Defining Uncertainty and Variability in Environmental Fate Models

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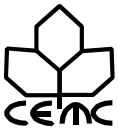

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EXECUTIVE SUMMARY

This report identifies the two main components of mass balance models of chemical fate in the environment as the equations describing the processes, and the parameters describing the chemical, the environment, and the emission. Uncertainty, variability, difference and error are defined within the context of determining model reliability. Studies of chemical, environmental, and emission data quality are discussed. There is a need for care in determining the relative importance of these data to a model outcome.

INTRODUCTION

It is useful, prior to embarking on any discussion of model reliability, to identify the model components, to consider some commonly used terms: their meaning in the context of the study, and their application in previous work.

MODEL COMPONENTS

Mathematical models of chemical fate in the environment are composed of equations and parameters. The equations describe quantitatively the natural processes being modelled, usually as equilibrium or rate expressions. The parameters describe relevant properties of the specific system under investigation. In the case of environmental fate models these parameters can be classified as chemical properties, discharge or emission data, and landscape parameters. Together the equations and parameters produce the model results to be used by those who interpret the results, including decision-makers. It is assumed that the equations and the parameters are correct in structure and approximate magnitude. However, models are necessarily a simplification of a complex system with an associated uncertainty due to the mathematical approximations and the uncertainty and variance in the parameters. As regulators and others in the chemical industry rely increasingly on models as decision-making tools, it is vital that the variance of the model outcome and its sources be thoroughly understood.

VALIDATION AND EVALUATION OF MATHEMATICAL DESCRIPTIONS OF ENVIRONMENTAL SYSTEMS

In the context of risk assessment and regulation, model validation becomes important, however environmental models can not be validated in the same sense as models of highly reproducible closed systems (Oreskes et al 1994; Oreskes 1998). Credibility, however, can be improved by documenting examples in which observed and predicted concentrations are compared, as single values or ranges with identification of dominant sources, fate processes, or partitioning characteristics. Such comparison studies have been performed on mass balance models of chemical fate with generally positive results (Devillers et al 1995; Mackay et al 1996c; Bintein and Devillers 1996a,b; Koprivnjak and Poissant 1997; MacLeod and Mackay 1999). These studies assume that the model equations are generally correct. The equations in different environmental fate models tend to be very similar (Cowan et al, 1995) indicating a high level of communication and confidence within the research community and making this not an unreasonable assumption. Unfortunately, it can be difficult to ascertain where differences occur due to the “black box” structure of many models.

In their comparison of model results, Cowan et al (1995) found that differences were largely attributable to differing landscape parameters and not to model structure. The chemical properties and discharge rates are typically provided by the user or decision-maker but environmental parameters may be either partially or wholly embedded in the program. For example, EQC has

properties typical of northeastern USA / southern Ontario partially embedded (Mackay et al 1996b) while EUSES, has properties typical of the Netherlands wholly embedded (Vermeire et al 1997, TSC Group Delft bv 1997).

Environmental, or landscape, properties are often selected by model developers. These models are designed to focus on chemical-to-chemical differences in environmental fate and facilitate regulatory assessments. The intent of the developers of the EQC model and other "evaluative" models was that they should provide the tool for one stage in a multi-stage analysis and their use is to be followed by a regional assessment (Mackay et al 1996a).

UNCERTAINTY, VARIABILITY, DIFFERENCE, AND ERROR IN MODEL PARAMETERS

The need for uncertainty and sensitivity analyses of model outcome has been long recognised (Slob 1994; Jager and Slob, 1995; Cowan et al 1995; Mackay et al 1996a; Vermeire et al 1997; Barnthouse et al 1998; Bennett et al, 1999). There is a general acceptance that every model outcome should be expressed as a distribution rather than a single value. Similar terminology has been used in a variety of contexts with different meanings to assign cause to the distribution in model outcome (Jager and Slob 1995; Bennett et al 1999; Huijbregts et al 2000). Here the following definitions are used to describe the quality of parameters.

