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## Exposure Assessment Methodology and Reference Environments for Synfuel Risk Analysis

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UNION CARBIDE CORPORATION  
FOR THE UNITED STATES  
DEPARTMENT OF ENERGY





830204

Health and Safety Research Division

EXPOSURE ASSESSMENT METHODOLOGY AND REFERENCE ENVIRONMENTS  
FOR SYNFUEL RISK ANALYSIS

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NOTICE: This document contains information of a preliminary nature. It is subject to revision or correction and therefore does not represent a final report.

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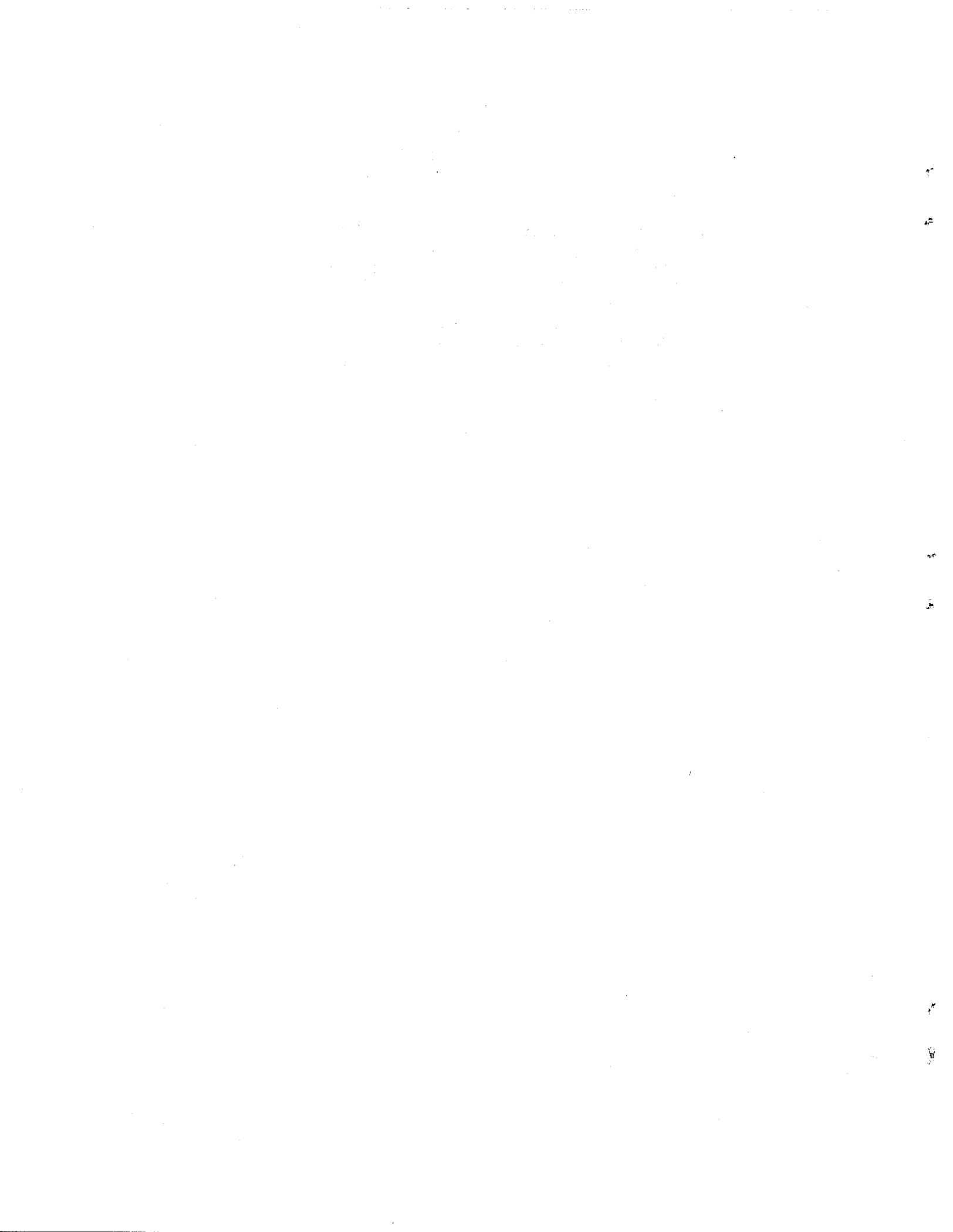
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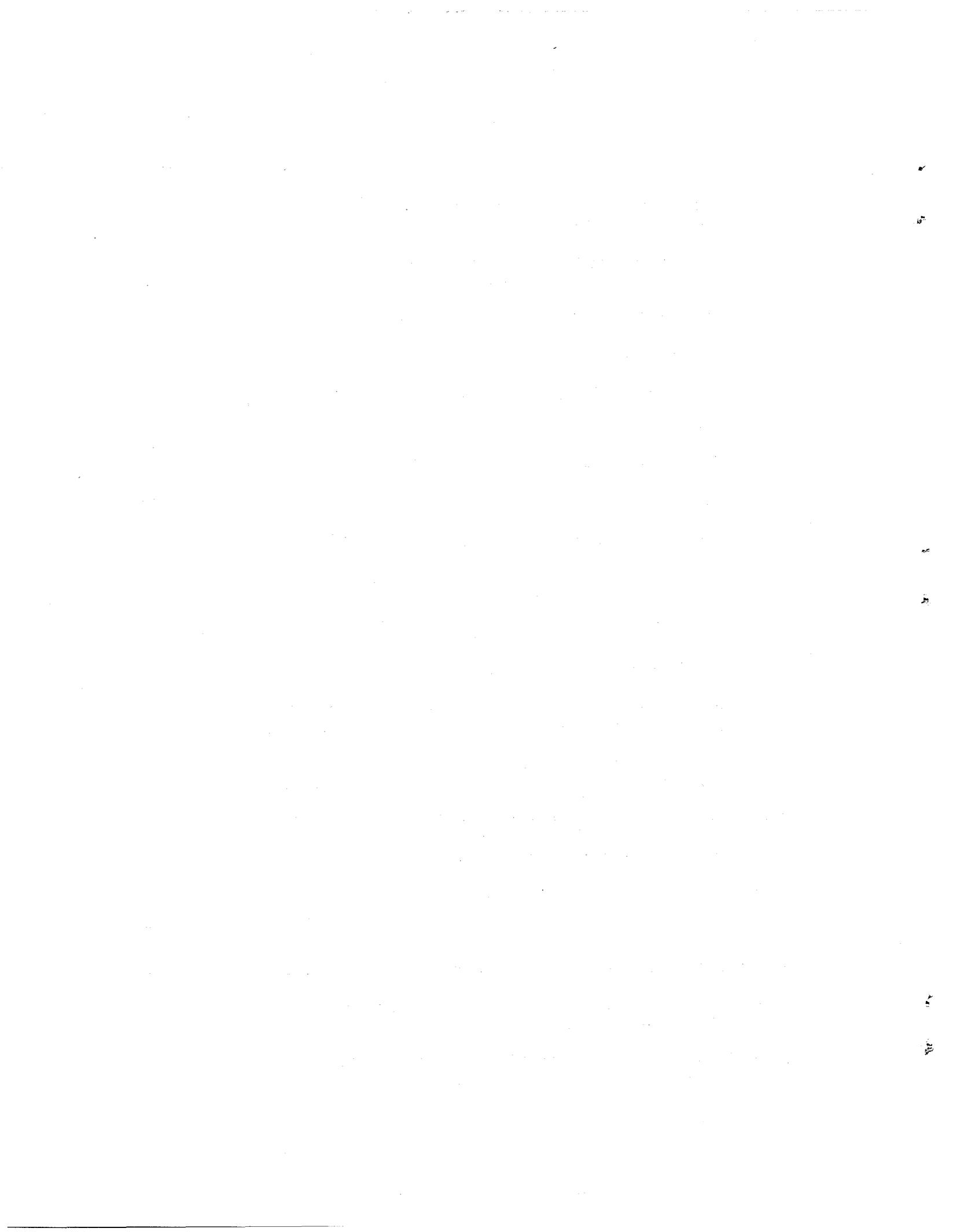
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## Abstract

