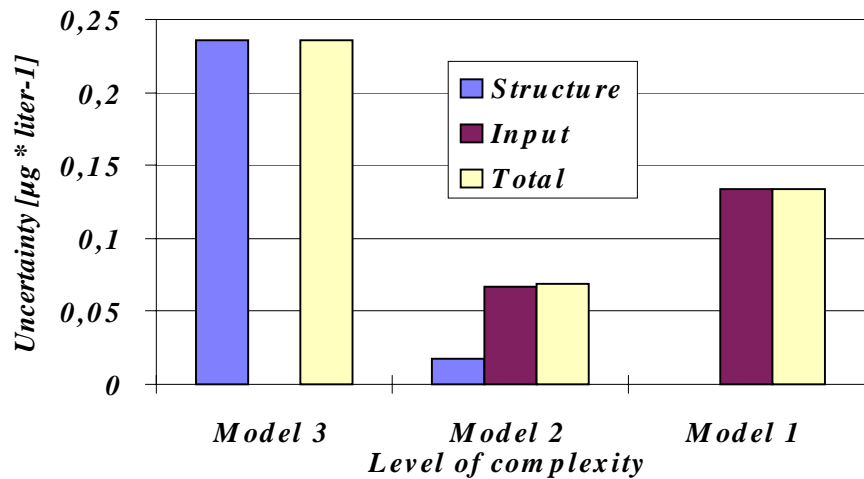|	*Model 1*	*Model 2*	*Model 3*
Structural uncertainty (Equation **7**)	0	0,02	0,24
Input uncertainty (Equation **8**)	0,13	0,07	0
Total uncertainty (Equation **9**)	0,13	0,07	0,24

Figure 2A. *Structural, input and total uncertainties for 3 different models of varying complexities. The models calculate the steady-state concentration at a depth of 1 cm in the sediment.*

The model complexity decreases from model 1 through 3 and accordingly the structural uncertainties increase from zero to approximately 0.238 for model 3. As previously noted model 1 is considered to produce the exact result but in reality this is not true and the structural uncertainty associated with model 1 will be different from zero, but still smaller than model 2 and 3. The more complex model 1 requires more input data and therefore the input uncertainty is larger than for model 2 and 3.

The differences in structural and input uncertainties between model 1 and 2 arise from the influence of diffusion. At a depth of 1 cm the substrate mass arising from molecular diffusion is larger than deeper down in the sediment which implies that the differences in structural and input uncertainties between model 1 and 2 are larger closer to the sediment surface, cf. Equations **7** and **8**. At larger depths, below approximately 0.5 m, the deviation between the output from model 1 and 2 is negligible and accordingly the structural, input and total uncertainties are identical. However, model 1 still requires more information about the input parameters, i.e. the diffusion coefficient.

The calculated dissolved concentrations at a depth of 1 cm in the sediment are thus

$C_{\text{model 1}} = 0.7667 \pm 0.1330 \, \mu g \cdot \text{liter}^{-1}$
$C_{\text{model 2}} = 0.7810 \pm 0.0699 \, \mu g \cdot \text{liter}^{-1}$
$C_{\text{model 3}} = 1 \pm 0.2376 \, \mu g \cdot \text{liter}^{-1}$

The distribution functions are shown in Figure 7.

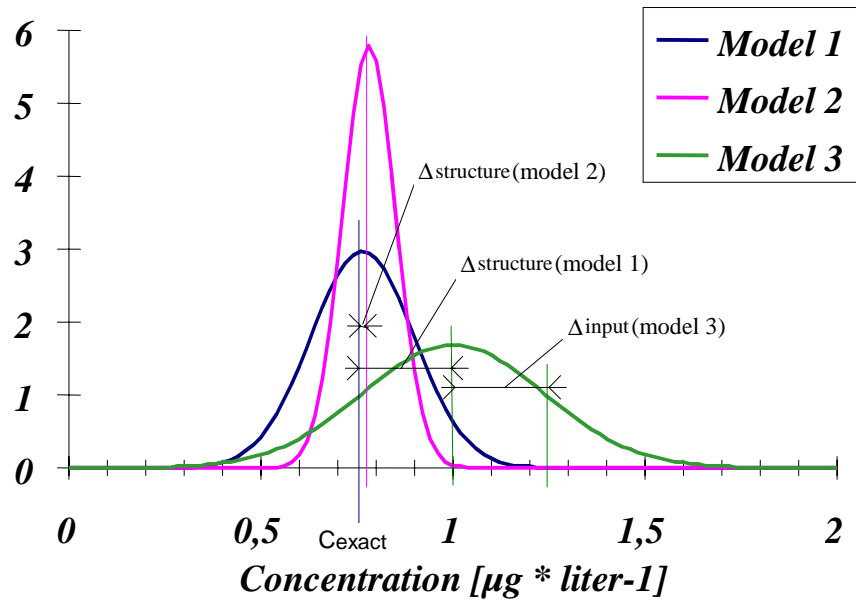**Figure 3A.** *Probability distribution functions for the steady-state dissolved pore water concentration 1 cm in the sediment. The standard deviation is the total uncertainty.*

The optimum model structure for describing the actual problem is therefore model 2. The accuracy is lower but the precision is higher than Model 1. Model 2 is simpler and requires less input information and is easier to use as a mathematical tool.

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