ESTABLISHING CREDIBILITY IN THE ENVIRONMENTAL MODELS USED FOR SAFETY AND LICENSING CALCULATIONS IN THE NUCLEAR INDUSTRY

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INTRODUCTION

Models that simulate the transport and behaviour of radionuclides in the environment are used extensively in the nuclear industry for safety and licensing purposes. They are needed to calculate derived release limits for new and operating facilities, to estimate consequences following hypothetical accidents and to help manage a real emergency. But predictions generated for these purposes are essentially meaningless unless they are accompanied by a quantitative estimate of the confidence that can be placed in them. For example, in an emergency where there has been an accidental release of radioactivity to the atmosphere, decisions based on a validated model with small uncertainties would likely be very different from those based on an untested model, or on one with large uncertainties.

This paper begins with a discussion of some general methods for establishing the credibility of model predictions. The focus will be on environmental transport models but the principles apply to models of all kinds. Experience in international model intercomparison programs such as BIOMOVS (Biospheric Model Validation Study (1)), VAMP (Validation of Model Predictions (2)) and BIOMOVS II (Phase II of BIOMOVS (3)) suggests that, although modelers know what they should do in the area of validation and uncertainty, they do not always do it. Establishing the credibility of a model is not a trivial task. It involves a number of tasks including face validation, verification, experimental validation and sensitivity and uncertainty analyses (4). Each of these tasks is inherently subjective in nature and must be addressed carefully if meaningful results are to be obtained. Each will be discussed in turn below. The work currently underway in the Canadian nuclear industry to validate safety assessment codes is using many of these tools.

The remainder of the paper will present quantitative results relating to the credibility of environmental transport models. Model formulation, choice of parameter values and the influence of the user will all be discussed as sources of uncertainty in predictions. The magnitude of uncertainties that must be expected in various applications of the models will be presented. The examples used throughout the paper are drawn largely from recent work carried out in BIOMOVS and VAMP.

FACE VALIDATION

A model possesses face validity if it and its parameter values are accepted by experts as being reasonable in the light of current scientific knowledge and practice. (This definition and others to follow are working definitions for use in this paper and are not offered as universal.) To demonstrate face validity, it is necessary to evaluate the assumptions made in developing the model, the processes included in it and how they are formulated mathematically. It must be shown that each of these components is treated appropriately, taking into account the purpose of the model and prevailing levels of understanding. This can be achieved in a number of ways. Initial construction of the model can be based upon scenario analysis, in which the features, events and processes that should be included are identified through a formal, structured procedure (5). The model can be shown to be consistent with ideas in the recent literature and with approaches taken by other groups working on the same types of problems. Its formulation and predictions can be compared with those of similar models through participation in international programs such as BIOMOVS and VAMP. Finally, it can be subjected to peer review through publication in the open literature. A model that performs well in each of these evaluation procedures can claim the credibility that attaches to scientific consensus.

VERIFICATION

Verification is the process of demonstrating that the equations representing the conceptual model are correctly coded and solved in the computer program. A verified code is not necessarily a good representation of reality, but is one that is working as its designer intended it to work. There are many ways to verify a computer code:

- Use a structured approach to code development, from task specification through code design to the coding itself. Use object-oriented programming techniques and modular structure in the coding.

- Use computer-aided software engineering to help design, generate, maintain and document codes (6). Use computer-aided tools such as unit checks to enhance quality assurance.

- Conduct code walkthroughs, examining each line in turn for errors.

- Compare the predictions of the code against known solutions and against the predictions of other codes.

- Ensure that the people involved in the development of the code are suitably trained. Use independent people in the verification phase, and challenge them to find errors.

- Thoroughly document all aspects of code development, changes, testing and use.

SENSITIVITY ANALYSIS

Sensitivity analysis quantifies the change in model output due to changes in the values of the input parameters, and ranks the parameters to which the model is most sensitive. It can increase understanding of a model by revealing the relationship between its parameters and its predictions, and by providing the opportunity to examine its behaviour under a variety of conditions. Confidence in the model is increased if it responds to changes in parameter values as expected on an intuitive basis and if good data are readily available for the most sensitive parameters. Sensitivity analysis can also aid in setting priorities for future development of the model. Work can focus on the sensitive processes and parameters, allowing improvements to be achieved with a minimum of resources and effort.

The results of a sensitivity analysis can depend very strongly on the model endpoint. For example, Table 1 shows the sensitivity of the function $Z = \exp(-H^2/2\sigma_z^2)/\sigma_z$, to which air concentrations are proportional in the Gaussian plume model of atmospheric dispersion. Here H is the release height and σ_z is a measure of the vertical spread of the plume at a given downwind distance. Close to the release point, the lower edge of the plume just reaches the ground and a small change in σ_z produces a very large change in Z as the exponential term increases rapidly. In contrast, at a downwind distance of 750 m, Z goes through a maximum and changes in σ_z have little influence on its magnitude. Therefore σ_z must be very precisely known in order to predict ground-level concentrations close to the source, but can be quite uncertain at greater downwind distances and still produce a good level of accuracy in the predicted concentration.