This document presents an exposure assessment methodology for evaluating health and environmental risk from synfuel technologies. It also provides a broad characterization of the reference environments in which synfuels facilities might be located. The exposure methodologies consider atmospheric, aquatic, and terrestrial food chain pathways. Both short- and long-range atmospheric transport and photochemical transformation methodologies are presented. The aquatic methodology considers surface and ground water transport. The foodchain methodology considers exposure pathways involving drinking water, agricultural produce, beef and milk, and contains a default data base of site-specific agricultural, meteorological, and land use parameters. Characterization of the generic environments is divided into three components: the physical environment, and the ecological and human populations at risk. The methodologies and parameters presented in this report are very generalized, and are intended to be used for screening purposes only.



## 1. INTRODUCTION

A growing demand for energy coupled with a shortage of oil has resulted in an increased interest in producing energy from domestically available fossil fuels. To assure that such development proceeds in a manner which protects both human health and the environment, the U.S. Environmental Protection Agency (USEPA) has commissioned staff of the Oak Ridge National Laboratory (ORNL) and Brookhaven National Laboratory to perform health and environmental risk analyses of the various synfuels technologies. Such analyses will allow for development of effective technology control modifications addressing prioritized public health and environmental concerns. These risk analyses are generic in that they do not utilize specific technological design or site-specific environmental data. The synfuel technologies selected for application of risk assessment methods are the Lurgi Fischer/Tropsch indirect coal liquefaction technology, the SRC-II direct coal liquefaction technology, and the underground mining, surface retorting of oil from shale.

This document defines the health and environmental exposure assessment methodologies that will be applied to these technologies. It is divided into two major sections. The first describes exposure assessment methodologies that can be used to quantify exposures to humans from the atmospheric, aquatic, and terrestrial pathways. The second section contains a description of general reference environments from which model parameters are obtained. Reference environments provide a broad characterization of the physical environment, and ecological and human populations-at-risk.

## 2. EXPOSURE ASSESSMENT METHODOLOGY

### 2.1 INTRODUCTION

Health and environmental risk analyses consist of two main components: exposure assessment and effects assessment. Exposure assessment is defined as the determination of the concentration of toxic materials in space and time at the interface with target populations. This description must include an identification of all major pathways for movement and transformation\* of a toxic material in a selected environmental setting. Ideally, concentrations as a function of time and location and all major transformation products should be identified.

It is not currently possible, nor is it necessarily desirable, to develop predictive methodologies which address all processes affecting movement of contaminants through the environment. Many environmental transport processes are extremely complex and not well understood. In addition, even when a sufficient conceptual basis exists for developing complex, process-oriented models, accurate physical and environmental data are generally not available to parameterize them. It is, therefore, often most appropriate to use simplifying assumptions when attempting to predict the environmental fate of pollutants.

