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# Report on the Workshop on Food-Chain Modeling for Risk Analysis

J. E. Breck
C. F. Baes III

ENVIRONMENTAL SCIENCES DIVISION
Publication No. 2340

OPERATED BY
MARTIN MARIETTA ENERGY SYSTEMS, INC.
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road, Springfield, Virginia 22161
NTIS price codes—Printed Copy: A05; Microfiche A01

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Environmental Sciences Division
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EPA Project Officer: A. A. Moghissi

Date of Issue - February 1985

Prepared for
Office of Research and Development
U.S. Environmental Protection Agency
Washington, D.C. 20460

EPA Interagency Agreement No. DW 89930292-01-0
(DOE 40-740-78)

Prepared by the
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37831
operated by
MARTIN MARIETTA ENERGY SYSTEMS, INC.
for the
U.S. DEPARTMENT OF ENERGY
under Contract No. DE-AC05-840R21400

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CONTENTS

LIST OF FIGURES

LIST OF TABLES

# ABSTRACT

BRECK, J. E., and C. F. BAES III. 1985. Report on the workshop on food-chain modeling for risk analysis. ORNL-6051. Oak Ridge National Laboratory, Oak Ridge, Tennessee. 82 pp.

The Workshop on Food-Chain Modeling for Risk Analysis was held in Washington, D.C., on March 22-24, 1983. The workshop was sponsored by the U.S. Environmental Protection Agency, Office of Research and Development (EPA/ORD), and supported under the Integrated Health and Environmental Risk Analysis Program (IHERAP) for Synfuels. Atmospheric and aquatic dispersion models, aquatic and terrestrial food-chain transport models, and models that estimate risks from calculated environmental exposures to synfuels effluents (dose-response models) are used to assess health risk from sunfuels effluents. The workshop focused on the aquatic and terrestrial food-chain models currently being used in the risk assessment process.

The workshop was attended by both modelers and experimentalists - all with some experience in risk assessment. During the first day, each participant presented a summary of recent work or a review of work of interest. After the presentations, topics of discussion included (1) models best suited for synfuels risk assessment, (2) best data sources and methods of estimating model input parameters, and (3) limitations inherent in the models used for risk analysis. However, discussions touched on all areas of food-chain modeling for risk assessment. Discussions on the complementary roles of the modeler and the experimentalist, estimation of model uncertainties, and

integration of food-chain models with other aspects of the assessment approach were particularly relevant. On the second day, discussions continued and participants logged the discussions and conclusions in which they took part. On the last day, a collective exposition was presented, discussed, and edited. This report details the presentations made by the workshop participants, the collective exposition on topics discussed, and the conclusions reached.

The workshop concluded that in aquatic food-chain modeling of chronic low-level releases of synfuels effluents, a simple concentration factor approach is appropriate. For terrestrial food-chain models the need for greater model complexity was recognized to account for location-specific variations in agricultural practice, although the estimation of terrestrial transport is also achieved through the use of concentration factors. For both aquatic and terrestrial models, using field data is the best method for estimating concentration factors, but where such data do not exist, laboratory data can be used. If no data exist for a particular compound or class of compounds, estimates can be made using partition coefficients based on structure-activity relationships. Finally, the workshop recognized the need to estimate the uncertainty associated with model output.

## ACKNOWLEDGMENTS

Dr. Lawrence W. Barnthouse, Charles F. Baes III, and Dr. James E. Breck, all of the Environmental Sciences Division of Oak Ridge National Laboratory (ORNL), planned and organized the technical program. Barnthouse was to be the Workshop Moderator, but because he was unable to attend, this duty was assumed by Mr. Baes and Dr. Breck.

Special thanks go to Dr. Melvin W. Carter of the Georgia Institute of Technology for making the meeting arrangements and coordinating travel plans and to Barbara Burns for typing assistance during the workshop. The workshop organizers also wish to thank the participants (listed in Appendix B) for their hard work at the conference.

This workshop was sponsored and supported by the Integrated Health and Environmental Risk Analysis Program for Synfuels of EPA's Office of Research and Development under Interagency Agreement No. DOE 40-740-78 (EPA No. DW 89930292-01-1) with the U.S. Department of Energy under Contract No. DE-AC05-840R21400 with Martin Marietta Energy Systems, Inc. The Project Officer is Dr. A. Alan Moghissi.

# 1. INTRODUCTION

## 1.1 OBJECTIVES

The Workshop on Food-Chain Modeling for Risk Analysis was held in Washington, D.C., March 22-24, 1983, and was sponsored and supported by the Integrated Health and Environmental Risk Analysis Program for Synfuels, U.S. Environmental Protection Agency Office of Research and Development (EPA/ORD). This particular workshop focused on applications in the area of synfuels and considered both terrestrial and aquatic food chains leading to man. The purpose of the workshop was to obtain the recommendations of experts on (1) terrestrial and aquatic food-chain models best suited to synfuels risk analysis, (2) data sources and parameter estimation methods best suited to synfuels risk analysis, and (3) major limitations on existing data and methods. Appendixes A and B, respectively, contain the agenda and list of participants.

The aquatic and terrestrial food-chain exposure models are parts of an overall assessment process that estimates the human health risk attributable to alternative synfuels technologies (Fig. 1.). These particular models estimate the concentrations of chemicals (or chemical groups) released from synfuels facilities in aquatic and terrestrial foods. From the concentrations in foods, exposures to individuals and populations are calculated; exposures (or intakes) are related to risks by applying models that incorporate dose/response relationships. The risk analyses in Fig. 1. are based on a characterization of synfuels

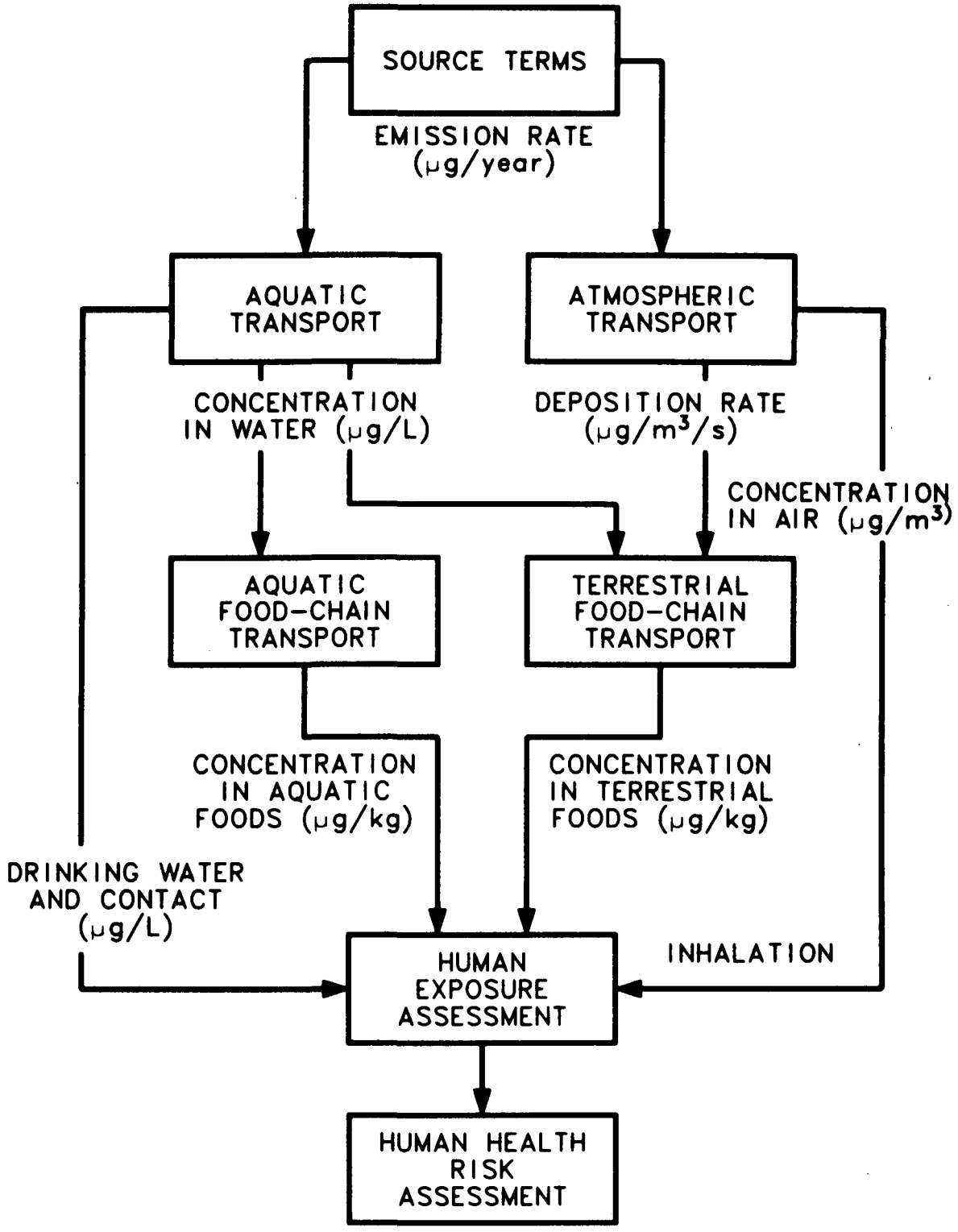


Fig. 1. Components of the overall human health risk assessment methodology for synfuels technologies.

plant waste streams by their risk analysis categories (RACs) content formerly Rish Analysis Units (RAUs). RACs are chemicals grouped for the purpose of risk analysis (Moghissi and Foley 1982). For this project, 39 RAUs have been defined (Table 1.).

The overall purposes of this risk assessment methodology for synfuels are to identify chemical groups (RACs) that could pose a problem for human health and to compare the health risks of alternative synfuels technologies. Several approaches could be taken in assessing the potential health effects of each RAC.

First, one could use the conservative approach used in certain screening assessments to identify potential problems. Parameter values used in the risk calculations could be chosen conservatively so that the human health risk is not likely to be underestimated. Chemical groups that do not produce significant risk, even with conservative calculations, are unlikely to cause problems. In this application, some RACs identified as being potential risks will not be shown to be of great risk upon more detailed investigation. However, for this type of screening, false positives (safe RACs identified as health risks) are more acceptable or tolerable than missed faults (problem RACs passed as safe).

A second approach is to use a single number for each parameter in the calculations that represents a typical or average value -- a best guess. Deterministic calculations would then produce a typical, average, or "best-guess" value for the risk associated with each RAC.