Table 1
Sensitivity of the Function $Z = \exp(-H^2/2\sigma_z^2)/\sigma_z$ to a 50% Increase in σ_z
for H = 50 m and Neutral Atmospheric Stability

Downwind Distance (m)	Change in Z
200	a factor of 34
750	10%

EXPERIMENTAL VALIDATION

Validation is the quantitative testing of model performance by comparing predictions with independent observations. The model should be tested only for the conditions in which it is meant to apply. The testing should be done at intermediate points in the calculations, as well as at the final endpoints, to check for the possibility of compensatory errors.

The process of comparing predictions and observations can be done either graphically or statistically (7). Graphical analysis is recommended in all validation exercises, as it provides a quick visual picture of the relationship between predictions and observations, especially if error bars are included. It is particularly useful when time series are involved, as it reveals at a glance whether the dynamics of the model and the data are the same. In addition, graphical analysis is usually fairly reliable in distinguishing between the performance of different models. But even if no formal statistical tests are applied, comparisons between predictions and observations should be quantitative. Statements such as "the predictions agree well with observations" are essentially meaningless and should be replaced, for example, with an estimate of the fraction of the results that are within a factor of two of the observations.

Statistical tests are required for drawing specific conclusions about the agreement between predictions and observations. But care must be taken in applying such procedures since statistical analysis is not well developed for the type of output produced by environmental transport models. Model predictions are usually not independent, normally distributed or drawn randomly from populations, and so violate the basic assumptions of many statistical tests. However, statistics can be useful for answering certain types of questions. For example, analysis of variance (8) can establish if the predictions of one model agree with those of another. Cluster analysis and principal component analysis (9) can help to identify similarities between models, and to determine if those similarities can be ascribed to specific model features. Measures such as normalized root mean square error (10) and mean fractional error (11) can show if one model performs better than another in reproducing a given data set, although they leave unanswered the question of whether the level of agreement between predictions and observations is adequate. When statistical tests are used, care must be taken to distinguish practical significance from statistical significance. Very small differences between two sets of predictions can cause one to fail a test in the statistical sense and the other to pass when the two sets are essentially identical on a practical level. Moreover, conclusions about model performance should never be drawn from statistical tests alone but should be based on the use of all tools available for establishing model credibility.

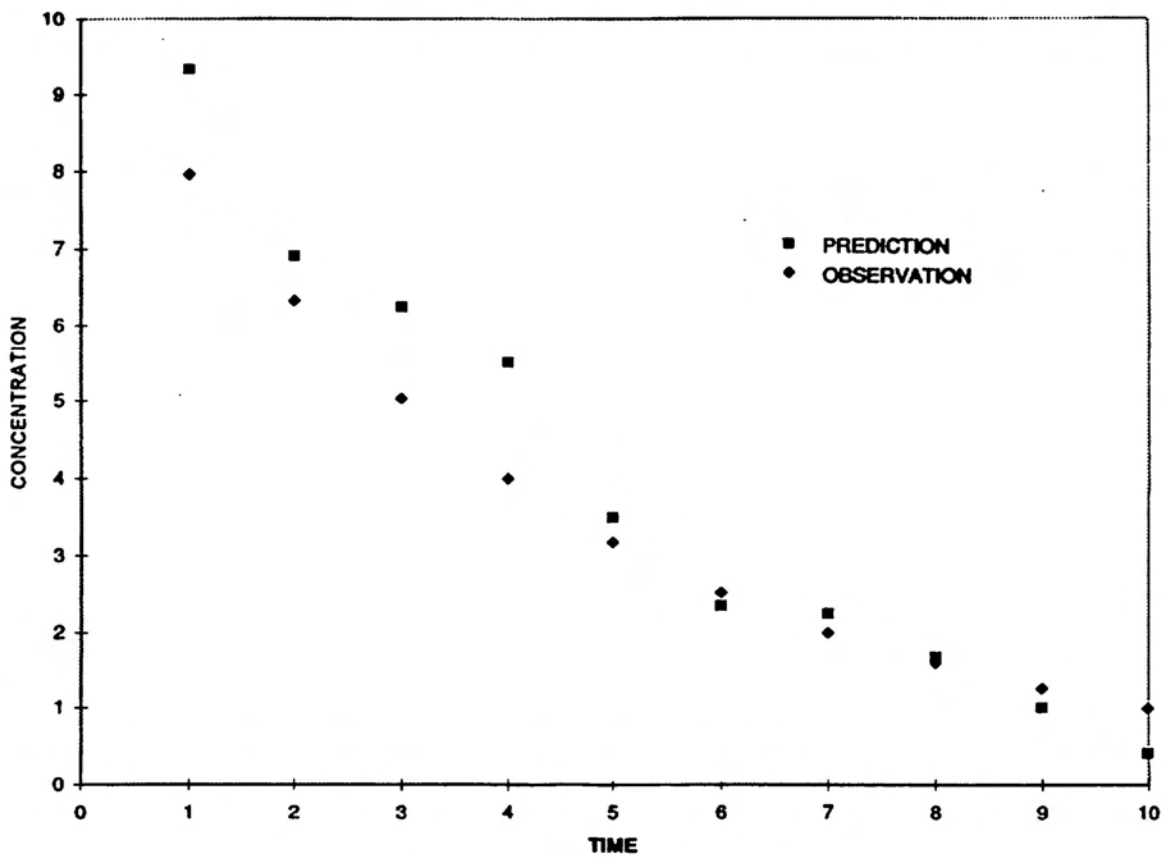
In any validation study, attention should be given to the observations as well as to the predictions. The two must be consistent for the comparison to be meaningful. Furthermore, where they disagree, the fault should not automatically be assumed to lie with the predictions. Experimental observations can be in error for many reasons, including the collection, preparation and analysis of the environmental samples. Cases arose in both BIOMOVS (12) and BIOMOVS II (13) in which the reasons for differences between predictions and observations could be traced to errors in the observations.