---

\*Transformation is a generic term used to describe any process in which a change takes place in molecular structure. Terms such as photolysis, degradation, or oxidation refer to specific transformation processes.

The methodologies presented here represent a reasonable compromise between model complexity\* and the ability to obtain realistic data characterizing model parameters. We have attempted to make reasonably conservative assumptions regarding environmental transport of materials released by synfuel technologies. The principal pathways considered are atmospheric and aquatic transport and transformation, and ingestion of toxic materials that have passed through the terrestrial foodchain.

It should be emphasized that the methodologies presented in this report are very generalized and are intended to be used when the predicted exposures to critical groups are at least an order of magnitude below the relevant exposure limit values. If an assessment undertaken using the procedures outlined in this report indicates that projected releases lead to exposures near the appropriate limit, then it will be necessary to carefully evaluate the extent to which the models and parameter values are representative of conditions prevailing at the specific site.

---

\* Although models employed are relatively simple, they reflect complex processes to a sufficient level that sensitivity studies can be utilized to determine those parameters whose uncertainty most influences confidence in overall assessment results. This approach can be used to help establish priorities for both research and environmental monitoring efforts.

## 2.2 ATMOSPHERIC METHODOLOGY

### 2.2.1 Atmospheric Transport

Synfuel technologies will result in atmospheric release of a variety of particulate and gaseous pollutants. Since atmospheric transport of these pollutants will be an important pathway of exposure to the general public, it is necessary to estimate the extent to which both transport and photochemical transformation affect concentrations reaching human populations.

### 2.2.2 Model Descriptions

#### 2.2.2.1 AIRDOS-EPA

The Gaussian plume model is a widely used method of estimating downwind concentrations of airborne material released to the atmosphere. This class of models is based on the assumption that the plume will spread both laterally and vertically in accordance with a Gaussian statistical distribution. While such models have limited applicability in instances of complex terrain and variable release rates, they have been successfully used for many years to predict ground-level concentrations where reasonably flat terrain exists and where an average, fairly stable release rate can be assumed. The physical processes generally included in Gaussian plume models are (1) dispersion by turbulent diffusion, (2) dry deposition onto the ground, (3) scavenging due to washout as

rain or snow pass through the plume, and (4) transformation of effluents as they are dispersed.

Within the first 50 km of a synfuels facility, we will apply the Gaussian plume dispersion code AIRDOS-EPA (Moore et al., 1979). This code is a modified version of AIRDOS-II (Moore, 1977), which has been used by the Environmental Sciences Division and the Health and Safety Research Division of ORNL for several years to assess radiological impact of routine operation of nuclear facilities. AIRDOS-EPA employs a modified Gaussian plume equation to estimate annual average, ground-level concentrations and surface deposition at various distances in a circular grid surrounding the release point. Air concentrations and ground deposition rates can be given as average values over each of sixteen 22.5° sectors surrounding the source. AIRDOS-EPA also contains subroutines to calculate population exposure to emitted pollutants in the area surrounding the proposed facility. Using user-supplied population data for each sector, AIRDOS-EPA combines air and food concentrations with average inhalation and food intake rates to calculate pollutant intake via ingestion and inhalation.

We now present a brief description of AIRDOS-EPA. A more detailed description may be found in Moore et al. (1979). The basic Gaussian equation used in AIRDOS-EPA for ground-level concentration ( $\chi$ ) is

$$\chi = \frac{Q_s}{\pi \sigma_y \sigma_z u} \exp \left[ -\frac{1}{2} \left( \frac{y}{\sigma_y} \right)^2 \right] \exp \left[ -\frac{1}{2} \left( \frac{h}{\sigma_z} \right)^2 \right], \quad (2-1)$$

where

$Q_s$  = source term (kg/s),

$\sigma_y$  = horizontal dispersion coefficient (m),

$\sigma_z$  = vertical dispersion coefficient (m),

$u$  = average wind speed (m/s),

$y$  = lateral location in (m), and

$h$  = effective stack height (m).

The downwind distance,  $x$ , enters Eq. (2-1) through  $\sigma_y$  and  $\sigma_z$ , which are functions of  $x$  as well as the atmospheric stability category.

The effective stack height,  $h$ , is estimated by

$$h = h_s + \Delta H \quad , \quad (2-2)$$

where

$h_s$  = the stack or release height (m), and

$\Delta H$  = plume rise (m).

Since plume rise calculations are subject to much uncertainty, the user of AIRDOS-EPA can elect either (1) to use the equation given by Rupp et al. (1948) to estimate plume rise for momentum-dominated plumes, (2) to use Briggs (1969) equations for hot plumes that rise because of bouyancy, or (3) to supply discretionary values for plume rise.

Annual-average meteorological data sets usually include frequencies for several wind speed categories for each wind direction and Pasquill atmospheric stability category. AIRDOS-EPA uses reciprocal-averaged wind speeds in the atmospheric dispersion equations. The reciprocal-averaged wind speed  $\mu_r$  for each direction and Pasquill category is defined by the equation

$$\mu_r = \sum f_k / (\sum f_k / \mu_k) , \quad (2-3)$$

where

$f_k$  = fraction of time in wind speed category  $k$ , and

$\mu_k$  = average wind speed within wind speed category  $k$  (m/s).