Table 1. Risk Analysis Categories (RACs)

| RAC No. | Category | Description/Chemical Makeup |
|---|---|---|
| 1 | Carbon monoxide | CO |
| 2 | Sulfur oxides | $SO_x$ |
| 3 | Nitrogen oxides | $NO_x$ |
| 4 | Acid gases | $H_2S$, HCN |
| 5 | Alkaline gases | $NH_3$ |
| 6 | Hydrocarbon gases | Methane through butanes, acetylene, ethene through butenes; $C_1$-$C_4$ alkanes, alkynes and cyclo compounds; bp < ~20°C |
| 7 | Formaldehyde | CHO |
| 8 | Volatile organochlorines | To bp ~120°C; $CH_2CL_2$, $CHCL_3$, $CCl_4$ |
| 9 | Volatile carboxylic acids | To bp ~120°C; Formic and acetic acids only |
| 10 | Volatile O&S heterocyclics | To bp ~120°C; Furan, THF, thiophene |
| 11 | Volatile N-heterocyclics | To bp ~120°C; pyridine, piperidine, pyrrolidine, alkyl pyridines |
| 12 | Benzene | Benzene |
| 13 | Aliphatic/alicyclic | $C_5$ (bp ~40°C) and greater; paraffins, olefins, cyclopcompounds, terpenoids, waxes, hydroaromatics |
| 14 | Mono/diaromatic hydrocarbons (excluding benzene) | Toluene, xylenes, naphthalenes, biphenyls, alkyl derivatives |
| 15 | Polycyclic aromatic hydrocarbons | Three rings and greater; anthracene, BaA, BaP, alkyl derivatives |
| 16 | Aliphatic amines(excluding N-heterocyclics) | Primary, secondary and tertiary nonheterocyclic nitrogen, $MeNH_2$, DiMeNH, TriMeN |
| 17 | Aromatic amines (exluding N-heterocyclics) | Anilines, napthylamines, amino pyrenes; nonheterocyclic nitrogen |
| 18 | Alkaline nitrogen heterocyclics [azaarenes] (excluding volatiles) | Quinolines, acridines, benzacridine; excluding pyridines |
| 19 | Neutral N, O, & S heterocyclics (excluding volatiles) | Indoles, carbazoles, benzofurans, dibenzothiophenes |
| 20 | Carboxylic acids (excluding volatiles) | Butyric, benzoic, phthalic, stearic |
| 21 | Phenols | Phenol, cresols, catechol, resorcinol |
| 22 | Aldehydes and ketones (carbonyls) (excluding formaldehyde) | Acetaldehyde, acrolein, acetone |
| 23 | Nonheterocyclic organosulfur | Mercaptans, sulfides, disulfides, thiophenols, $CS_2$ |
| 24 | Alcohols | Methanol, ethanol |
| 25 | Nitroaromatics | Nitrobenzenes, nitropyrenes |

Table 1. (continued)

| RAC No. | Category | Description/Chemical Makeup |
|---|---|---|
| 26 | Esters | Acetates, phthalates, formates |
| 27 | Amides | Acetamide, formamide, benzamides |
| 28 | Nitriles | Acrylonitrile, acetonitrile |
| 29 | Tars | |
| 30 | Respirable particles | |
| 31 | Arsenic | As, all forms |
| 32 | Mercury | Hg, all forms |
| 33 | Nickel | Ni, all forms |
| 34 | Cadmium | Cd, all forms |
| 35 | Lead | Pb, all forms |
| 36 | Other trace elements | |
| 37 | Radioactive materials | Ra-226 |
| 38 | Photochemical oxidants | Ozone |
| 39 | Other materials | |

A third approach, similar to the second, attempts to propagate the variance associated with each parameter. In the best case, the uncertainty or variability associated with each parameter would be characterized by a distribution of values, and the resulting assessment calculations would produce a probability distribution of the risk associated with each RAC. This approach is more complicated and requires acquisition of more data and, consequently, requires more effort. However, in the best case, it could produce results that include and surpass the results of both methods mentioned previously: the mean or median of the distribution of risk is similar to the result from the second approach mentioned, and the 95th or 99th (or 99.99th or other selected) percentile of the risk distribution may approximate the result obtained by the first screening method.

The purpose of these synfuels risk assessments is not regulatory screening in which regulatory action would be initiated or recommended if conservative screening levels are exceeded. Rather, the purposes of these synfuels risk assessments are to identify RACs likely to cause significant health risks and to compare alternative synfuels technologies using the best available estimates of their risks to human health. At this stage of the evaluation of the alternative technologies, both missed faults and false positives are to be avoided. (Reducing the probability of one type of error tends to increase the probability of the other; a single method cannot simultaneously minimize each type of error.) Users of the food-chain risk assessment methodology described in this report will need to decide the approach that best fits their assessment goals.

This workshop is one in a series covering different aspects of the Integrated Health and Environmental Risk Analysis Program (IHERAP) for synfuels. The workshop considered contaminant accumulation and transfer in food chains, not physical transport in the ambient environment. A previous workshop (Georgia Institute of Technology, Atlanta, Georgia, January 18-20, 1983) covered aquatic transport modeling for risk analysis (Donigian and Brown 1983).

## 1.2 ACTIVITIES

The agenda for the workshop is presented in Appendix A. After a welcome by Dr. Mel Carter and some introductory remarks by C. Fred Baes III, Dr. Alan Moghissi gave a charge to the workshop. Several of the attendees presented short talks to the entire group about recent research they have conducted in workshop-related areas. These presentations are summarized in Sect. 1.3 of this report.

The workshop was then divided into aquatic and terrestrial discussion groups. Each group reviewed and discussed the issues and wrote a several-paragraph summary of their discussion. These summaries were combined, typed, and reviewed by the group on the final day of the workshop. This report is an edited and expanded version of this combined report.

## 1.3 PRESENTATIONS

After a welcome from Dr. Melvin W. Carter (Georgia Institute of Technology), Dr. A. Alan Moghissi, EPA Project Officer for the Integrated Health and Environmental Risk Analysis Program (IHERAP) for

Synfuels of EPA's Office of Research and Development, gave a charge to the workshop participants. He briefly described the synfuels activities currently supported by IHERAP. Dr. Moghissi explained the use of RACs in relation to the risk analysis of synfuels chemicals. He defined the objective of the workshop as using the expertise of the participants to assist risk analysts in deciding which food-chain model to use.

In his presentation titled "Conceptual Framework for Foodchain Exposure Assessment," Charles F. Baes III (ORNL) described the terrestrial food-chain model he has been using (see Sect. 3.1) as it has been applied in assessments of exposures to synfuels chemicals. The four key issues Baes suggested for consideration in examining food-chain models for risk analysis of synfuels were:

1. Is the model structure appropriate?
2. How should parameters be quantified?
3. What are the major sources of uncertainty, and how can they be quantified?
4. Where should future efforts be directed?

James E. Breck (ORNL) discussed estimation of food-chain uptake of chemicals by fish by expansion of a structure-activity relationship that considers only chemical uptake from water. The structure-activity relationships used are regressions between some chemical parameter, such as the octanol-water partition coefficient or solubility in water, and some biological activity of the compound, such as bioaccumulation. By applying some simplifying assumptions, the octanol-water partition

coefficient $K_{ow}$ can be used to compute the steady-state contaminant concentration in fish resulting from both direct uptake from water and uptake from food (see Sect. 2.1). The results of such computations suggest that for chemicals that bioaccumulate because they are lipophilic, a $K_{ow}$ exists below which food-chain uptake is negligible and may be ignored. For such chemicals, a bioconcentration factor (BCF) model should adequately predict the contaminant concentration in fish.

James Falco (EPA/ORD) described recent work in estimating human exposures from hazardous waste sites and from contaminated foods. Recent assessments have moved away from "worst-case" analyses toward methods that estimate upper and lower bounds of exposure or, preferably, the entire distribution of exposure. Human exposures from contaminated foods are estimated by (1) monitoring food contaminated by chemicals such as pesticides and (2) modeling chemical transport and transformation up the human food chain. Bioconcentration factors have been used to predict the concentration of chemicals in fish. Concentration ratios of chemicals in fish to chemicals in sediment are useful when the contaminant is undetectable in the water; however, such ratios are not accurate for running waters, where concentrations observed in catfish and other bottom feeders are only 5% of the calculated values.

Jerry Eisele (Oak Ridge Associated Universities, Comparative Animal Research Laboratory) presented information on his experiments with poultry, swine, and dairy cattle. He described movement of several

RAUs [naphthalene (RAC 14), α-naphthol (RAC 21), and 7-methyl benz(c)acridine (RAC 18)] through animals to human food products (e.g., meat, eggs, and milk). Chemical distribution and concentration differed among the animals tested. For example, naphthalene fed to dairy cows reached an approximate equilibrium concentration in milk within 30 d, but naphthalene fed to chickens remained far from equilibrium concentration in eggs after 30 d.

Craig McFarlane (EPA Corvallis) described his planned experiments to quantify the rates of transfer of chemicals to plants. After some introductory remarks on plant physiology, he described the laboratory apparatus constructed for plant uptake experiments. He plans to study chemicals that span a range of values for $K_{ow}$ and Henry's Law constants, beginning with the compound bromacil. The results are intended for use in terrestrial food-chain models.

Chuck Garten (ORNL) discussed his study of empirical and statistical terrestrial food-chain models. Working with John Trabalka (ORNL), he developed regression models that predict the chemical concentration factor (CF) for ruminant fat, nonruminant fat, and avian fat based on a chemical's water solubility or its $K_{ow}$. They found that the coefficient of determination for the regressions decreased as additional chemicals were included in the analysis and that error bounds on the predicted CF were large -- plus or minus two orders of magnitude. The CFs for mammalian fat, nonrodent fat, and avian fat could be estimated ($r^2$ = 0.91 and 0.72, respectively) from a chemical's CF in rodent fat. A chemical's persistence in the soil

half-life, however, could not be predicted adequately from $K_{OW}$ or water solubility.

John Connolly (Manhattan College) presented the results of research on modeling the bioaccumulation of contaminants by several trophic levels in aquatic systems. Using a bioenergetics approach, a detailed model simulates the assimilation of polychlorinated biphenyls (PCBs) by lake trout in Lake Michigan. The model accounts for direct uptake from the water as well as food-chain transfer from phytoplankton to the opossum shrimp (Mysis) to the alewife to the lake trout. The model has also been applied to the accumulation of PCBs by yellow perch in Saginaw Bay of Lake Huron and kepone by striped bass and croakers in the James River. Connolly compared field data and simulated kepone concentrations in croakers; good agreement existed between the two.