UNCERTAINTY ANALYSIS

Uncertainty analysis provides a quantitative statement of the range of model predictions that results from uncertainties in model structure or parameter values (14,15,16). The importance of uncertainties in establishing model credibility cannot be overstated. They make validation possible by providing a measure against which to decide if differences between predictions and observations are significant. The range of applicability of a model can be defined as the domain in which uncertainties are acceptably small. Finally, the magnitude of the uncertainties often affects the decisions that are based on the predictions of the model.

Some of these concepts can be made more concrete by considering the comparison of hypothetical predictions and observations shown in Figure 1. Most radioecologists would

Figure 1
Hypothetical Observations and Predictions of Radionuclide Concentration
as a Function of Time



likely be impressed with the evident level of agreement demonstrated in this figure. But there is in fact no agreement in the normal sense of the word since at no point in time are the predictions and observation numerically equal. Apparently, agreement in the context of validation allows for some degree of difference, which is quantified by the uncertainty estimates. The impression of good agreement in Figure 1 would be warranted if the data pertained to the loss of activity over time from an environmental compartment such as the soil following a deposition event. Past experience with situations of this sort suggests that the expected uncertainties would be much larger than the differences in the figure, implying that the model is performing well. But if instead the data describe the radioactive decay of a particular nuclide, the level of agreement is not so impressive. The uncertainties in this case should be less than the differences between predictions and observations shown in the figure, and the model would be judged inadequate. Thus two diametrically opposite interpretations of Figure 1 can be made depending on the uncertainties assigned to the predictions. Conclusions regarding model performance cannot be drawn without taking uncertainties into account.

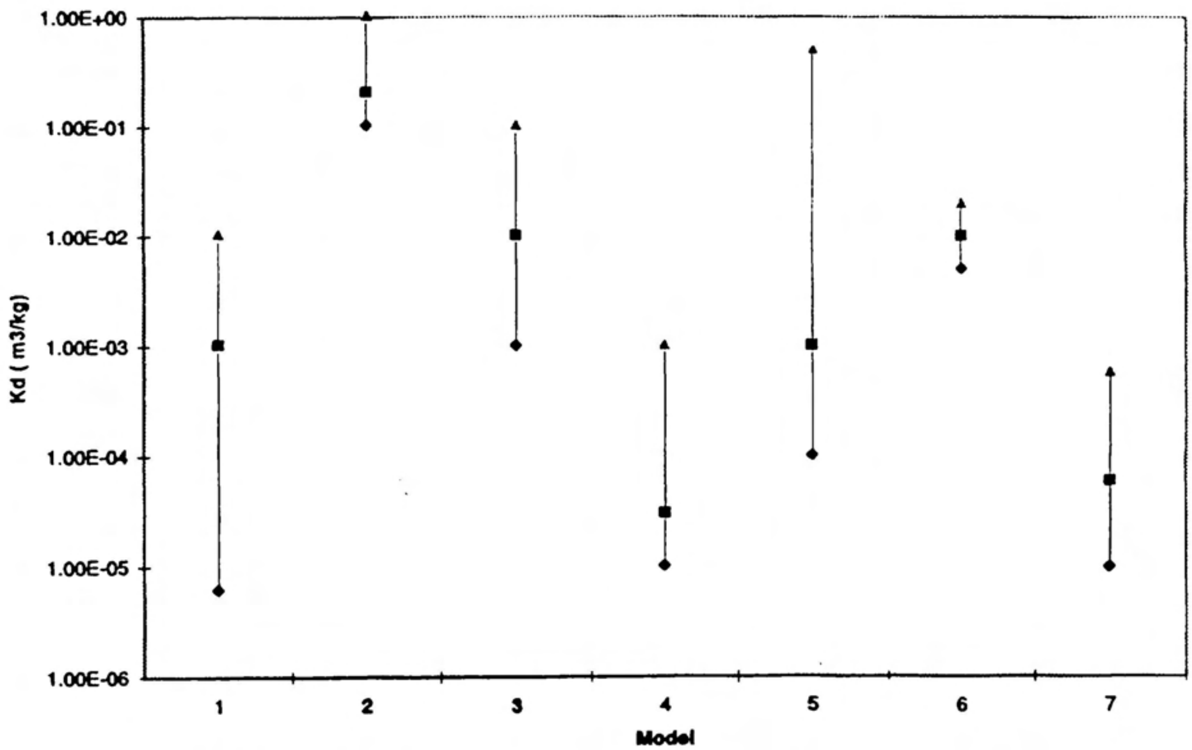
Uncertainty in model predictions can arise from many sources, the most common being parameter values, model conceptualization and formulation, and user interpretation. These sources will be discussed in turn below. Uncertainty analysis can help to identify the main sources of uncertainty and so point the way to priorities for future research.