> ***Uncertainty*** is a measure of the knowledge of the magnitude of a parameter. Uncertainty can be reduced by research, i.e., the parameter value can be refined. Uncertainty is quantified as a distribution. For example the volume of a lake may be estimated from its surface area and an average depth. This estimate can be refined by measurement.
>
> ***Variance*** is a measure of the heterogeneity of a landscape parameter or the inherent variability in a chemical property. Variance can not be reduced by further research. It is quantified as a distribution. For example, the organic carbon content of the soil in a region may vary, even over short distances. The soil is not homogenous and thus the organic carbon content can be described with a distribution of values.
>
> ***Difference*** is a measure of the uniqueness of the substance or region described. It is not described by a distribution. It is not the result of a lack of knowledge, inherent variation, nor an incorrect assignment. For example, the surface area of Lake Ontario is different from the surface area of Lake Superior.
>
> ***Error*** is an invalid or incorrect parameter assignment. It is not described by a distribution. Research is required, not to refine the value but to correct it.

UNCERTAINTY AND SENSITIVITY IN MODEL OUTCOME

Model outcome is uncertain due to parameter uncertainty and variability as defined above. This is often determined using Monte Carlo techniques. While alternate methods have been proposed (Slob, 1994; MacLeod et al 2002), Monte Carlo analysis remains the standard for this type of study.

Model outcome is sensitive to each parameter. This sensitivity has been quantified as the relative change in outcome divided by a small relative change in parameter, i.e., the partial derivative (Mackay et al 1996c).

The role of uncertainty and sensitivity analyses differs with model applications. When models are being used to rank chemicals, products, processes, or systems, it is necessary to determine whether differences in model outcome are significant and whether such differences are real or artifacts of uncertainty and variance in parameters. By contrast, in single chemical, product, or system evaluation uncertainty analysis provides the distribution of the model outcome while sensitivity analysis shows the relative contribution of each parameters uncertainty and variance to the outcome variance thus facilitating outcome variance reduction.

CHEMICAL PARAMETER QUALITY

Chemical-to-chemical differences in the environmental fate of substances are controlled by the physical-chemical properties. When measuring physical-chemical properties, an identified chemical is tested and properties are determined with a precision defined by the experiment. This is often given as a mean value with a normal or lognormal distribution. For some properties such as individual media degradation half-lives, there is also variation unrelated to experimental precision. Factors such as the intensity and duration of sunlight, and the concentration of hydroxyl radicals make it impossible to assign the substance a single, discrete value for the degradation half-life in air, for example. For the half-lives in water, soil, or sediment, the nature of the microbial community is a major confounding factor. (Mackay et al 2000) These variations are also generally characterised by lognormal distributions. Mackay et al (2000) suggest assigning half-life classes on a logarithmic scale with variation of one or two classes to each degradation rate.

When assessing the variance, or uncertainty, in model outcome Monte Carlo analysis has become the standard for environmental fate and effects models (Calabrese, 1996). These analyses are often preformed for a number of chemicals in a single environment, with either realistic discharges or hypothetical emissions depending on the focus of the study (Kühne et al 1997; Bennett et al 1999; Hertwich et al 1999; Huijbregts et al 2000; Maddalena et al 2001; MacLeod et al 2002). Half-lives are typically the least well-defined chemical property, i.e., have the highest standard deviation, and thus are often the critical properties in determining the variance in model outcome.

It must be recognized that such an assessment of variance presupposes that the chemical has been correctly identified, that is, that the physical-chemical properties are correct. If even one of the property values is incorrect, the model outcome is, effectively, that of a different chemical.

Certain parallels can be drawn between this case of "chemically-specific physical-chemical properties" when considering the importance of regionally-specific landscape parameters.

ENVIRONMENTAL PARAMETER QUALITY

Region-to-region differences in the environmental fate of a substance are controlled by the landscape properties. When measuring a landscape parameter for an identified region a value can be assigned with a precision defined by the method. Whether that method involves traditional surveying techniques or the analysis of satellite images there is an associated uncertainty. There is an additional uncertainty caused by such decisions as, whether ponds, streams, and wetlands are considered in the same category as other surface waters, i.e., a water-body size cut-off must be selected. These sources of variance have also been characterised by normal and lognormal distributions and the resulting model outcome variances determined using Monte Carlo analysis (Hertwich et al, 1999; Huijbregts et al 2000; Maddelena et al 2001, MacLeod et al 2002).