John Nagy, Brookhaven National Laboratory (BNL), presented concerns of human health risk analysts about the uncertainty of the data used in food-chain models. As data are passed from scientists involved in basic research to environmental modelers to risk analysts, information about the uncertainty associated with the data and the applicability of the data for particular purposes should be passed on. Nagy critically examined the reported BFs for vinyl chloride and polyaromatic hydrocarbons (PAHs) in fish. He suggested that risk analysts should be aware of the variation among reported values and the importance of considering the influence of the fish lipid level in selecting the appropriate value to use in a particular application.

Paul Moskowitz (BNL) described the use of food-chain model output in assessing the risk of synfuels technologies to human health. The health risk is initially being assessed by estimating, for each route of exposure (aquatic foods, terrestrial foods, inhalation, drinking water, etc.), the annual cancer incidence rate induced by emissions from synfuels plants. Dose-response models are used to predict the annual cancer incidence rate from the total mass of each RAC in aquatic or terrestrial foods consumed by people. Comparisons can then be made of the differences in cancer incidence rate among the pathways of exposure, among RACs, and among alternative synfuels technologies.

F. Owen Hoffman (ORNL) discussed uncertainties associated with the output of models. He distinguished between research models, that are used to enhance understanding of mechanisms and processes and assessment models that are used to make predictions upon which decisions are made. Several sources of model uncertainty are (1) a particular model's abstraction of reality, (2) variability in the model's parameters, (3) correlations among parameters, (4) site-specific capabilities, and (5) deterministic estimates that ignore system variability.

## 2. AQUATIC FOOD-CHAIN MODELS

Aquatic food-chain models are used to estimate the concentration and total amount of each RAC in the edible fraction of aquatic foods consumed by man. Estimates of RAC concentrations in water and sediment and other relevant physiochemical variables are calculated using an

aquatic transport model (e.g., Travis et al. 1983). The eventual impact of ingesting a particular RAC, taking into account the effects of any food processing on toxicity, is addressed in the human exposure and human health risk components of the overall assessment methodology (Fig. 1.).

Some very similar and frequently used terms are defined here to facilitate understanding of the subsequent discussion. Concentration factor (CF) refers to the ratio between the concentration of a chemical in an organism and in water. There is no implication that the concentration in the organism is at steady state, though it may be. All uptake pathways are considered, as they are in CFs derived from field data. Bioconcentration factor (BCF) also refers to the ratio between the concentration of a chemical in an organism and in water. The concentration in the organism is assumed to be at steady state, and only uptake from water is considered. (This same term is used in some terrestrial papers to mean the ratio between a concentration in an organism's fat and the concentration in its diet.) Biomagnification factor (BMF) is the ratio of the steady-state concentration in an organism to the concentration in its food when food is the only route of exposure (i.e., when the concentration in water is negligible). Bioaccumulation factor (BAF) is the ratio of the steady-state concentration in an organism to the concentration in water, if both food and water contribute to the organism's exposure.

## 2.1 MODELS BEST SUITED TO SYNFUELS RISK ANALYSIS

Estimation of the risk posed to humans by the components of synfuels released to natural water systems requires estimation of the concentration of these components in aquatic species consumed by humans. It was the opinion of the human health risk analysts at the workshop that the uncertainty associated with the human health dose-response estimates was approximately plus or minus two orders of magnitude (i.e., given an accurate estimate of dose, that the response could be predicted within a factor of 100). It should be noted that the level of knowledge about the dose-response relationship varies among RACs; thus, the level of uncertainty associated with the response estimates varies accordingly. Knowing this level of uncertainty may be helpful in selecting an appropriate aquatic food-chain model.

### 2.1.1 Concentration Factor Model

The analysis of chemical accumulation in aquatic species has been approached from several levels of detail. The simplest method computes the concentration of a chemical in a species as the product of a CF and the concentration of dissolved chemical in water. This method was used in recent assessments of synfuels wastes (Moskowitz et al. 1983) and has been used by the U.S. Environmental Protection Agency (EPA) in developing water quality criteria (EPA 1980) and by the U.S. Nuclear Regulatory Commission (NRC) for radionuclide assessments (NRC 1977). The CF is obtained from field data, from laboratory testing, or from an empirical relationship between CF and the octanol-water partition coefficient ($K_{OW}$). For these assessments of synfuels technologies, a

CF is needed that makes the best prediction of the contaminant concentration in fish chronically exposed under field conditions. The CF should account for all important routes of uptake. A CF estimated from field data is preferred only if the exposure is chronic. If such a field CF is not available, an appropriate CF must be estimated. If the elimination rate of the chemical from fish is rapid, (1) the food chain is unlikely to be an important route of uptake and (2) the BCF is likely to be a good approximation of the CF (Macek et al. 1979; Thomann 1981; Bruggeman et al. 1981; Oliver and Niimi 1983). Chemicals having rapid elimination rates will include those that are not highly lipophilic. [Chemicals, such as methyl mercury, which have a low $K_{OW}$ but are accumulated by mechanisms unrelated to lipophilic characteristics must be given separate and special consideration.]

The experiments and field data of Oliver and Niimi (1983) suggest that the BCF will approximate the field CF for chemicals having a log $K_{OW}$ less than about 4.3; Bruggeman et al. (1981) suggest that the food chain will make an important contribution only for chemicals having log BCF greater than about 5. Since the workshop, approximately 60 possible synfuels chemicals have been assessed at ORNL, and the concentrations in fish appear to be adequately estimated by the CF method; for these chemicals, either a field CF is available, the chemical is not highly lipophilic, or the chemical is rapidly metabolized by fish (e.g., PAHs, RAC 15). Section 2.2 discusses the estimation of BCFs and field CFs, and Sect. 2.1.2 discusses models that can be used when the food-chain pathway to fish is likely to make an important contribution to the total contaminant concentration in fish.

### 2.1.2 Dynamic, Bioenergetics-based Models

Dynamic, bioenergetics-based models consider the uptake and depuration dynamics of one or more trophic levels in the food chain. These models can account for the influence of factors such as body size and water temperature on contaminant dynamics through effects on growth rate, respiration rate, and consumption rate. Detailed models based on a bioenergetics approach can give good estimates of contaminant concentration in fish (estimated by the aquatics group to be within a factor of three), given a good estimate of depuration rates and the contaminant concentrations in water and food (e.g., Weininger 1978; Thomann and St. John 1979; Thomann 1981; Thomann and Connolly 1984). These models may be required for the best estimates of concentrations in fish of compounds having very low depuration rates (e.g., PCBs) because these compounds take a long time to reach equilibrium. Because such models can account for effects of fish age, size, and fish lipid content, they can provide the high-level resolution required for risk analysis of critical human populations.

Bioenergetics-based models have already been developed for several fish species and have been applied to several specific situations: PCBs in lake trout, coho salmon, and alewives in Lake Michigan; kepone in striped bass and croakers in the James River; methyl mercury in pike and roach in Swedish lakes; and PCBs and methyl mercury in Ottawa River yellow perch [Connolly and Tonelli (in press); Fagerstrom and Asell 1973; Fagerstrom et al. 1974; Norstrom et al. 1976; Weininger 1978; Thomann and St. John 1979; Thomann and Connolly 1984]. Because of the

level of detail used in these models, the resulting equations are complex and application to a specific food chain requires knowledge of many parameters, some of which are hard to obtain and/or are site specific. However, once the biological data are accumulated for a particular species and location, it is relatively easy to apply the model to additional chemical contaminants having similar properties. These models can give detailed, time-varying estimates of contaminant concentration in fish of several ages. The risk analyst should consider the following criteria in deciding whether or not to use these detailed models:

1. chemicals of interest should have low depuration and biotransformation rates [i.e., long times to reach steady state (Thomann 1981)] such that the steady-state assumption of certain simpler models is violated;
2. a model and paramter, or the resources to develop them, should be available for the chemical, species, and location of interest; and
3. the level of accuracy or detail that these models can provide should be worth the increased effort required.

Considering these criteria, it appears that the detailed models are currently inappropriate for synfuels risk analysis.

One of the possible shortcomings of BCF models is that the potential contribution of the food chain to bioaccumulation may be ignored. A relatively simple model that includes the food chain can be constructed based on the following assumptions:

1. the food chain is linear,
2. each trophic level is represented by fixed bioenergetic parameters,
3. the concentration of chemical in the food chain is in dynamic equilibrium with the concentration of chemical in water, and
4. the rate of direct uptake from water is independent of trophic level (it may be easy to relax this assumption by accounting for body size).

The resulting model may be termed a bioenergetic-based equilibrium food-chain model or an "equilibrium food-chain model." The model presented by Thomann (1981) did not assume a constant BCF. Bruggeman et al. (1981) independently derived a similar model. The Thomann model calculates the steady-state BAF for the $n^{th}$ trophic level ($BAF_n$) in a linear food chain. The "food-chain transfer number" $f_n$ (Thomann 1981) or "biomagnification factor" (Bruggeman et al. 1981) depends on the assimilation efficiency of ingested chemical, the consumption rate, the contaminant elimination rate, and the growth rate of organisms in trophic level n (Thomann 1981). The model is highly sensitive to elimination rate. Errors in its estimation will produce rather large errors in $BAF_n$.

To simplify further it may be inferred from Bruggeman et al. (1981) that the food-chain transfer number $f_n$ is (approximately) directly proportional to the bioconcentration factor (i.e., $f_n$ will be on the order of $10^{-5}$ to $10^{-6}$ times $BCF_n$). As Bruggeman et al.

(1981) point out, this suggests that chemicals in the food will make an important contribution to the concentration in an organism only for chemicals with a $BCF_n$ of $10^5$ or greater. This result is shown in Fig. 2, where the additional assumption has been made that the food-chain transfer numbers ($f_n$) and the BCF from water ($BCF_n$) are the same for all trophic levels. In this figure, the log $BCF_1$ vs log $K_{ow}$ relation is taken from Oliver and Niimi (1983), who corroborated their laboratory measurements of BCF with field data on fish/water contaminant ratios in Lake Ontario rainbow trout. This figure shows the importance of considering the food-chain pathway to fish for chemicals with very low elimination rates (i.e., chemicals having very high BCFs).

The accuracy of the equilibrium food-chain model is dependent on the validity of the four assumptions indicated earlier and the uncertainty associated with the input parameters. The amount of reduction in uncertainty resulting from the increase in process specification in this model, relative to the simple water BCF approach, is unknown and remains to be quantified.

A major assumption of this model is that equilibrium or steady state is closely approached. Work in progress by Breck (ORNL) suggests that chemicals for which the food-chain pathway is a dominant uptake route are likely to have very low depuration rates (and high $K_{ow}$ values), so that a fish may not reach a steady state within its lifetime. The simple equilibrium models of Thomann (1981) and Bruggeman et al. (1981) are easily modified to account for this deviation from steady state without greatly increasing model complexity.