Particulate material and reactive or soluble gases may deposit on ground or water surfaces through two distinctly different processes: (1) dry deposition, and (2) scavenging by rain or snow. Dry deposition is estimated by

$$R_d = V_d \chi , \quad (2-4)$$

where

$R_d$  = surface deposition rate ( $\text{kg}/\text{m}^2 \cdot \text{s}$ ),

$V_d$  = dry deposition velocity (m/s), and

$\chi$  = atmospheric concentration at ground level ( $\text{kg}/\text{m}^3$ )

Scavenging is estimated by

$$R_s = \Phi \chi_{\text{ave}} L , \quad (2-5)$$

where

$R_s$  = surface deposition rate ( $\text{kg}/\text{m}^2 \cdot \text{s}$ ),

$\Phi$  = scavenging coefficient ( $\text{s}^{-1}$ ),

$x_{ave}$  = average concentration in vertical column up to lid height  
(kg/m<sup>3</sup>), and

L = lid height (m).

The value for total ground deposition used in AIRDOS-EPA is the sum of  $R_d$  and  $R_s$ .

AIRDOS-EPA also allows for depletion of the plume through chemical transformation via first-order reactions. Thus, as the airborne plume is blown downwind from the release point, it is depleted by three processes: dry deposition, scavenging, and chemical transformation. Depletion is taken into account by substituting a depleted source term  $Q_p$  for the original source term  $Q_s$  in Eq. (2-1) for each downwind distance  $x$ . For scavenging, the depletion fraction  $Q_p/Q_s$  for each  $x$  value is given by

$$Q_p/Q_s = \exp^{-t}, \quad (2-6)$$

where the value of  $t$  is the time in seconds that is required for the plume to reach a point  $x$  meters downwind. For dry deposition, the depletion fraction for any downwind distance  $x$  is given by

$$Q_p/Q_s = \exp \left\{ -(2/\pi)^{1/2} \frac{V_d}{u} \int_0^x \left[ \frac{\exp -\frac{1}{2} \left( \frac{h - V_g x/u}{\sigma_z} \right)^2}{\sigma_z} \right] dx \right\}, \quad (2-7)$$

where  $V_g$  is the gravitational settling velocity (m/s). The depletion fraction for degradation is

$$Q_p/Q_s = \exp^{-kt} \quad , \quad (2-8)$$

where  $k$  is the chemical degradation constant and  $t$  is the time in seconds required for plume travel. The overall depletion fraction used in AIRDOS-EPA is the product of the depletion fractions for dry deposition, scavenging, and chemical transformation.

We now present a brief justification for our selection of AIRDOS-EPA. Since there are literally hundreds of computer codes available for prediction of the local atmospheric dispersion of toxic contaminants, we make no claim as to having performed an exhaustive review of the literature. The codes reviewed were AIRDOS-EPA (Moore et al., 1979), ATM (Culkowski and Patterson, 1976), CRSTER (USEPA, 1977), ISC (Bowers, Bjorklund and Cheney, 1979), MESOPUFF (Berkley and Bass, 1979), and RAM (Turner and Novak, 1978). Criteria used in selection of a model were as follows:

- The modeling region of interest is assumed to be within 50 km of the individual sources being considered.
- The time-averaging periods of interest are both short-term (8-24 hours) and long-term (annual averages).
- The model must be able to simulate chemical degradation and must provide surface deposition rates for use in foodchain modeling.
- The model should account for complex terrain.

- It is desirable that the atmospheric model interact directly with demographic data to estimate population exposures.

None of the codes reviewed met all of these criteria (Table 2-1). The AIRDOS-EPA code meets all assessment requirements except that of analysis over complex terrain.\* All other models, except ISC, were eliminated from consideration because of their failure to allow for both chemical degradation and surface deposition of pollutants. The ISC code was eliminated because its methodology for estimating surface deposition is based on reflective coefficients not applicable to complex terrain nor readily available in the literature.

#### 2.2.2.2. RETADD-II

At distances greater than 250 km from a synfuels facility, we will apply a long-range trajectory-type code, RETADD-II (Murphy, Ohr, and

---

\* Most air quality models use diffusion coefficients and eddy diffusivities developed from studies over flat, homogeneous terrain such as the grasslands of western Kansas (Drake, Barrager, and Lavlaine, 1979). Locations associated with this synfuels assessment will be the Piceance Basin in the Rocky Mountains (for oil shale development) and Eastern Kentucky (for coal conversion technologies). In these areas of mountain ranges and deep valleys, wind and temperature fields produce complicated atmospheric dispersion patterns and distributions that are difficult to simulate.

The USEPA is aware of this problem and is currently funding research to develop a complex terrain model for the Piceance Basin (Huber, 1981) and elsewhere (Holzworth, 1980). The U.S. Department of Energy (USDOE) has similarly funded studies in the Appalachians (Cushman and Suter, 1981) and the Geysers region of California (Dickerson and Gudiksen, 1980) to improve knowledge of transport processes in complex terrain.

Table 2-1. Simulative capabilities of a selected group of atmospheric dispersion codes

Attribute	Atmospheric codes					
	AIRDOS	ATM	CRSTER	ISC	MESOPUFF	RAM
≤24-h averaging	Yes*	Yes	Yes	Yes	Yes	Yes
Annual averaging	Yes	Yes	Yes	Yes	Yes	No
Chemical removal	Yes	Yes	No	Yes	Yes	Yes
Surface deposition	Yes	Yes	No	Yes	No	No
Complex terrain	No	No	Yes	Yes	No	No
Population exposure	Yes	No	No	No	No	No
Sector averaging	Yes	Yes	No	No	No	No

\* AIRDOS-EPA only estimates worst-case, short-term concentrations.