Parameter Uncertainty

The parameter values used in a given model may be uncertain for a number of reasons. Observations on which to base the values may be scarce, and invariably will contain measurement errors. Data derived from laboratory experiments may be quite different from values that are appropriate in the field. Empirical parameters may be used outside of their range of applicability. Spatial and temporal averaging may not be consistent with model objectives. Lumped parameters that represent the net effect of several processes may not describe those processes well.

The propagation of parameter uncertainties through a model is usually done by Monte Carlo analysis. Each variable parameter is first assigned a probability density function (PDF) that reflects the degree of belief that the parameter will take on given values within its range. The model is then run a large number of times, with a different set of parameter values chosen each time by random or stratified sampling from the PDFs. Uncertainties in the predictions are determined from the distribution of outputs. These techniques are well known and will not be discussed further here, except to point out that specification of the PDFs is the critical step. Very rarely are there enough data to derive the PDFs objectively and it is usually necessary to resort to subjective assignments. In this case it is vital that the distributions be set by consensus. Formal expert elicitation, which is expensive and time-consuming, is normally not required, but informal input from a number of experts will help to avoid the bias that a single individual inevitably brings to the process. To illustrate this, Figure 2 shows the distributions chosen by seven different modelers, each working alone, for the ^{99}Tc soil solid/liquid partition coefficient (K_d) in the BIOMOVS B2 scenario (Irrigation with contaminated groundwater (17)). Although each participant had access to the same database, their best-estimate values extended over four orders of magnitude and the uncertainty ranges varied from one to four orders of magnitude. Had the participants been able to meet and discuss this parameter, it is likely they would have agree on intermediate values, and reduced the substantial variability that the original range induced in the predicted ^{99}Tc concentrations in soil.

Figure 2
K_d Values and Uncertainty Ranges for ^{99}Tc Adopted by Participants in the BIOMOVS B2 Scenario (Irrigation with Contaminated Groundwater)



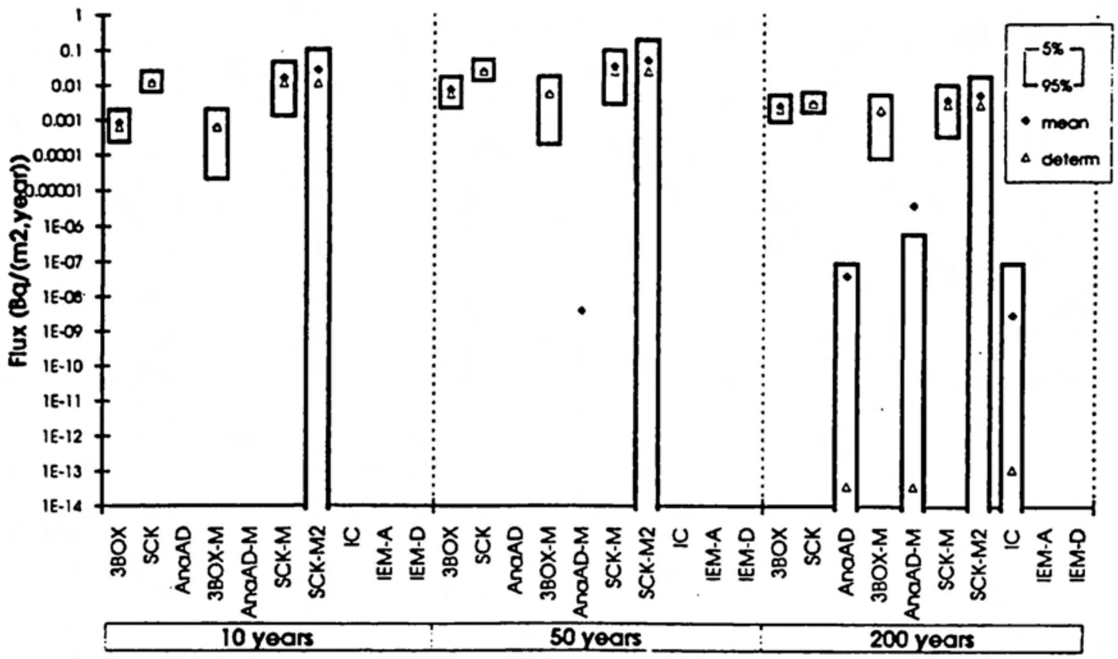
Model Uncertainty

The simplifications inherent in all models lead to uncertainties in their predictions. These may arise because it is not clear what processes are operating in the system, or because the processes are too poorly understood or too complex to be modeled adequately. Most models cannot account for the large natural spatial and temporal variability found in the environment.