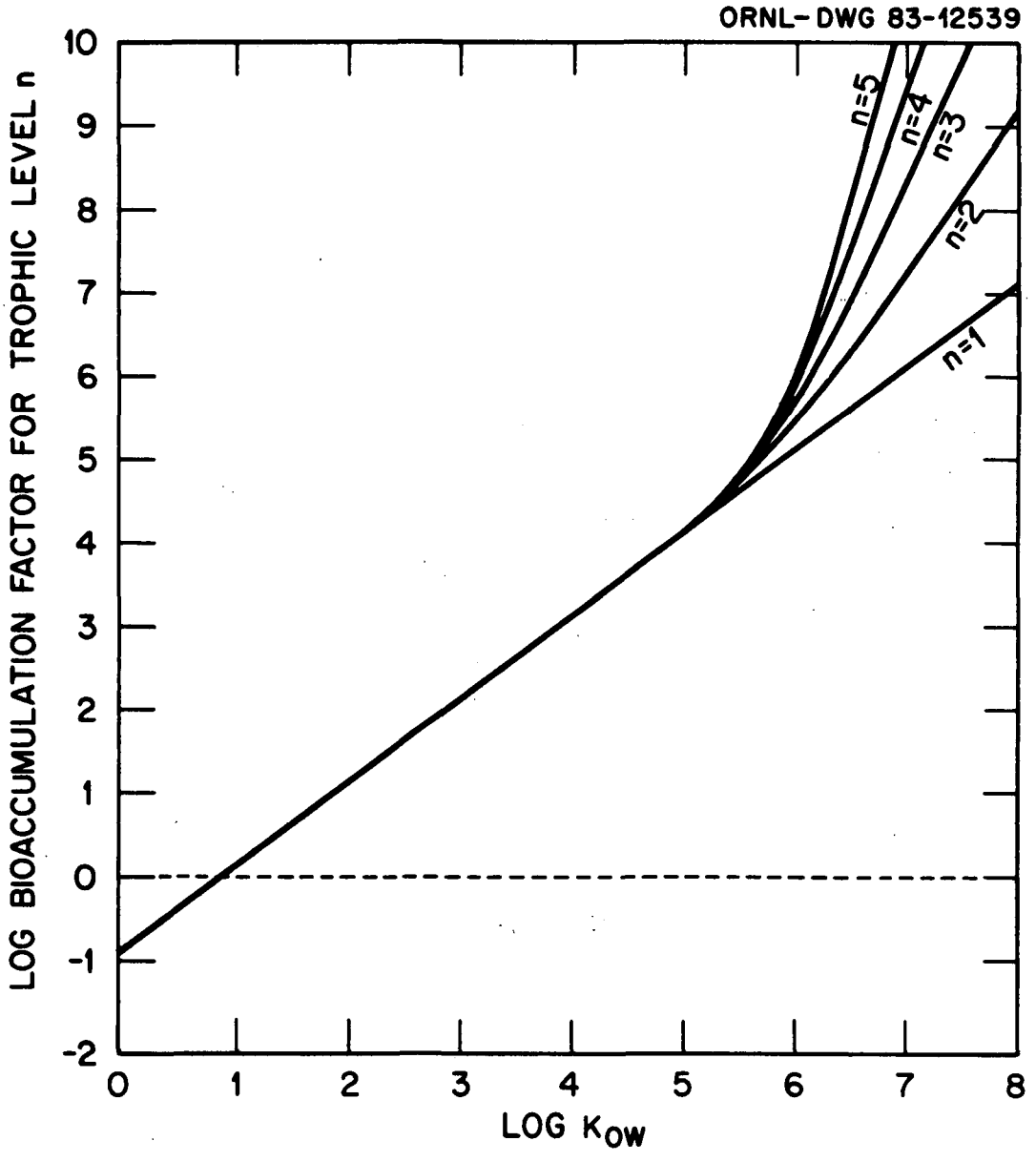


Fig. 2. Bioaccumulation factor (BAF) vs octanol-water partitioning coefficient ($K_{OW}$) for different trophic levels in a linear food chain. The line for n = 1 reflects contaminant bioconcentration from water only, as measured a low-exposure experiment (Oliver and Niimi 1983). The line for n = 2 includes contaminant uptake from water plus food-chain transfer from trophic level 1. The line for n = 3 includes direct uptake from water plus food-chain transfer from trophic levels 1 and 2. Lines for trophic levels 4 and 5 are computed similarly.

For the 60 or more synfuels chemicals considered thus far in synfuels assessments at ORNL, concentrations in fish appear to be adequately estimated by a simple CF model (see Sect. 2.1.1). However, if chemicals are encountered that do not fit the requirements of the CF model (e.g., chemicals for which there are no field estimates of CFs and for which depuration and biotransformation rates are very low and values for $K_{ow}$ very high, suggesting that the food chain is the dominant uptake pathway), then a dynamic bioenergetic model would be appropriate. The scientists at the workshop believed that if use of this type of model were necessary, then data currently available in the literature could be used.

### 2.1.3 Comments For All Models

Concentration factors for aquatic organisms can vary among taxa, trophic levels, and sizes of individuals. If aquatic foods represent a major source of exposure or risk for a particular chemical (or group), as determined by preliminary analyses, such differences should be accounted for in synfuels risk analyses. For example, some crustaceans and molluscs lack the ability of fish to rapidly metabolize PAHs (RAC 15), so that BCFs are higher for certain of these organisms than for fish (Malins et al. 1979; Southworth et al. 1980; Farrington et al. 1983). Differences among taxa in growth rate and trophic level also contribute to variations in CFs (Thomann 1981). Larger body size is correlated with a lower elimination rate; this has been observed for methyl mercury in fish (Norstrom et al. 1976), and for PCBs in macrozooplankton and phytoplankton (Brown et al. 1982). Because

elimination rate influences the CF, and most laboratory measurements of BCF have been made on much smaller sizes of fish than those typically consumed by humans, it would be useful to know the contribution of body size to increased uncertainty in estimated CF. A literature survey should be done to quantify the uncertainty in CF (or BCF) resulting from variations among taxa, trophic levels, and sizes of individuals.

If justified by the results of such a literature survey, the aquatic food of humans could be categorized as follows:

Level 1, a phylogenetic classification. Data on the harvest and consumption of aquatic foods from commercial and sport fisheries and aquaculture would be directly or indirectly available on a taxonomic basis. Species specification would allow determination of the feeding habit class (Level 2) and the parameter values (e.g., lipid content) required for estimating the CFs. The important taxa in the aquatic food chain are (1) Pisces, (2) Mollusca, (3) Crustacea, and (4) Aves/Anseriformes.

Level 2, feeding habit (or some trophic-level scheme). Recognizing that combinations are the rule rather than the exception, these might include (1) detritivore, (2) phytoplanktivore, (3) zooplanktivore, (4) macroherbivore, (5) benthic invertebrate feeder, and (6) piscivore. Other distinctions may be necessary (e.g., feeding on aquatic benthic invertebrates vs feeding on invertebrates of terrestrial origin). Not all feeding habit classes will be represented in a given phylogenetic group.

Other possible, important classifications would distinguish between freshwater, saltwater, and estuarine species and between flowing- and standing-water species or populations.

The method of classification described here is general, possibly exceeding the needs of an assessment program. IF a preliminary analysis using the simplest approach showed that greater resolution is required for particular chemicals in aquatic foods, then, depending on the results of a literature survey, the method could be expanded to a more complex form.

A workshop participant suggested that a data book documenting the derivation of CFs should be kept. This would include sections on each substance/RAC, including pertinent math, biology, and chemistry, computations performed; a qualitative review of uncertainty, both at individual compound and RAC levels; and, if possible, quantification of uncertainty via confidence intervals and/or probability distribution functions (PDFs) for possible use in stochastic assessment models. It is recognized that these intervals or PDFs will vary according to the question addressed by the model; larger uncertainties will be associated with initial group assessments than with assessments of risk to large populations.

As discussed in the Introduction, the overall purposes of this risk assessment methodology are to identify chemical groups (RACs) that could pose human health problems and compare the health risks of alternative synfuels technologies. Therefore, it is suggested that calculations of food-chain exposure to each RAC use values for a

typical chemical or a value obtained by averaging across several chemicals in the RAC, noting and carrying through the variance or variability in output; an alternative method would be to do the calculations for several representative chemicals within each RAC to account for the variability among chemicals within a RAC. The purpose here is not regulatory screening (i.e., regulatory action would not be initiated or recommended if conservative screening levels were exceeded). For the regulatory screening case, upper-bound estimates would be more appropriate than average or typical values for CFs. Depending upon the goals of a particular risk assessment, different methods might be used to select parameter values and to account for the variability among chemicals.

For the purposes of the EPA synfuel assessment, then, at least best guess estimates of uncertainty are needed although ideally PDFs would be available for all substances and aquatic food types. The workshop aquatic food-chain group did not, however, reach a consensus on this point. The following two paragraphs represent a strongly felt minority opinion.

Currently, uncertainties in 95% upper-bound risk estimates warrant only an order-of-magnitude accuracy for estimates of BAFs. However, even when ranges are specified for BAF values, their derivation has been usually associated with conservative bias. Therefore, because of limitations in available data, current models are not capable of producing a best-estimate value or of values. Thus, the most appropriate use of BAF values to date is in screening calculations.

In all cases, however, it is desirable to preserve the range or distribution of uncertainty of BAFs with stochastic modeling. It is not appropriate to use single values in deterministic models unless the approach is known to be sufficiently conservative for screening calculations. Deterministic calculations based on indiscriminate use of geometric means may be particularly misleading.

In view of the location of possible synfuel plants, specification of the following variables/parameters for freshwater fishes have the highest priority: CF (else BCF) by RAC, a factor to convert whole-body concentration to concentration in the edible portion of the aquatic food, and a factor to account for changes in concentrations resulting from food processing and cooking. A survey of the literature should be done to quantify the uncertainty in CF (else BCF) resulting from variations among taxa, trophic levels, and sizes of individuals. To estimate the mass of each RAC in aquatic foods ingested by humans, the following information is needed as well to complete the exposure assessment: the mass of each aquatic food type taken from each stream reach or water body, the fraction that goes to human consumption, the edible fraction, and the number of people eating food of each subtype from each stream reach/water body.

## 2.2 DATA SOURCES AND PARAMETER ESTIMATION METHODS

*When a CF method is to be used in risk analysis as suggested here,* the best way to estimate the factor is to use field data on the ratio of the concentration of contaminant in fish to the concentration of

contaminant in water. This approach has been found to be useful for estimating BAFs for radionuclides in freshwater biota (Vanderploeg et al. 1975). Data on the concentration in fish categorized by species, lipid level, and weight and age will be needed for later, more detailed risk analyses.