Begovich, in preparation), developed at ORNL for the USEPA. This code is based on the RETADD code of Begovich, Murphy, and Nappo (1978) which, in turn, was an ORNL version of a code described by Heffter and Taylor (1975). Ground-level concentrations and depositions are computed along trajectories composed of a series of 3-h segments. The direction and length of each segment are determined by upper air wind data reported closest to the position and time of the segment. The major differences between RETADD-II and both the Heffter and original RETADD codes are that RETADD-II allows for an elevated source, it has a modified treatment of dry deposition, and it calculates growth and decay of a chain of species.

RETADD-II operates by calculating tropospheric wind trajectories which advect material away from the source of emission. Superimposed on these trajectories are the vertical and horizontal diffusion rates which are a function of travel time. Loss of material by deposition on the ground is also accounted for in RETADD-II, as is chemical decay. The source of emission can be considered to be either at ground level or elevated. This option allows for realistic treatment of plume depletion from elevated sources during the initial part of the advection and diffusion process.

The calculation of wind trajectories is effected by accessing a data base of historical upper-air wind data. The premise behind this approach is that a climatology typical of the assessment period is chosen from the historical record and used in the simulation. For instance, to predict dispersion patterns during a given time period with

RETADD-II, one would use upper-air wind data for that month, season, or year of interest.

Four wind trajectories are calculated for each day of a RETADD-II simulation. These trajectories pass through the source of emission at 0, 6, 12, and 18 hours Greenwich Mean Time (referred to as 0 Z, 6 Z, 12 Z, and 18 Z, respectively). The user chooses a rectangular grid area to include the assessment area, and the trajectories are followed by the code until they exit the grid. The grid may encompass a regional area the size of a few states or the entire conterminous United States. Upper-air wind data are available for the continental United States, adjacent parts of Canada and Mexico, and the Caribbean. The code subdivides the assessment grid into 315 cells, and calculates average ground-level air concentrations and ground deposition rates for each of the 315 cells.

The RETADD-II code was selected over other models primarily because of its state-of-the-art computational algorithms and the compatibility of model output with our intended uses. Of particular interest was its ability to handle chemical degradation and provide pollutant deposition rates on soil for use in foodchain modeling. Availability, adaptability, and previous familiarity with the code were also factors in our choice. The Heffter code has been used for several years at ORNL to assess the health impact of various technologies. One application was an assessment for the U.S. Nuclear Regulatory Commission (USNRC) of the health risk of radon released by uranium mills in the United States (Travis et al., 1979), in which the code was used to estimate inhalation of  $^{222}\text{Rn}$  and ingestion of deposited daughter  $^{210}\text{Pb}$  by residents of the United States, Canada, and Mexico.

### 2.2.2.3 Intermediate-Range Atmospheric Transport

We have proposed using a Gaussian plume dispersion code for predicting atmospheric concentrations within 50 km of a synfuels facility and a long-range trajectory-type code for distances greater than 250 km. The intermediate distances pose somewhat of a problem. Plume transport beyond 50 km may require substantial travel time. As travel time increases, diurnal variations in meteorological conditions, movement of weather systems, and mesoscale terrain effects alter the assumptions of steady-state conditions and spatial homogeneity upon which short-range atmospheric transport models are based. While techniques are available to analyze these effects (Miller, Cotter, and Hanna, 1981), only limited experience is available in their use. Miller, Cotter, and Hanna (1981) suggest that a simple Gaussian plume model may be adequate to describe intermediate range atmospheric transport in some situations. However, many applications may present more complex situations than can be adequately described through the use of short-range models. Among the refinements which characterize state-of-the-art intermediate-range atmospheric transport models are the following: (1) temporal and spatial changes in the boundary layer, (2) variations in trajectories, (3) windfield modeling techniques, and (4) improved techniques for advection and diffusion. These refinements are necessary to account for the high degree of spatial and temporal inhomogeneity inherent in complex intermediate-range transport situations.

In their 1978 guidelines on air quality models, EPA recommended that simple Gaussian models be used as screening techniques for transport beyond 50 km, and that "more refined models" be considered only on a "case-by-case basis" (USEPA, 1978).

Given the uncertainty surrounding both the choice of an intermediate atmospheric transport model and data necessary for its application, we do not recommend a specific intermediate model. We do recommend that EPA sponsor further research on intermediate-range and long-range transport modeling of nonnuclear pollutants. This research should include both model development and adaption, as well as field validation studies to distances of at least 250 km.

### 2.2.3 Photochemical Transformation

Pollutants emitted from a synfuels facility may undergo photochemical transformations which significantly alter their chemical and physical nature. For some pollutants such as selected polycyclic aromatic hydrocarbons (PAH), transformation products may exhibit greater bioactivity than the parent pollutant (Pitts et al., 1980; National Academy of Sciences, 1972; USEPA, 1979). Other emitted pollutants, such as carbon monoxide (CO) or nitrous dioxide (NO<sub>2</sub>), oxidize to products that are less harmful or which have shorter atmospheric residence times.