It is generally difficult to quantify the uncertainty in a conceptual model or in its mathematical representation. The exception is the case in which more than one process may be responsible for a given consequence. For example, it is not clear whether the formation of organically-bound tritium (OBT) in plants at night is due to residual photosynthetic processes or to other chemical reactions. In such a case both processes are coded into the model and a new binary parameter P_b defined that implements one or the other depending upon its value. The model is run a large number of times as in an ordinary uncertainty analysis, with values of P_b chosen to reflect the degree of belief that one process or the other causes the OBT formation. In this way the uncertainty in the conceptual model is quantified in the analysis.

The magnitude of model uncertainty can sometimes be quite large. Figure 3 shows results from the Model Complexity Working Group of BIOMOVS II (18). Participants were asked to calculate the flux of ^{137}Cs to groundwater as a function of time following contamination of the surface soil layer. This was done using models of varying complexity,

Figure 3
Predictions and Uncertainty Estimates of the ^{137}Cs Flux to Groundwater by Models of Different Complexity (Model Complexity Working Group of BIOMOVS II)



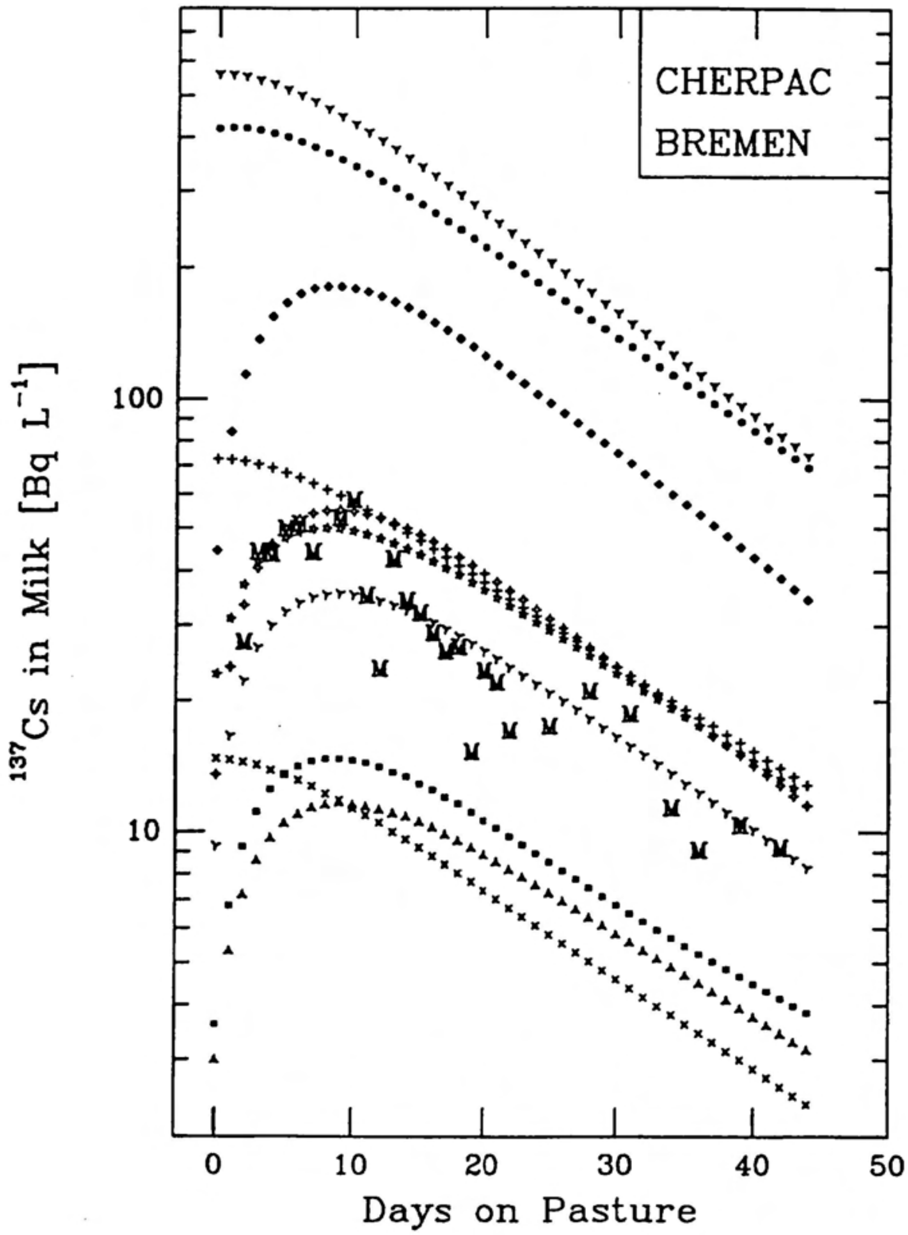
ranging from simple box models (3BOX, SCK) to sophisticated numerical solutions of the advection-diffusion equation (AnaAD, IC). The box models tended to predict much larger fluxes than the advection-diffusion models because the assumption of instantaneous mixing within a box resulted in artificially-enhanced diffusion and faster downward migration of the radioactivity through the soil profile. Although this is a well-known deficiency in box models, none of the participants took it into account when they calculated the uncertainty in the fluxes, leading to estimates that were unrealistically small. The gap between the error bars associated with the box and advection-diffusion codes at 200 years suggests that model uncertainty in this case amounted to several orders of magnitude.