Field data should be included in risk assessment only if:

1. the concentration of a chemical in aqueous solution is measured,
2. the concentration in fish is measured (may be whole organism or a portion), and
3. the exposure concentration is reasonably constant for an adequate period of time (i.e., the rate of approach to steady-state CF is chemical-dependent) -- not the result of a local spill or other temporary or localized condition.

This approach to the estimation of concentration ratios includes all pathways of exposure for aquatic organisms under the most realistic conditions. Unfortunately, such measurements are not available for many of the synfuels organics. Data from acute field exposures are also valuable but need to be analyzed carefully to yield CFs appropriate for the risk analyses of chronic exposures discussed here.

As previously mentioned (Sect. 2.1.1), if an appropriate field CF is not available, then an appropriate CF must be estimated. If either the elimination rate or the rate of biotransformation of the chemical is rapid, the BCF is likely to be a good approximation of the CF

(Thomann 1981; Bruggeman et al. 1981), and estimates are needed of the BCF of the chemical. This is likely to be the case for most synfuels chemicals, according to recent assessments of synfuels chemicals at ORNL (Breck, in preparation). If both the elimination rate and the rate of biotransformation are very low, the food-chain uptake pathway may contribute significantly to the chemical's concentration in fish, and additional information will be needed to estimate an appropriate CF, as discussed in the following.

The laboratory and field data of Oliver and Niimi (1983) suggest that the steady-state BCF measured in the laboratory will be a good approximation of the field CF for chemicals having a log $K_{ow}$ of about 4.3 or less. (It should be noted that the Oliver and Niimi values for BCF were higher than thse measured by some other workers, perhaps because Oliver and Niimi used the large-size fish or very low exposure concentrations.) Bruggeman et al. (1981) suggest that the food-chain uptake pathway is probably not significant for chemicals having a log BCF of less than about 5.

A measured BCF is generally preferred over an estimated BCF. The fish/water concentration ratio should be measured very close to steady state or the steady-state fish/water ratio (i.e., BCF) should be estimated from the ratio of uptake rate to elimination rate (including the biotransformation rate). The results of Kosian et al. (1981) suggest that the BCF is appreciably influenced by the method of calculation of BCF from laboratory measurements. The ratio of uptake rate to elimination rate seems to be more appropriate for estimating

the BCF of very lipophilic chemicals than are the 28-d values of the fish/water concentration ratio.

If field or laboratory CFs are not available for the compound of interest, BCFs should be estimated from regression models developed for homologous chemicals (these will often be members of the same RAC). For example, separate regression models for PAHs, chlorinated benzenes (Oliver and Niimi 1983), and phenols (Saarikoski and Viluksela 1982), could be used. Estimates from other homologs should be especially useful for cases like the PAHs, in which BCFs are relatively low, despite high log $K_{ow}$s, as a result of metabolism of the compound by fish. If data on homologs are not sufficient to estimate a BCF, BCF should be estimated from the octanol-water partition coefficient by using regression models based on a wide variety of chemicals (e.g., Trabalka and Garten 1982; Veith et al. 1980).

Chemicals that ionize to a significant extent at field pHs have a reduced potential for accumulation, as Saarikoski and Viluksela (1982) found for certain substituted phenols. For such chemicals, the reduction in BCF resulting from ionization at a given pH can be estimated if the dissociation constant is known (Saarikoski and Viluksela 1981; Goldstein et al. 1974).

BCF data for fat-soluble RACs should be accompanied by lipid content information so that the BCF values can be expressed on either a whole-body or lipid-weight basis, as necessary. BCFs represented on the basis of lipid content can be easily converted to either edible-portion or whole-weight basis using reasonable estimates of

lipid content in tissues. For example, if the BCF on a lipid basis is 10,000, whole fish are 3% lipid, and the edible portion is 5% lipid, then the BCF in whole fish would be 300 and the BCF in edible portion would be 500. General estimates of the percentage of lipid content are available for many commercial species (Sidwell et al. 1974; Kinsella et al. 1977; Rottiers and Tucker 1982). The workshop group felt that such estimates are generally useful for a risk assessment.

In the event that a linear food-chain model is required (Sect. 2.1.2), values for the BCF, elimination rate, consumption rate, assimilation efficiency of ingested chemical, and growth rate would be required for each trophic level. The BCF and the excretion rate can be determined from laboratory experiments or estimated from the $K_{ow}$ (e.g., Oliver and Niimi 1983; Spacie and Hamelink 1982; Trabalka and Garten 1982; Mackay 1982; Veith et al. 1980; Kenaga and Goring 1980). Growth rate can be obtained from the literature or may be estimated from general functions relating these parameters to the size of the organism. Assimilation efficiency of the chemical can be obtained from laboratory experiments or estimated from the $K_{ow}$ (see Schanker 1960). Consumption rate, which varies with body size, can be obtained from the literature or estimated from the growth rate, respiration rate, and food assimilation efficiency (Norstrom et al. 1976; Thomann 1981).

Models having two body compartments for the organism are not necessary if the bioaccumulation ratio is derived from a log $K_{ow}$ correlation, chronic laboratory exposure, or field data. However, they

may be considered if the food-chain model is developed from uptake- and elimination-rate constants measured in the laboratory (Ellgehausen et al. 1980). In some cases, the elimination-rate constant can be overestimated by making observations only during the beginning of depuration. Elimination of organics is often made up of "fast" and "slow" phases. If the initial slope of a biphasic depuration curve is used as an estimate of the elimination-rate constant, then the half-life of the chemical will be underestimated and the calculation:

$$BCF = \frac{\text{uptake rate}}{\text{elimination rate}} \qquad (2.1)$$

will produce an underestimation of BCF.

## 2.3 MAJOR LIMITATIONS ON EXISTING DATA AND METHODS

Concentration factors measured from chronic field exposures would provide the most appropriate values for use in synfuels risk analyses, given the conditions listed in Sect. 2.2. Such field exposures include several uptake pathways and more realistic conditions than laboratory exposures. Measurements of CFs observed in the field are valuable sources of information about the behavior of organic chemicals, and such measurements provide a way to calibrate and verify the models. However, it should be understood that the results will probably vary from one ecosystem to another because of factors such as food-chain length, bioavailability of the chemical, and species characteristics. Compilation of results from different systems will allow the magnitude of this variation to be estimated.

If Thomann's (1981) equilibrium food-chain model (see Sect. 2.1.3) is used to calculate the CF, estimates will be needed of the BCF from water only. Several limitations exist on the use of structure-activity relationships (SARs) to estimate BCF. First, an appropriate equation must be used (Trabalka and Garten 1982; Oliver and Niimi 1983; Veith et al. 1980), as discussed in Sect. 2.2. Second, for benthic species, a concentration ratio relative to the concentration of chemical in sediment may be more appropriate than a ratio relative to the water concentration. Third, it must be recognized that there is generally uncertainty associated with the value of the $K_{ow}$ (the independent variable in the regression) as well as error associated with the dependent variable (here, BCF) in the regression (Trabalka and Garten 1982; Veith et al. 1980).

The regressions relating BCF and $K_{ow}$ that are currently used were developed mainly for organo-chlorines and other organics that are poorly metabolized by fish. To a close approximation, these chemicals remain unchanged throughout the partitioning process and throughout the food chain. These regressions work rather well for such materials. However, many of the organics associated with synfuels (e.g., PAHs) are known to undergo biotransformation in some aquatic organisms (Southworth et al. 1980; Spacie et al. 1983). Usually, but not always, the metabolites formed are more polar and are, therefore, eliminated more quickly from the body. In effect, the organism has the ability to lower the partition coefficient of the parent material. Thus, estimates based on the log $K_{ow}$ of the original chemical may produce

overestimates (conservative estimates) of BCF and food-chain transport. Enzyme induction may also lower BCF.

It would be extremely useful to collect information to group aquatic organisms on the basis of their biotransformation abilities. For example, fish and chironomid midges readily metabolize many PAH compounds, whereas bivalves and Daphnia are poor hydrocarbon converters. Categorization of this type would dramatically facilitate our estimates of BCF and food-chain transfer for synfuel chemicals. Currently, no good structure-activity models exist for predicting in advance which taxa will or will not metabolize a particular organic compound.

A fourth limitation on the use of SARs to estimate BCFs concerns the variable(s) used to quantify a chemical's structure. The most commonly used regressions predict BCF from $K_{ow}$. As others have pointed out (e.g., Trabalka and Garten 1982), such relations will underestimate the bioconcentration of chemicals such as methyl mercury. This is because methyl mercury bioaccumulation is not related to lipid partitioning, but to bonding with the sulfhydryl groups of certain proteins (Reichert and Malins 1974). Therefore, its bioaccumulation would not be expected to correlate with a variable ($K_{ow}$) related to lipid partitioning. Fortunately, however, there appears to be only a very small portion of chemicals that behave like methyl mercury.

A final limitation on the use of regressions to estimate BCFs is the relatively large degree of uncertainty about the predicted values.

Regression equations developed for a homologous group of chemicals will have a smaller range of uncertainty about the predicted values than will regressions developed from a wide variety of chemicals. Trabalka and Garten (1982) compiled bioconcentration information on more than 100 chemicals. In their regression of log BCF vs log $K_{OW}$ "the 95% confidence limits about the predicted value at the mean log [$K_{OW}$] are greater than $\pm$2 orders of magnitude." They note, however, that "the bulk of the extreme data scatter occurs below the regression line...and overpredictions by the model are more acceptable than underpredictions."

A limitation of the structure of the models (presented in Sect. 2.1) is that they are based on the concentration of the chemical in water. Situations in which the concentration of sediment-associated chemical is important (e.g., through a benthic component of the food chain) may require that this benthic component be separated and referenced to the sediment rather than to the water column. Factors such as adsorption to dissolved organic matter (e.g., humic acid) may also reduce the concentration available in water and, therefore, reduce the amount of chemical absorbed by the organism. Such factors should be accounted for by the aquatic transport model.

## 2.4 CONCLUSIONS

The aquatic food-chain group at the workshop agreed that for chronic low-level releases of synfuels effluents, the concentration factor approach is relevant and appropriate for assessing risks. Application of field data based on the ratio of a chemical's

concentration in fish to the concentration in water is the best way to estimate the CF. If field data are not available, laboratory measurements of BCFs should be used. If no measured BCF is available, then the factor can be estimated using regressions of log BCF vs log $K_{ow}$.