#### 2.2.3.1 Chemical Removal Processes

To approximate chemical transformation processes which convert harmful pollutants to less harmful products, a first-order degradation constant which considers photolytic transformation and reactions with hydroxyl radicals (OH) and ozone (O<sub>3</sub>) will be used. This technique, based on those of Aravamudan et al. (1980) and Cupitt (1980), assumes that most

pollutant photochemical activity results from photolysis and oxidation by either OH or O<sub>3</sub>. A first-order rate constant K is found from the expression

$$K = \phi K_p + K_{OH}[\overline{OH}] + K_{O_3}[\overline{O_3}] \quad , \quad (2-9)$$

where

$\phi$  = the quantum yield of the photolysis,

$K_p$  = the photolysis rate constant for the pollutant,

$K_{OH}$  = the OH + pollutant reaction rate constant,

$K_{O_3}$  = the O<sub>3</sub> + pollutant reaction rate constant, and

$[\overline{OH}]$  and  $[\overline{O_3}]$  = average concentrations of OH and O<sub>3</sub>.

The rate and quantum yield of photolytic transformations are difficult to estimate and this process will be considered only when data are available.\* Rates of oxidation can be found in the literature (National Bureau of Standards, 1980) or through comparison with other chemical compounds of similar structure and properties. Approximations of average atmospheric concentrations of OH and O<sub>3</sub> are quite variable and dependent on many factors. Consequently, we intend to estimate  $[\overline{OH}]$

---

\*Photolysis is an important removal process only for chemicals which strongly absorb light within the solar radiation region of the lower troposphere; otherwise, reaction with OH or O<sub>3</sub> is likely to dominate the removal process (Cupitt, 1980).

and  $[O_3]$  by a procedure outlined below. Use of these average values within the rate expression for K will enable the second-order oxidation reactions to be approximated by a first-order rate. AIRDOS-EPA and RETADD-II can accommodate such a first-order treatment.

### 2.2.3.2 Photochemical Oxidants

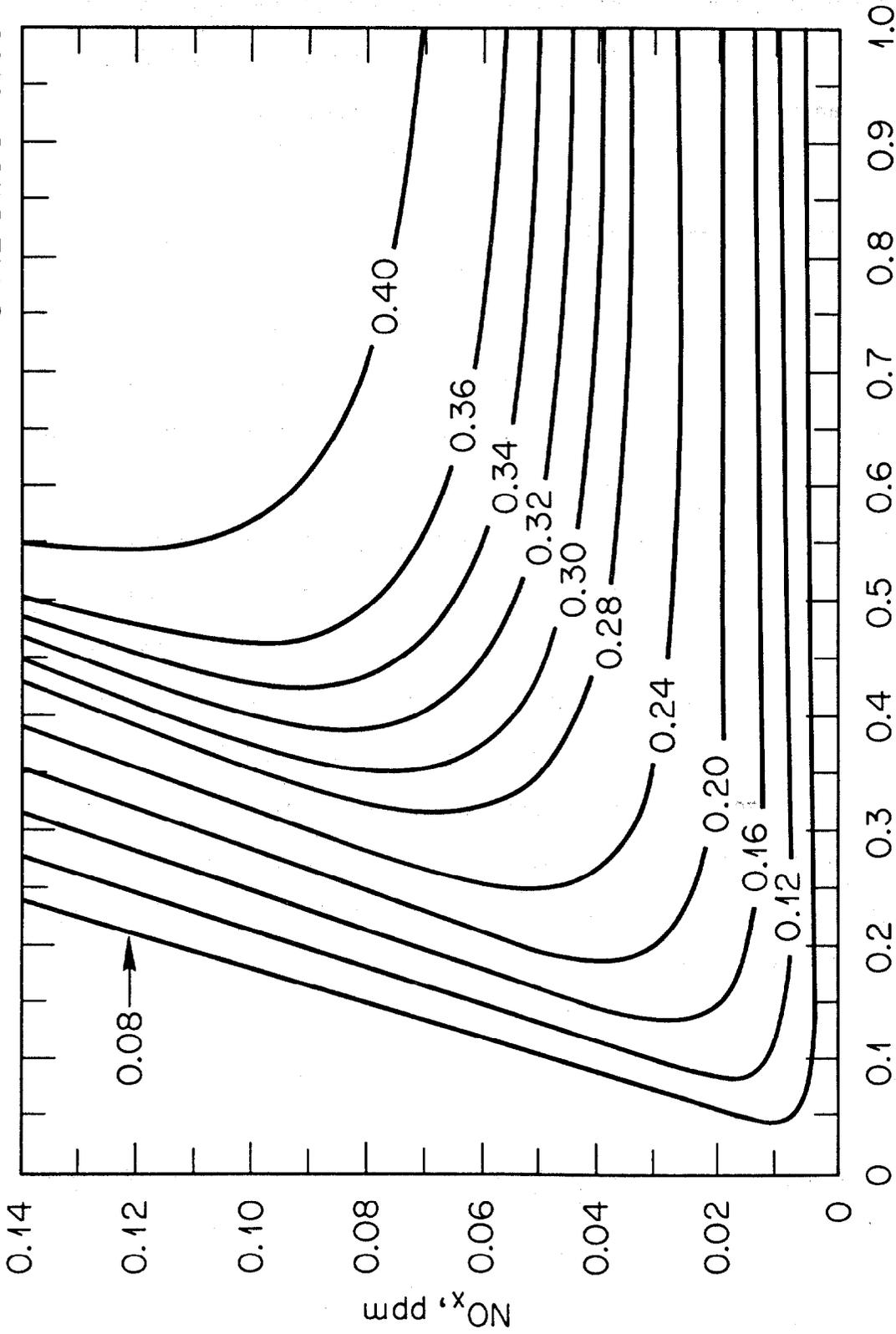
The Criteria Pollutant  $O_3$  is photochemically produced from oxides of nitrogen ( $NO_x$ ) and nonmethane hydrocarbon (HC) precursors. It is known that photochemical ozone production depends nonlinearly on  $NO_x$  and HC concentrations (see Figure 2-1 for a plot of an ozone-precursor surface). Light intensity profiles, initial hydrocarbon reactivities, and other photochemical mechanisms produce specific effects that alter the ozone-precursor surface. A simple mathematical model consisting of a few parameters that account for these effects has been developed by Holton and Jeffries (1979), and improved by Holton (1981).