In the Sacramento air basin study by Maddelena et al (2001), total potential dose was selected as the model outcome of interest and for the emission scenarios selected. For benzene, wind speed controlled the variance, for fluoranthene, the depth of the surface soil was key to the variance, and for hexachlorobenzene, the variance was more sensitive to rain rate than any other landscape parameter. Hertwich et al (1999), evaluated the variance in potential dose for 236 chemicals in the California region. They found that the contribution of landscape parameters to the overall variance in potential dose was typically less than 10% while, not surprisingly, individual media reaction half-lives often contributed most to the variance. MacLeod et al (2002) found, that for benzo[a]pyrene emitted into the air at a fixed rate in southern Ontario, the aerosol deposition velocity contributed most the variance in their chosen endpoint of total mass of chemical present in the environment, assuming the emission rate is known absolutely.

Model sensitivity to landscape parameters appears less consistent than for chemical properties. However, this may be due to the approach used by those conducting the study. For examinations of model sensitivity to chemical properties, a single landscape is chosen; for examinations of model sensitivity to landscape properties, many chemicals may be used. By analogy with the first examination which uses a single "generic" landscape, the second should be conducted using a single "generic" chemical. Of course, this introduces a severe difficulty. It is impossible to define a single "generic" chemical. Sensitivity of the model outcome depends on both the region selected and the chemical chosen. It is expected that such a study would show that degradation half-lives continue to contribute most to variance in model outcome due to the extremely high variation and uncertainty in these parameters.

EMISSION PARAMETER QUALITY

Uncertainty in emission or discharge data can be very high and is often difficult to estimate (Maddelena et al 2001). In cases where this uncertainty was included in the analysis of outcome variance, it played a significant role (Bennett et al 1999; Huijbregts et al 2000). Exposure (Bennett et al 1999) and LCA (Hertwich et al, 1999; Huijbregts et al 2000) studies with estimated emissions have been performed. It was found that uncertainty in chemical properties contributed more to outcome variance than either emission or landscape variance. Other researchers have chosen to use generic emissions and assumed that these were known absolutely or otherwise removed from consideration so that the analysis could highlight other sources of outcome variance (Kühne et al 1997; Maddelena et al 2001; MacLeod et al, 2002).

CONCLUSION

There are three sources of uncertainty and variance contributing to uncertainty in the outcome from models of chemical fate in the environment; chemical properties, landscape properties, and emission data. There is an incentive to minimize error and uncertainty in all three. In focussing data research efforts, sensitivity analyses are helpful but care must be exercised to avoid misleading evidence. The cost of the effort to define or refine a parameter should be balanced against the expected reduction in outcome uncertainty.

REFERENCES

Barnthouse, L, Fava, J., Humphreys, K., Hunt, R., Laibson, L., Noesen, S., Norris, G., Owens, J., Todd, J., Vigon, B., Weitz, K., Young, J., 1998. Life-Cycle Impact Assessment: the State-of-the-Art. Report of the SETAC Life-Cycle Assessment (LCA) Impact Assessment Workgroup. Society of Environmental Toxicology and Chemistry (SETAC).

Bennett, D.H., Kastenberg, W.E., McKone, T.E. 1999. A multimedia, multiple pathway risk assessment of atrazine: the impact of age differentiated exposure including joint uncertainty and variability. *Reliability Engineering and System Safety.* 63: 185-198.

Bintein, S., Devillers, J., 1996a. Evaluating the environmental fate of lindane in France. *Chemosphere.* 32: 2427-2440.

Bintein, S., Devillers, J., 1996b. Evaluating the environmental fate of atrazine in France. *Chemosphere.* 32: 2441-2456.

Calabrese, E.J., 1996. Special Issue: Commemoration of the 50th anniversary of Monte Carlo. *Hum. Ecol. Risk Assess.* 2: 627-1038.

Cowan, C.E.; Mackay, D.; Feijtel, T.C.J.; van de Meent, D.; Di Guardo, A.; Davies, J.; Mackay, N., 1995. The Multi-Media Fate Model: A vital tool for predicting the fate of chemicals. Proceedings of a workshop organized by the Society of Environmental Toxicology and Chemistry (SETAC), SETAC Press: Pensacola, FL.