The data of Oliver and Niimi (1983) suggest that simple BCF models adequately predict the concentration in fish of chemicals with a log $K_{ow}$ of about 4.3 or less. The great majority of synfuels chemicals fall in this category. Those synfuels chemicals that have a log $K_{ow}$ greater than about 4.3 are typically metabolized rapidly (e.g., PAHs, RAC 15), consequently, they are not accumulated significantly through food chains and are adequately described by a BCF model. Chemicals having low depuration and biotransformation rates are candidates for significant uptake via the food chain, making models that explicitly account for food-chain uptake applicable. No such synfuels chemicals have yet been identified, except for those for which field estimates of CFs are already available (i.e., mercury, RAC 32).

Although information is currently available on the uncertainty associated with regression models (i.e., log BCF vs log $K_{ow}$), further research is needed to quantify (1) the level of uncertainty associated with CFs estimated from field data and (2) the differences among taxa and among trophic levels.

# 3. TERRESTRIAL FOOD-CHAIN MODELS

## 3.1 MODELS BEST SUITED TO SYNFUELS RISK ANALYSIS

The appropriateness of a terrestrial food-chain model for synfuels risk assessment may be judged by its usefulness to the risk analyst, who must not only perform the initial risk estimates but also identify critical pathways, uncertainties, and research needs. The model currently used at ORNL for terrestrial food-chain exposure calculations is based on a modification of the traditional multiplicative chain approach used by the NRC in making radionuclide dose assessments (NRC 1977; Travis et al. 1983). The computer code incorporating this model, TERREX (Baes et al. in preparation), is a modified version of the TERRA computer code for radionuclide transport (Baes et al. 1983). The various pathways addressed in the TERREX code are shown in Fig. 3. The breakdown and interrelationships among these pathways are based on a review and analysis of agricultural practice in the United States, by Shor et al. (1982).

The terrestrial food-chain transport model includes produce, milk, and beef pathways to humans. Input into the terrestrial model is via atmospheric dispersion and deposition. Plant compartments are contaminated via root uptake of material that has deposited and accumulated in soil and via direct contamination of foliar surfaces. The root uptake component of plant contamination is calculated through the use of soil/plant CFs that are specific for either leafy ($B_{iv}$) or reproductive/storage ($B_{ir}$) organs of the plant. These CFs relate the dry weight concentration of compound i in the edible plant part to its

## CONCEPTUAL GENERIC TERRESTRIAL FOODCHAIN

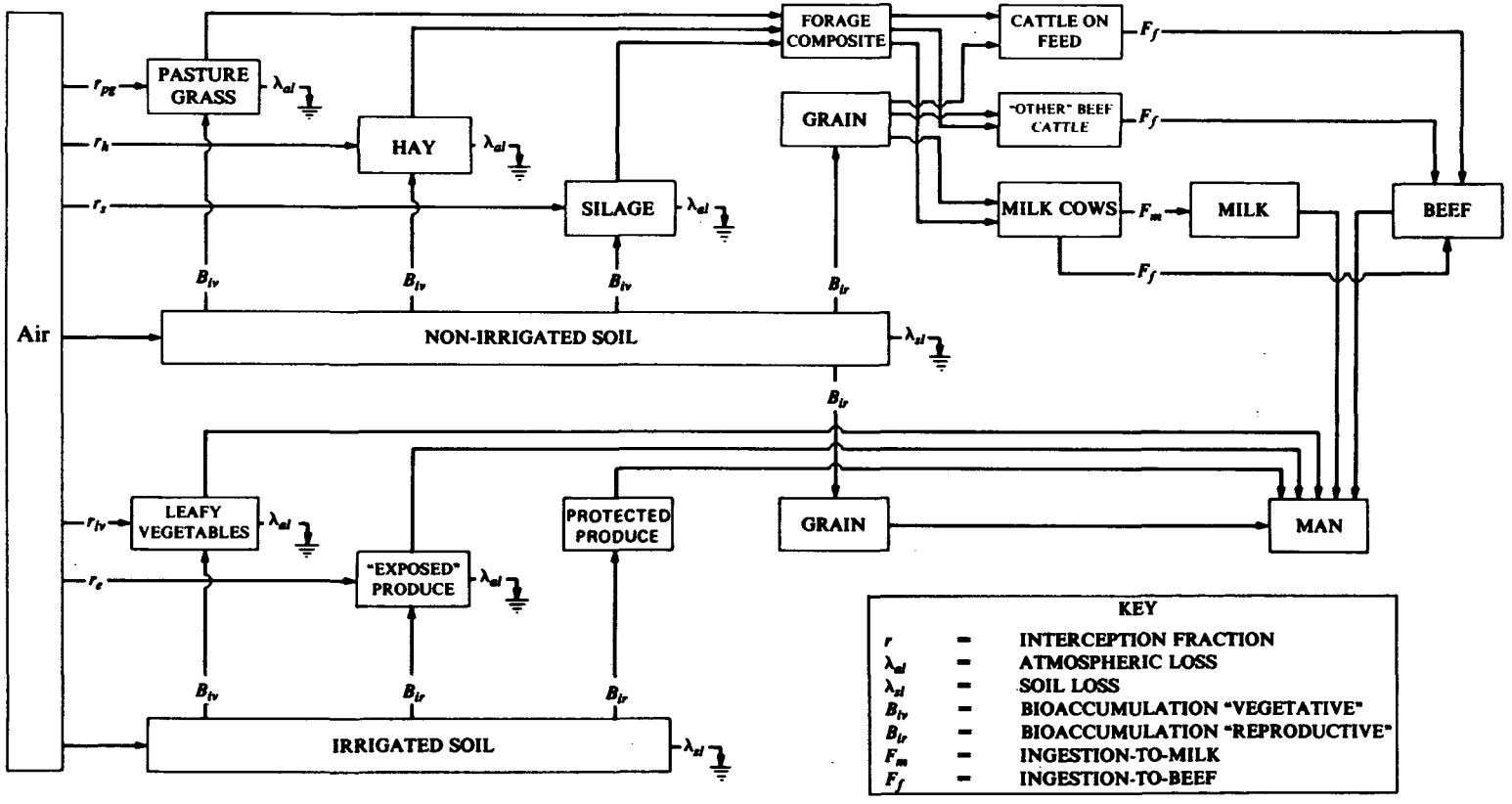


Figure 3. Pathways addressed in the terrestrial food-chain computer code TERREX.

dry weight concentration in root zone soil (assumed to be to a 15-cm depth). Meat- and milk-producing cattle are assumed to feed on grain and locally-contaminated forage. The grain may be grown locally or imported from offsite, depending on sizes of local livestock herds and grain production within the assessment area. Beef and milk concentrations are calculated via beef and milk transfer coefficients ($F_f$ and $F_m$, respectively), which relate daily intake of the contaminant to equilibrium concentrations in the food products. The derivation of the soil/plant CFs and beef and milk transfer coefficients relies heavily on structure/activity relationships (based on log $K_{ow}$) reported in the literature (Briggs 1981; Kenaga 1980; Baes 1982).

The terrestrial transport model is coupled with a data base (SITE) of default location-specific parameters describing agricultural, meteorological, and land-use characteristics for each cell of a rectangular grid superimposed on the conterminous United States. The dimension of each grid cell is 0.5° x 0.5° latitude-longitude; and for each cell, 36 parameters are defined (Table 2). In performing an assessment of a synfuels plant, the assessment grid defined by the atmospheric dispersion model (for distances less than 50 km, this is usually a polar grid) is superimposed on the data base grid and parameters are recalculated to the assessment grid. This process allows the assessment model to reflect, in a general way, the actual agricultural practices and characteristics of the area being modeled. The details of the data base and the sources of the parameter values within it are described by Baes et al. (1984b).

Table 2. Variable names and descriptions of parameters in the SITE* data base.

| Variable name | Units | Description |
|---|---|---|
| CELLON | °W | longitude of the southeast corner of the SITE data cell |
| CELLAT | °N | latitude of the southeast corner of the SITE data cell |
| ET | mm/y | evapotranspiration |
| IRRI | mm/y | irrigation |
| PRECIP | mm/y | precipitation |
| YEV | kg(fresh)/$m^2$ | yield of exposed produce |
| AYBF | kg(dry)/y/$m^2$ | areal yield of hay feed |
| YLV | kg(fresh)/$m^2$ | yield of leafy vegetables |
| YSF | kg(dry)/$m^2$ | yield of (corn and sorghum) silage feed |
| AREAP | $m^2$ | total area of pasture |
| NUMCC | head | cattle and calf inventory |
| SALFC | head/y | number of cattle on feed sold |
| NUMMC | head | number of milk cows |
| NUMSHP | head | number of sheep |
| PGF | kg | production of grain for feed |
| PHF | kg | production of hay feed |
| PSF | kg | production of (corn and sorghum) silage feed |
| HUMID | g/$m^3$ | average annual absolute humidity |
| AREAT | $m^2$ | total area of cell |
| POP | number | population of cell based on 1980 census |
| FRUNF | unitless | fraction of 1980 population classed as rural non-farm |
| FRUFM | unitless | fraction of 1980 population classed as rural farm |
| FURBN | unitless | fraction of 1980 population classed as urban |
| PLV | kg | production of leafy vegetables |
| PEV | kg | production of exposed produce |
| PPV | kg | production of protected produce |
| PGH | kg | production of grain for human consumption |
| MNIXHT | m | morning mixing height |
| AMIXHT | m | after noon mixing height |
| YPV | kg(fresh)/$m^2$ | yield of protected produce |
| YGF | kg(fresh)/$m^2$ | yield of grain food |
| YGH | kg(dry)/$m^2$ | yield of grain feed |
| FFDAYS | number | number of frost-free days in a year |
| NUMBC | head | number of beef cattle |

Table 2. Continued.

| Variable name | Units | Description |
|---|---|---|
| CFLAG | number | the caution flag: 1 means cell on atlantic coast. 2 means cell on Mexican border. 3 means 1 and 2. 4 means cell has interior body of water. 5 means 1 and 4. 6 means 2 and 4. 8 means cell on pacific coast. 12 means 4 and 8. 16 means cell on Canadian border. 20 means 4 and 16. 21 means 1 and 4 and 16. 24 means 8 and 16. 32 means cell has desert or barren land. Finally, 36 means 4 and 32. |
| DUMLF | number | A five digit number of the form FLPPP is printed out. F = 1 if the cell is more than 50% federal land, i.e., land type is undefined. F = 0 if less than 50% of the cell is federal land. L = 1 means tall row crops. L = 2 means short row crops. L = 3 means has or tall grass. L = 4 means urban area. L = 5 means small lakes. L = 6 means short grass. L = 7 means forest. Finally, PPP = the percentage of the dominant land type (may be 0 if the SITE cell is 100% federal land). |

*Baes et al., 1984.