The entire ozone-precursor surface can be described by the following two equations in L, the distance up the ridge line in ppm units and D, the distance to the left (negative) or right (positive) of the ridge line in ppm units:

for  $D \geq 0$ ,

$$[O_3] = (CL^N) \left[ 1.00 - \left( \frac{D}{L \tan \theta} \right)^G \right]^H, \quad (2-10)$$

ORNL-DWG 81-6956



HC, ppmC  
Figure 2-1

Ozone-precursor surface with indicated ozone isopleths as a function of HC and NO<sub>x</sub> precursors, generated using the Carbon-Bond II Mechanism with an initial olefin/paraffin ratio of 25/75 (Whitten et al., 1979).

and for  $D < 0$ ,

$$[O_3] = (CL^N) e^{-Q \frac{|D|}{L}} R, \quad (2-11)$$

where

$$L = [HC]_0 \cos \theta + [NO_x]_0 \sin \theta, \text{ and}$$

$$D = [HC]_0 \sin \theta - [NO_x]_0 \cos \theta,$$

and

$\theta$  is the ridge line angle,

C is the ozone produced for 1 ppm total reacting material on the ridge line, and

N, G, H, Q, and R are mechanism-dependent constants.

Equations (2-10) and (2-11), specialized to various conditions of mechanism surface, light profile, and hydrocarbon reactivity, are contained in Table 2-2.

Briefly, application of the photochemical methodology is as follows:

(1) From source term estimates of  $NO_x$  and HC releases, calculate  $[NO_x]$  and  $[HC]$  data pairs with AIRDOS-EPA using desired meteorological conditions (worst case, annual average, etc.). During these calculations, assume no degradation.

(2) From monitoring data on reference site, estimate background  $[O_3]$ ,  $[NO_x]$ , and  $[HC]$ . From source term and background data, estimate olefin fraction of HC in plume.

(3) After selecting conditions of mechanism surface, light profile and hydrocarbon reactivity, use appropriate equation from Table 2-2 to

Table 2-2. Evaluated mathematical models for eight ozone-precursor surfaces with measures-of-fit values (Holton, 1981)

Mechanism Surface	Light Profile	Hydrocarbon Reactivity	D ≥ 0.000 ppm				D < 0.000 ppm			
			Equation <sup>a,b,c</sup>	e <sup>b</sup>	r <sup>2</sup>	RMS <sup>d</sup>	Equation <sup>b,c,e</sup>	r <sup>2</sup>	RMS <sup>d</sup>	
Dodge-1	High	Medium	$[O_3] = 0.346 L^{0.688} [1 - (4.80 D/L)^{1.96}]^{0.483}$	11.8	1.000	0.002	$[O_3] = 0.346 L^{0.688} e^{-7.07( D /L)^{1.67}}$	0.988	0.011	
Dodge-2	Medium	Medium	$[O_3] = 0.282 L^{0.683} [1 - (5.49 D/L)^{1.97}]^{0.518}$	10.3	1.000	0.001	$[O_3] = 0.282 L^{0.683} e^{-9.11( D /L)^{1.68}}$	0.994	0.007	
Dodge-3	Low	Medium	$[O_3] = 0.186 L^{0.696} [1 - (7.11 D/L)^{1.98}]^{0.582}$	8.01	0.999	0.001	$[O_3] = 0.186 L^{0.696} e^{-24.97( D /L)^{2.01}}$	0.996	0.004	
CBII-4	High	Medium	$[O_3] = 0.608 L^{0.631} [1 - (4.17 D/L)^{1.67}]^{0.512}$	13.5	0.999	0.005	$[O_3] = 0.608 L^{0.631} e^{-4.67( D /L)^{1.40}}$	0.998	0.007	
CBII-5	Medium	Medium	$[O_3] = 0.504 L^{0.638} [1 - (4.72 D/L)^{1.66}]^{0.558}$	12.0	0.999	0.003	$[O_3] = 0.504 L^{0.638} e^{-5.43( D /L)^{1.49}}$	0.999	0.004	
CBII-6	Low	Medium	$[O_3] = 0.340 L^{0.655} [1 - (5.98 D/L)^{1.96}]^{0.765}$	9.49	0.999	0.002	$[O_3] = 0.340 L^{0.655} e^{-7.91( D /L)^{1.53}}$	0.999	0.003	
CBII-7	Medium	High	$[O_3] = 0.611 L^{0.629} [1 - (3.07 D/L)^{1.81}]^{0.751}$	18.0	0.998	0.007	$[O_3] = 0.611 L^{0.629} e^{-3.94( D /L)^{1.68}}$	0.999	0.004	
CBII-5	Medium	Medium	$[O_3] = 0.504 L^{0.638} [1 - (4.72 D/L)^{1.66}]^{0.558}$	12.0	0.999	0.003	$[O_3] = 0.504 L^{0.638} e^{-5.43( D /L)^{1.49}}$	0.999	0.004	
CBII-8	Medium	Low	$[O_3] = 0.418 L^{0.642} [1 - (6.90 D/L)^{1.65}]^{0.527}$	8.25	1.000	0.002	$[O_3] = 0.418 L^{0.642} e^{-8.37( D /L)^{1.38}}$	0.997	0.007	

<sup>a</sup>Mathematical model equation:  $[O_3] = CL^N \left[ 1 - \left( \frac{1}{\tan\theta} D/L \right)^G \right]^H$ .