User Interpretation

If two different modelers were asked to perform a given assessment using the same code, it is likely that their predictions would be substantially different. In carrying out the task, each modeler must make many decisions, most of which are highly subjective. He or she must first interpret the scenario and determine how best to match the given information, which is often incomplete and inconsistent, to the input requirements of the code. The code itself must be understood and its various options selected in such a way that the output provides a suitable answer to the assessment question. Finally, values for all of the parameters required by the model must be chosen to best reflect the situation being simulated. There are usually no "right" responses in any of these tasks and the different choices made by different modelers contribute to the uncertainty in the model predictions.

A Working Group was set up in BIOMOVS II to quantify the effect of the user on uncertainty for assessments dealing with radionuclide transfer through terrestrial food chains (19). The same three codes and the same three scenario descriptions were distributed to ten different modelers, each of whom worked independently to obtain the specified outputs. Results produced using the CHERPAC code (20) are shown in Figure 4 for the Bremen scenario, which involved the transfer of ^{137}Cs to milk from plants and soil contaminated by deposition of airborne activity following the Chernobyl accident. The predictions all show roughly the same dynamics as the observations, suggesting that the modelers were able to implement the code as desired, but the spread in the magnitude of the concentrations at any time is almost a factor of 100. These results were typical of other codes, scenarios and endpoints, and were obtained by modelers who were experienced in these sorts of assessments. Choice of parameter values was identified as the primary cause of the different predictions, although the assumptions made in deriving input data from the scenario descriptions was also a major contributor. The Working Group recommended that all important assessments be carried out by at least two different groups or by teams of experts. In this way the magnitude of the uncertainty due to user interpretation can be estimated and, through consensus, reduced.

Figure 4
Time-Dependent Predictions of ^{137}Cs Concentrations in Milk by 10 Modelers using the CHERPAC Code for the Bremen Scenario (User Interpretation Working Group of BIOMOVS II). 'M' denotes measurements.



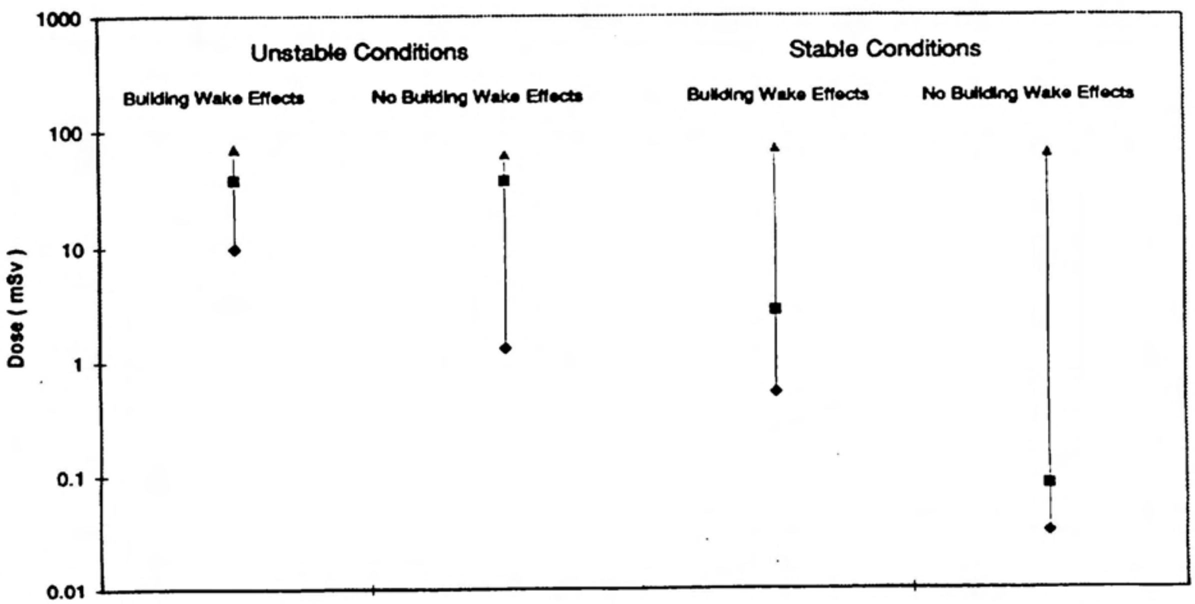
CURRENT STATUS OF MODEL CREDIBILITY

The level of confidence that can be placed in the predictions of current environmental transport models is discussed below for three different applications.