Although the food-chain model represented by Fig. 3 appears to be more complex than the aquatic food-chain model, both are based on the use of BCFs to calculate accumulation in various food-chain trophic levels. The apparent complexity of the terrestrial model arises from the necessity of considering the many varied components of agricultural food chains (e.g., produce exposed to and produce protected from direct contamination of edible parts and management practices for milk, feedlot, and other cattle). From the standpoint of the uncertainty in model predictions, the participants at the workshop felt that increased complexity did not improve the model's accuracy as compared to a simpler model. However, those workshop participants who have performed risk calculations felt that a simpler approach would not provide sufficient detail in addressing the complex differences, identifying important exposure pathways, and highlighting research needs. Workshop attendees involved in work in which model input parameter values are experimentally determined argued that the model is too simple to address real-world transport processes and provides little guidance in their work. However, they agreed that, within the context of the overall assessment procedure, the model is a reasonable approach, provided there is an ongoing dialogue between the modeler and the experimentalist. This latter point will be addressed subsequently in Sect. 3.2.

Because of the limited data base on terrestrial transport and behavior of synfuels effluents, many potentially important pathways are not included in the terrestrial food-chain model. Recognizing the

difficulty in quantifying many of these transport process, the workshop attendees, nevertheless, identified several potentially important issues that should be considered at some point in the modeling process. These issues include foliar adsorption and translocation to edible produce parts; the effects of food processing (especially cooking) on human exposures; the prediction of soil degradation kinetics based on structure/activity relationships; the contribution of animal products other than beef and milk (e.g., eggs, chicken, and pork); differences in transfer coefficients as a result of livestock management practice; ingestion of water and soil by livestock; and irrigation water as a source term to the terrestrial food chain. The attendees ranked the first three issues as being more important than the latter four. Each of these issues is discussed in Sect. 3.3.

## 3.2 DATA SOURCES AND PARAMETER ESTIMATION METHODS

Early in the workshop, the methods for estimating model parameter values and the available data sources were discussed. The agricultural production and practice parameters in the SITE data base are derived from a Census of Agriculture conducted by the U.S. Department of Commerce (DOC 1977). These data are summarized by county and were converted to the uniform 0.5° x 0.5° cell grid by methods described in Baes et al. (1984b). A more recent Census of Agriculture is available, but differences in agricultural practice and production represented by the more current census were thought to be relatively small (less than 10%). The meteorological data are 30-year averages collected from over

200 U.S. weather stations maintained by the National Oceanic and Atmospheric Administration (Ruffner 1978; DOC 1968; DOC 1979). Other information, including land-use data, are taken from ORNL's Geoecology Data Base (Olsen, Emerson, and Nungesser 1980).

These data sources were generally viewed as being appropriate to the risk assessment methodology, which is concerned with annual-average or equilibrium conditions and population exposures. Of greater concern are the methods used to estimate the terrestrial transfer coefficients in the model. Because information in the literature on food-chain transport characteristics for synfuels compounds is scarce, most transport parameters must be estimated from structure/activity relationships. Table 3 lists the soil/plant, milk, and beef transport parameters currently used at ORNL and indicates which are derived from literature sources and which have been estimated from structure/activity relationships. The parameters derived from literature sources represent an "average" value for an "average" compound within the RAC. That is, if references were found for more than one compound within an RAC, a geometric mean (exponential of the mean of the log-transformed data) of all values found was used. Typically, this procedure required determination of a geometric mean value for each literature reference and determination of a geometric mean of all of these mean values. However, in most cases, multiple references or information on more than one compound within an RAC was not available; thus, most parameters in Table 3 are based on only one reference for each compound.

Table 3. Transport parameters for synfuels food-chain exposure assessment

| RAC # | Log $K_{OW}$ [1] | $\lambda_d$ [2] (s-1) | $K_d$ [3] (ml/g) | $B_{iv}$ [4] | $B_{ir}$ [5] | $F_m$ [6] (d/kg) | $F_f$ [7] (d/kg) |
|---|---|---|---|---|---|---|---|
| 9 | [-0.36][8] | 2 E-6[9] | 7 E-2 | 8 E+2 | 8 E+1 | 5 E-7 | 5 E-6 |
| 10 | [2.00] | 1 E-5 | [1 E+0] | 3 E+1 | 3 E+0 | 8 E-6 | 7 E-5 |
| 11 | [-1.00] | 7 E-6 | [3 E-2] | 2 E+3 | 2 E+2 | 2 E-7 | 2 E-6 |
| 12 | [2.09] | 1 E-6 | [1 E+0] | 3 E+1 | 3 E+0 | 8 E-6 | 8 E-5 |
| 13 | [4.00] | 8 E-6 | [1 E+1] | 2 E+0 | 2 E-1 | 8 E-5 | 7 E-4 |
| 14 | [3.18] | 1 E-5 | [5 E+0] | 5 E+0 | 5 E-1 | [5 E-5] | [6 E-4] |
| 15 | [5.28] | [5 E-8] | [7 E+1] | [2 E-1] | [3 E-2] | 3 E-4 | 3 E-3 |
| 16 | [0.57] | 3 E-6 | 2 E-1 | 2 E+2 | 2 E+1 | 2 E-6 | 1 E-5 |
| 17 | [1.19] | 7 E-6 | 4 E-1 | 9 E+1 | 9 E+0 | 3 E-6 | 3 E-5 |
| 18 | [2.65] | 4 E-6 | [3 E+0] | 1 E+1 | 1 E+0 | [4 E-5] | [1 E-3] |
| 19 | [2.96] | 1 E-5 | [4 E+0] | 7 E+0 | 7 E-1 | 2 E-5 | 2 E-4 |
| 20 | [1.97] | 2 E-6 | 1 E+0 | 3 E+1 | 3 E+0 | 7 E-6 | 7 E-5 |
| 21 | [1.55] | [8 E-8] | 7 E-1 | 6 E+1 | 6 E+0 | [2 E-4] | [4 E-4] |
| 22 | [0.90] | 2 E-5 | 3 E-1 | 1 E+2 | 1 E+1 | 2 E-6 | 2 E-5 |
| 23 | [2.52] | 4 E-6 | 2 E+0 | 1 E+1 | 1 E+0 | 1 E-5 | 1 E-4 |
| 24 | [-0.50] | 3 E-6 | 6 E-2 | 1 E+3 | 1 E+2 | 4 E-7 | 4 E-6 |
| 25 | [2.31] | 1 E-6 | 2 E+0 | 2 E+1 | 2 E+0 | 1 E-5 | 1 E-4 |
| 27 | [0.64] | 4 E-6 | 2 E-1 | 2 E+2 | 2 E+1 | 2 E-6 | 2 E-5 |
| 28 | [-0.92] | 3 E-6 | 3 E-2 | 2 E+3 | 2 E+2 | 3 E-7 | 3 E-6 |
| 31 | | | [2 E+2] | [4 E-2] | [6 E-3] | [6 E-5] | [2 E-3] |
| 32 | | | 1 E+1 | [9 E-1] | [2 E-1] | [5 E-4] | 3 E-1 |
| 33 | | | 2 E+2 | [6 E-2] | [6 E-2] | [1 E-3] | 6 E-3 |
| 34 | | | [7 E+0] | [6 E-1] | [2 E-1] | [1 E-3] | [6 E-4] |
| 35 | | | [9 E+2] | [5 E-2] | [9 E-3] | [3 E-4] | [3 E-4] |

1. Logarithm of the water/octanol partitioning coefficient (unitless)
2. The soil degradation constant (1/s)
3. The soil/water distribution coefficient (mL/g)
4. The soil/plant bioaccumulation factor for vegetative plant parts (unitless)
5. The soil/plant bioaccumulation factor for reproductive/storage plant organs (unitless)
6. The milk transfer coefficient which relates daily intake to milk concentration at equilibrium (d/kg)
7. The beef transfer coefficient which relates daily intake to beef concentration at equilibrium or slaughter (d/kg)
8. Bracketed values have either been measured directly or are based on experimental data reported in the literature
9. Read as $2 \times 10^{-6}$.

The distribution coefficient $K_d$ is the ratio of solute concentration in soil to that in water. This parameter is used to predict leaching removal from root zone soil after the method of Baes and Sharp (1983). More importantly, this parameter is used to predict the soil/plant concentration factors $B_{iv}$ and $B_{ir}$ defined in Sect. 3.1. The prediction of $K_d$ is based on the relationship given by Briggs (1981),

$$\log K_d = -0.99 + 0.53 (\log K_{ow}) . \qquad (3.1)$$

The estimation of $B_{iv}$ is based on the relationship given by Baes (1982) between $K_d$ and $B_{iv}$. Substitution of Eq. (3.1) into that relationship gives

$$\log B_{iv} = 2.71 - 0.62 (\log K_{ow}) . \qquad (3.2)$$

The soil/plant CF for reproductive/storage plant organs $B_{ir}$ is assumed to be 0.1 $B_{iv}$, based on the work of Baes et al. (1984b) on inorganic compounds. This relationship also fits measured CFs for benzo(a)pyrene (Kolar et al. 1975; Ellwardt 1977; Skcodich 1979). Finally, the milk and beef transfer coefficients are derived by incorporating into Kenega's (1980) relationship between bovine fat BCFs and log $K_{ow}$ the average fat content of milk and beef (Spector 1956), and feed intake rates for milk cows and beef cattle (Shor et al. 1982). These substitutions yield for milk,

$$\log F_m = -6.12 + 0.50 (\log K_{ow}) \qquad (3.3)$$

and for beef,

$$\log F_f = -5.15 + 0.50 (\log K_{ow}) . \qquad (3.4)$$

The soil degradation constant $\lambda_d$ is assumed to be equal to the air degradation constant if no measured values are available. This approach is taken because no structure/activity relationships for soil persistence have been published.

The workshop participants recognized many limitations in current procedures for estimating transfer parameters. These limitations include (1) the use of a single transfer coefficient to represent an entire RAC, which may contain compounds having highly variable transport properties (perhaps spanning four or five orders of magnitude), (2) use of relationships derived from work done with inorganic compounds for organic compounds, and (3) heavy dependence on log $K_{ow}$ as the measure of structure for the RAC. None of the participants was able to outline more appropriate procedures for parameter determination, although there was general agreement on the need to find better approaches. Also, there was a general consensus that for a first-cut screening-level assessment, the parameter estimation procedures were reasonable. Some participants suggested that future assessments include uncertainty estimates based on either analytical or numerical error propagation techniques, but the estimation of probability density functions for the transport parameters will be difficult in the absence of experimental data.