Devillers, J.; Bintein, S.; Karcher, W., 1995. Chemfrance: a regional level III fugacity model applied to France. *Chemosphere.* 30: 457-576.

Hertwich, E.G., McKone, T.E., Pease, W.S., 1999. Parameter Uncertainty and Variability In Evaluative Fate and Exposure Models. *Risk Analysis.* 19: 1193-1204.

Huijbregts, M.A.J, Thissen, U., Jage, T., van de Meent, D., Ragas, A.M.J., 2000. Priority assessment of toxic substances in life cycle assessment. Part II: assessing parameter uncertainty and human variability in the calculation of toxicity potentials. *Chemosphere.* 41: 575-588.

Jager D.T., Slob, W., 1995. Uncertainty analysis of the Uniform System for the Evaluation of Substances (USES). Report no. 679102027. RIVM. Bilthoven, The Netherlands.

Koprivnjak, J.F., Poissant, L., 1997. Evaluation and application of a fugacity model to explain the partitioning of contaminants in the St. Lawrence River Valley. *Water, Air, and Soil Pollution* 97: 379-395.

Kühne, R., Breitkopf, C., Schüürmann, G., 1997. Error propagation in fugacity Level III models in the case of uncertain physicochemical compound properties. *Environ. Toxicol. Chem.* 16: 2067-2069.

Maddalena, R.L., McKone, T.E., Hsieh, D.P.H., Geng, S., 2001. Influential input classification in probabilistic multimedia models. *Stochastic Environmental Research and Risk Assessment.* 15: 1-17.

MacLeod, M., Mackay, D., 1999. An assessment of the environmental fate and exposure of benzene and the chlorobenzenes in Canada. *Chemosphere*. 38: 1777-1796.

MacLeod, M., Fraser, A., Mackay, D., 2002. Evaluating and Expressing the Propagation of Uncertainty in Chemical Fate and Bioaccumulation Models. *Environ. Toxicol. Chem*. 21: 700-709.

Mackay, D., Di Guardo, A., Paterson, S., Kicsi, G., Cowan, C.E., 1996a. Assessing the Fate of New and Existing Chemicals: A Five Stage Process. *Environ. Toxicol. Chem*. 15: 1618-1626.

Mackay, D., Di Guardo, A., Paterson, S., Cowan, C.E., 1996b. Evaluating the Environmental Fate of a Variety of Types of Chemicals Using the EQC Model. *Environ. Toxicol. Chem.* 15: 1627-1637.

Mackay, D., Di Guardo, A., Paterson, S., Kicsi, G., Cowan, C.E., Kane, D.M., 1996c. Assessment of Chemical Fate in the Environment Using Evaluative, Regional and Local-Scale Models: Illustrative Application to Chlorobenzene and Linear Alkylbenzene Sulfonates. *Environ. Toxicol. Chem*. 15: 1638-1648.

Mackay, D., Shiu, W.Y., Ma, K.C., 2000. Physical-Chemical Properties and Environmental Fate and Degradation Handbook. CRCnetBASE 2000, Chapman & Hall CRCnetBASE, CRC Press LLC., Boca Raton, FL. (CD-ROM.)

Oreskes, N., Shrader-Frechette, K., Belitz, K., 1994. Verification, validation, and confirmation of numerical models in the earth sciences. *Science*. 263: 641-646.

Oreskes, N., 1998. Evaluation (not validation) of quantitative models. *Environmental Health Perspectives.* 106 (Suppl. 6): 1453-1460.

Slob, W., 1994. Uncertainty Analysis in Multiplicative Models. *Risk Analysis.* 14: 571-576.

TSA Group Delft bv., 1997. EUSES: the European Union System for the Evaluation of Substances 1.00 User Manual. The Netherlands Ministry of Housing, Spatial Planning, and the Environment, the European Commission, the UK Department of the Environment, the Danish EPA, the German Umweltbundesamt, and the Swedish National Chemicals Inspectorate.

Vermeire, T.G., Jager, D.T., Bussian, B., Devillers, J., den Haan, K., Hansen, B., Lundberg, I., Niessen, H., Robertson, S., Tyle, H., van der Zandt, P.T.J., 1997. European Union System for the Evaluation of Substances (EUSES). Principles and structure. *Chemosphere.* 34: 1823-1836.