Short-Range Atmospheric Dispersion Models

Atmospheric dispersion is a well-studied and reasonably well-understood subject. Models for short-range dispersion have high face validity and have been tested against experimental data in many studies. However, dispersion is a stochastic phenomenon and there is no general theoretical relationship connecting turbulence to diffusion. Concentrations measured at the same location under ostensibly identical meteorological conditions can vary by up to a factor of two. Current models are unable to account for this, and so their predictions contain an inherent uncertainty of this order of magnitude. To this must be added uncertainties due to parameter values. Figure 5 shows the results of work in progress on the parametric uncertainty of a Gaussian Plume model. The end point of the calculations was the total thyroid dose, summed over inhalation, cloudshine and groundshine, to an adult located 1000 m downwind of an elevated source of ^{131}I of source strength 10^{14} Bq. The stack gas temperature was 70°C above ambient, and the release was subject to the wake effects of a nearby building. Rain was falling at the rate of 3 mm/h during the release. Probability density functions for the variable parameters were set using a process of informal expert elicitation and uncertainties were determined from 100 model runs in which parameter values were selected using Latin Hypercube Sampling. Figure 5 shows that, for unstable conditions in the presence of building wakes, the 95% confidence interval on the total dose spans almost an order of magnitude. The interval is much larger for stable conditions with no building wake effects.

Figure 5
Uncertainties in the Predictions of a Gaussian Plume Dispersion Model for Different Release and Meteorological Conditions

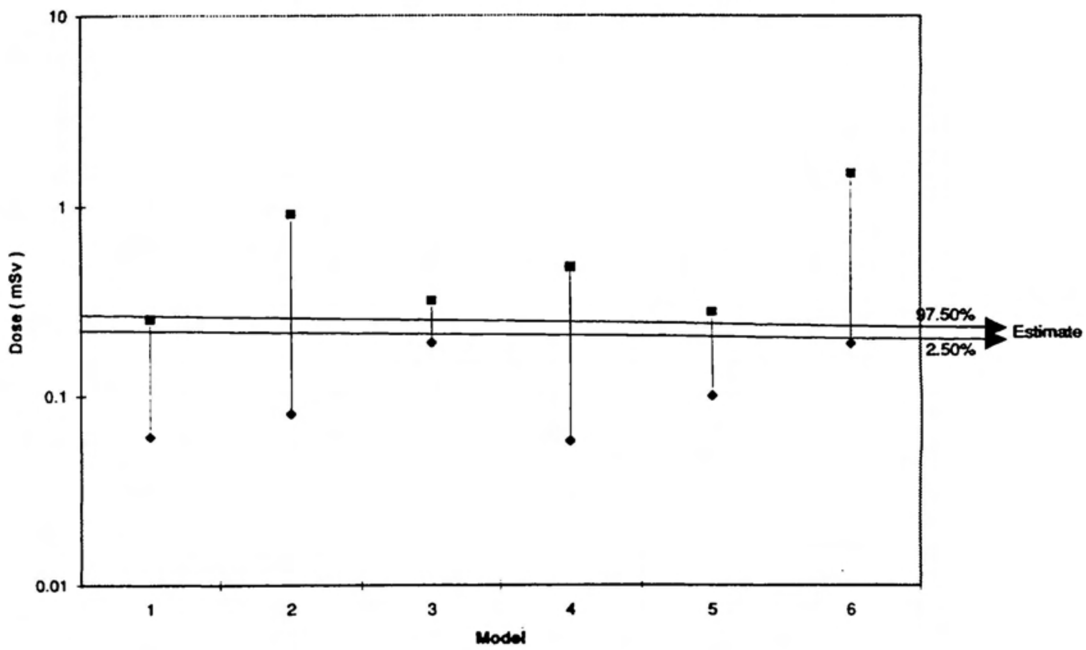


The key to understanding these results is to note that the lower edge of the plume just reaches the ground at the downwind distance considered. Concentrations and doses at ground level are therefore very sensitive to the effective release height and the vertical dispersion parameter (Table 1). The sensitivity is greatest for stable conditions, when the plume is still largely elevated, and the uncertainties are correspondingly large. They are smaller when the plume is influenced by the building wake, which mixes the plume more effectively down to the ground and reduces the sensitivity of the concentrations. This is an example of a case in which increased model complexity leads to lower uncertainties.

Terrestrial Food Chain Models

There is general agreement on which processes govern radionuclide transfer through terrestrial food chains. But many of these processes are poorly understood and there is often no consensus on how best they should be simulated. The credibility of model predictions depends very much on the radionuclide under consideration. The accident at the Chernobyl Nuclear Power Plant generated a large amount of field data that has subsequently been used for model testing, but most of the information is restricted to ^{131}I and ^{137}Cs. An example of the performance of current terrestrial food chain models is shown in Figure 6, which is based on calculations done in the VAMP Multiple Pathways Working Group (21). The figure displays the confidence intervals of six different models

Figure 6
Confidence Intervals on Predicted Ingestion Doses to Inhabitants of Finland Following the Chernobyl Accident (Scenario S from the VAMP Program). The Horizontal Lines Mark the 95% Confidence Interval on the Doses Estimated from Measured Body Burdens.