## 3.3 MAJOR LIMITATIONS ON EXISTING DATA AND METHODS

The workshop participants felt that one of the major shortcomings of the current model and, indeed, the available data base is the lack

of a food contamination pathway via foliar adsorption and translocation to edible produce parts. This pathway would be important for both direct deposition of atmospherically released pollutants and pollutants dissolved in irrigation water. Once deposited, pollutants can remain on leaf surfaces, be removed from the plant via weathering, or be passed through the cuticle or stomata and be redistributed within the plant. The first two processes are modeled in the current ORNL model, but the latter is not.

Foliar absorption may be the primary route of entry for some chemicals (e.g., herbicides and pesticides); however, information is too sparse to develop predictive models based on structure/activity relationships. Foliar interception of synfuels compounds, such as gasses, particulates, or hydrosols, is primarily a function of leaf surface morphology and structure. Adsorption through the cuticle can be a significant route of entry for particulates and liquids and may be related to lipid solubility, molecular size, and free energy. Stomatal absorption occurs primarily with gasses and should be a function of plant transpiration. The workshop participants recommended that the foliar absorption/translocation pathway be included in the terrestrial food-chain pathway model. It was suggested that absorption and translocation be measured in experimental determinations of plant uptake and distribution of synfuel compounds so that predictive models based on the above relationships can be developed. Finally, it was suggested that the existing data on pesticide foliar absorption/translocation pathways be examined for structure/activity relationships.

A second area deemed important is the soil compartment. Here, two areas were cited. First is the prediction of soil degradation kinetics based on structure/activity relationships, and second is the calculation of the synfuel compound concentration in the soil solution. The former is considered an essential improvement of the assessment methodology, and the second allows much closer communication between modeler and experimentalist.

The current model assumes first-order kinetics for the degradation of organics in soil. Data from field and laboratory studies of organics (mostly pesticides) indicate that the assumption of first-order kinetics is not always appropriate method in modeling degradation in the soil. Rates of degradation in soil sometimes depend on the concentrations in soil and on environmental variables such as soil temperature, moisture, etc. Adaptation of soil microorganisms to organics can increase degradation rates. In such cases, there may be a significant departure from first-order kinetics.

An associated problem is the lack of a model for predicting the soil degradation constants ($\lambda_d$). The current approach is to assume the same value for $\lambda_d$ as for $\lambda_a$ (the atmospheric degradation constant). A good predictive model for soil degradation would incorporate structure/activity relationships based on easily measured chemical or structural properties (e.g., molecular size, functional groups, and/or water solubility). The group recommended examination of the pesticide data base for such structure/activity relationships.

The prediction of a soil solution concentration is an important consideration from the standpoint of integrating results of experimental plant uptake studies with modeling activities. Experimental studies of root uptake of synfuel compounds must necessarily be based on hydroponic solutions for practical reasons. Constant measurable substrate concentrations must be maintained and soil kinetics must be eliminated. Recognizing these requirements, workshop participants felt that the model should be modified to accommodate the experimental data, rather than vice versa. Additionally, a soil solution submodel would allow the prediction of the traditional soil/plant concentration factor from hydroponic data and would also provide a means of assessing impact of synfuels compounds on crops, because the majority of toxicological data is based on hydroponic studies.

Another important area for further improvement in the model is the consideration of the effects of food processing (especially cooking) on human exposures. Exposure from leafy vegetables and exposed produce would be expected to be significantly reduced by food processing, including washing, trimming, and removal of outer exposed plant parts. All of the attendees felt that, especially for organic compounds, the effects of heating during cooking would tend to significantly reduce human exposures because of thermal degradation. The EPA is currently developing loss estimates for the various food preparation processes. Preliminary results are highly variable and highly dependent on individual preparation practices. Nevertheless, the unanimous opinion

of the participants was that this consideration is an important one for all meat and that most milk and vegetable pathways should be further researched.

Other areas needing attention are (1) the inclusion of animal products other than beef and milk into the model, (2) accounting for differences in transfer coefficients resulting from livestock management practice, (3) consideration of water and soil ingestion by livestock (in addition to feed), (4) addition of irrigation water as a source term to the terrestrial system, (5) capability to model acute exposures and sensitive populations, and (6) estimation of uncertainty associated with model predictions. These additional capabilities were not unanimously considered to be essential by the workshop, although one or more of the participants felt strongly about each. The reason that these issues were not collectively considered to be as important as the issues previously described is probably that their inclusion in the model is not expected to change model results significantly, or, in the case of the uncertainty issue, the uncertainty estimate could only be tested through model validation, which could be difficult.

The food-chain model considers only cow's milk and beef pathways in its current form. The workshop participants suggested that chicken, pork, and egg pathways be considered as well. It was pointed out that poultry and swine are significant components of the American diet. Rupp (1980) found these two sources to constitute 11 and 13% of the total annual consumption of meat and other animal products, respectively, for the over-18 age group. By contrast, milk (and milk

products) and beef constitute 51 and 14%, respectively. A first solution to account for poultry and swine would be to adjust the beef consumption rates used in the risk assessment model upward to reflect consumption of all meats. However, this approach assumes that beef transfer coefficients are appropriate to poultry and swine. Eisele, Traylor, and Schwarz (1983) demonstrate this not to be the case for three organic compounds. In general, the ordering of transfer coefficients was found to be poultry > swine > bovine. Therefore, a better approach would be to include poultry and swine in the model.

The use of a single transfer coefficient for an animal product was criticized because livestock management practice is thought to significantly influence contaminant metabolism. Two examples are the differences between broilers and egg-laying hens and between beef and dairy cattle. Egg laying in poultry and milk production in cows can be significant routes of depuration of ingested synfuels compounds because these two excretory pathways are very important for these animals. In the absence of these excretory pathways (broilers and beef cattle), higher accumulations of organics in body tissues would be expected. However, because this effect is not proven for synfuel compounds, it was suggested that further research be done to examine this question. If it is found that management practice does influence the measured livestock transfer coefficients, the model should be modified accordingly.

Also of concern in the modeling of livestock pathways is the consumption of contaminated soil and water during grazing. It was

pointed out that cattle consume roughly 0.5 to 1 kg of soil per day while grazing pasture; poultry and swine, to a lesser extent, also consume soil. If soil/plant CFs are low (as indeed they are for most synfuel compounds as currently modeled), then soil may be an even more important pathway than ingestion of feed. To a lesser extent, contaminated water may also be considered an ingestion source. These additional contamination sources may be more important in certain areas of the United States than in others, depending on livestock management practices. The workshop participants could not arrive at a consensus as to whether incorporation of these pathways would significantly alter model results. In the interest of conservatism, however, it was generally agreed that provisions for these pathways should be examined in the food-chain model.

Another recommended addition to the food-chain model is the contribution of contamination of agricultural plants via irrigation water. In many parts of the country, irrigation waters are derived from groundwater supplies, and organics deposited on or in soil could reach these reservoirs. In other parts of the country, surface waters contaminated via atmospheric, aquatic, and surface runoff inputs, are used for irrigation of crops. It was suggested that simple bounding analyses be performed to determine the importance of this source term. If this is found to be a critical pathway, data collection and model modifications should be undertaken. Inclusion of this pathway is appealing because it would link the terrestrial and aquatic transport models. If irrigation proved significant, the addition of a groundwater transport model would also be needed.

The workshop addressed issues that went beyond the scope of the food-chain model itself, including the capability to assess acute exposures and sensitive populations and to estimate uncertainties. The current assessment strategy addresses chronic population exposures after 35 years of synfuel plant operation. Because these facilities have a projected lifetime of 30 years, the assessment scenario now used should provide maximum average exposure estimates. However, participants recognized the need to address acute exposures from intermittent pollutant releases and exposures to sensitive populations (nursing mothers, children, vegetarians, individuals growing their own food, etc.). Acute exposures and exposures to sensitive populations should eventually be addressed in both the transport modeling and in the determination of risk estimates. Currently, simple bounding estimates to address these needs should be performed in both the transport and risk methodologies.

Finally, although sensitivity analyses have been performed on the food-chain model, numeric determination of model uncertainties have not been performed. Stochastic variability could be examined using available numerical and analytic tools [e.g., ORNL's Monte Carlo techniques (Gardner and O'Neill 1983) and Carnegie-Mellon University's DEMOS model (Henrion and Morgan, in press)]. Model results would then be presented as distributions rather than as single-value estimates. These techniques allow important contributors to overall model uncertainty to be specified as a guide to further research. Also, methods for examining systematic error need to be developed. Of

course, the best method to address systematic error would be model validation. The workshop concluded that validation is really the only method not only to ensure that the assessment model is both appropriate and accurate but also to specify definitively the uncertainty associated with model predictions. Validation would also determine whether the various concerns about the current model expressed above are important.

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# APPENDIX A. AGENDA

# WORKSHOP ON FOOD CHAIN MODELING FOR RISK ANALYSIS

Capitol Hill Hotel - Washington, D.C.

March 22-24, 1983

## AGENDA

Tuesday, March 22, 1983 - All Day

Welcome: Mel Carter, Georgia Inst. of Tech.

Introduction to the Workshop: C. Fred Baes III, ORNL

Charge to Workshop Participants: Alan Moghissi, EPA

Presentations:

- C. Fred Baes III, ORNL
- James Breck, ORNL
- Jim Falco, EPA
- Jerry Eisele, ORAU/CARL
- Craig McFarlane, EPA
- Chuck Garten, ORNL
- John Connolly, Manhattan College
- John Nagy, Brookhaven National Laboratory
- Paul Moskowitz, Brookhaven National Laboratory
- F. Owen Hoffman, ORNL

Break into working groups: Aquatic and Terrestrial

Wednesday, March 23 - All Day

Working group discussions and report writing

Topics discussed by each group:

1. Significance of potential uptake pathways
2. Lessons from radionuclide assessment
3. Extrapolation from laboratory to field
4. Major uncertainties in food chain assessment

Thursday, March 24 - A.M.

Presentation, discussion, and review of draft recommendations

1. Food chain models best suited to synfuels risk analysis
2. Data sources and parameter estimation methods best suited to synfuels risk analysis
3. Major limitations on existing data and methods

Noon: Adjournment

# APPENDIX B. LIST OF PARTICIPANTS

# WORKSHOP ON FOOD CHAIN MODELING FOR RISK ANALYSIS

Capitol Hill Hotel - Washington, D.C.

March 22-24, 1983

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# WORKSHOP ON FOOD CHAIN MODELING FOR RISK ANALYSIS

Capitol Hill Hotel - Washington, D.C.

March 22-24, 1983

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