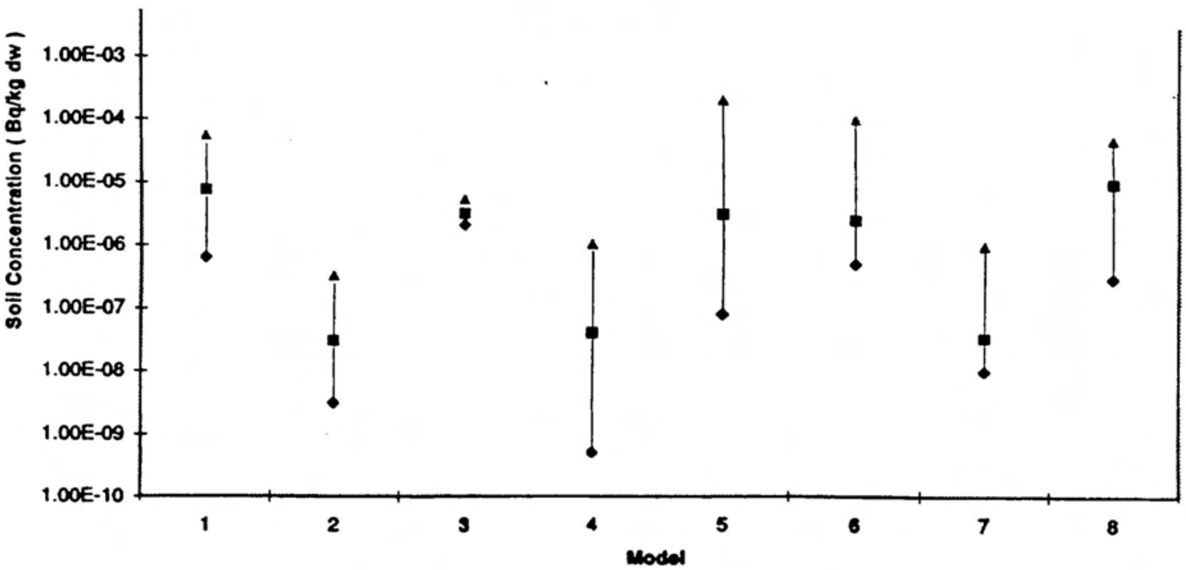


for the effective dose to the inhabitants of Finland due to ingestion of food supplies contaminated by Chernobyl fallout. The intervals typically extend over an order of magnitude, but within this accuracy agree with the doses estimated on the basis of measured body burdens. Note, however, that the performance of the models may have been enhanced by lessons learned in a similar test scenario undertaken previously in VAMP using data from Central Bohemia. The predictions would be less credible if the models were applied to a different radionuclide or to a different type of accident.

Models to Assess Nuclear Fuel Waste Disposal

Modeling radionuclide migration in the context of nuclear fuel waste disposal presents challenges not found in more traditional environmental transport applications. The source of the activity is in the geosphere and its upward migration depends on processes not normally modeled when the release occurs directly to the biosphere. Very long time frames must be considered, during which the biosphere and human lifestyles might undergo profound and essentially unpredictable changes. The testing of model predictions against field data is possible only for the first very small fraction of the total simulation time. There exists little information on many of the radionuclides involved. For these reasons, the credibility of waste management assessments depends primarily on face validation, and uncertainties in the predictions are large. Figure 7 shows results from the B6 Scenario of BIOMOVS, which involved the prediction of ^{129}I concentrations in soil, plants and animal products due to the upward migration of activity from a contaminated water table (22).

Figure 7
Best Estimate and Uncertainty Ranges for ^{129}I Concentrations in Soil at Steady State for the BIOMOVS B6 Scenario (Groundwater Discharge to a Terrestrial Area)



Participants were faced with the problem of migration across the geosphere-biosphere boundary, and their best-estimate predictions varied by almost three orders of magnitude. Confidence intervals for a given model were typically two to three orders of magnitude, and the range from the lowest confidence limit to the largest across all models was about five orders. The variability in results can be reduced through a more precise scenario description and discussion among participants (23), but the uncertainties in predictions of this sort will remain large.

PRECEPTS FOR ESTABLISHING MODEL CREDIBILITY

The key concepts to emerge from the above discussion are summarized below as a guide to good scientific practice in determining the level of confidence to be placed in the predictions of environmental transport models and in reducing their uncertainties:

- choose approaches to establishing model credibility that are consistent with the purpose of the assessment, the quality of the data and the capabilities of the model
- take advantage of all opportunities to test model predictions against observations
- supplement quantitative statistical procedures with graphical analysis, qualitative evaluation, sensitivity and uncertainty analyses and verification tests
- include uncertainty estimates with all model predictions, and include all sources of uncertainty in the estimates
- reduce the subjectivity in the process by gaining consensus from teams of experts on all major decisions required in the analysis

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