<sup>b</sup> $L = [HC]_0 \cos\theta + [NO_x]_0 \sin\theta$ , where  $\theta$  is the ridge line angle,  $\arctan([NO_x]_0/[HC]_0)$ , in degrees.

<sup>c</sup> $D = [HC]_0 \sin\theta - [NO_x]_0 \cos\theta$ .

<sup>d</sup>Residual root mean square.

<sup>e</sup>Mathematical model equation:  $[O_3] = CL^N e^{-Q(|D|/L)^R}$ .

calculate  $[O_3]$ . Isopleth diagrams of Whitten et al. (1979) can be used to estimate  $[OH]$ .

(4) Use estimated  $[O_3]$  and  $[OH]$  together with Eq. (2-9) to calculate degradation rates for desired organic chemical.

(5) Rerun AIRDOS-EPA with calculated degradation rates to obtain atmospheric concentrations of desired organic chemicals.

#### 2.2.3.3 Other Secondary Products

To approximate production of aldehydes, ketones, hazardous gases, and nitrogen dioxide, isopleth diagrams (which express the compound of interest as a function of  $NO_x$  and HC) of Whitten et al. (1979) are used. These diagrams, in conjunction with HC- $NO_x$  dispersion modeling data and a detailed trajectory-type photochemical model (Jeffries, 1979), can be applied to estimate atmospheric concentrations of these harmful secondary products.

The transformation processes which convert "parent" compounds to more hazardous PAH "daughter" compounds are more difficult to approximate. Information on atmospheric transformations of PAH is scant and often conflicting (Andon et al., 1979). Accordingly, treatment of these processes is as follows. For PAH compounds with researched and identified degradation rates, degradation is approximated using the techniques of Aravamudan et al. (1980) and Cupitt (1980) described above. Where degradation information is not known, degradation possibilities are ignored. Reasons for this decision involve the large uncertainties of health risk associated with these compounds and the current inability to document the photochemical degradation composition and yield.

## 2.3 AQUATIC METHODOLOGY

### 2.3.1 Groundwater Transport

Contaminants produced by synfuel processes can enter groundwater either by direct release or by deposition from the atmosphere onto the ground with subsequent infiltration to the water table. Once in the ground, many contaminants interact strongly with soil. Such interactions can result in large fractions of the contaminants being adsorbed onto soil, thus greatly retarding their movement relative to that of groundwater. In addition, overall concentrations of many compounds in soil are decreased by various degradation processes during transport.

In this work, simple models to describe both the transport of the contaminants through the ground and their concurrent interactions with the soil were used. The emphasis is on models which include consideration of all important interactions and yet for which necessary data can be obtained or straightforwardly estimated.

#### 2.3.1.1 Contaminant-Soil Interactions

The soil is an exceedingly complex system. Not only is it composed of a solid, liquid, and gaseous phase, but each of these phases possess organic and inorganic constituents as well as inert and active compounds. This heterogeneous character strongly influences the physical and chemical properties of soil, thereby having a direct effect on solute transport and sorption in soil.

Given the total complexity of the solute-water-soil complex, a completely predictive simulation capability may never be possible. Nevertheless, significant progress has been made in understanding this complexity, and models formulated to date appear to provide a reasonably good basis for extrapolation and interpolation of data. There is a continuing need, however, to upgrade these methodologies as demand for accuracy and realism increases.

The transport of a reactive solute through soil is dependent on the rate of the sorptive-desorptive reaction between the soil solution and the solid phase. In general, this reaction can be either a kinetic one in which the relative amount of solute in the soil solution and in the soil matrix is changing with time, or it can be an equilibrium situation in which the above relationship is attained rapidly and thereafter remains constant. For a review of both kinetic and equilibrium sorption models for reactive solutes in soil, see Travis and Etnier (1981).

The simplest and most widely used sorption relationship is the linear adsorption isotherm. Here a linear equilibrium is assumed to exist between material in solution and that sorbed onto soil. Therefore, at any point the relative concentrations of a compound in the groundwater and in the soil may be given by

$$C_{\text{water}} = C_{\text{soil}}/K_d \quad (2-12)$$

where

$c_{\text{water}}$  = concentration of the compound in water ( $\mu\text{g}/\text{m}^3$ ),

$K_d$  = distribution coefficient for the compound in the particular soil under consideration ( $\text{m}^3/\text{kg}$ ), and

$c_{\text{soil}}$  = concentration of the compound in soil ( $\mu\text{g}/\text{kg}$ ).

In general,  $K_d$  reflects the amount of adsorption to the soil; consequently, it depends strongly on both the compound and the soil type. It is generally used to describe adsorption of inorganic compounds on soil. For most organics, it is possible to express their tendency for adsorption on soil in terms of a parameter which is largely independent of the properties of the soil. The concentration of organics is usually described using the parameter  $K_{oc}$ , the soil sorption coefficient for the compound relative to the organic carbon content of the soil; that is,

$$c_{\text{water}} = c_{\text{soil}}/K_{oc} \times (\text{fraction of organic carbon in soil}) . \quad (2-13)$$

The soil sorption coefficient of many organic compounds in soil and groundwater can be estimated from known physicochemical properties of the compounds. For instance,  $K_{oc}$  can be estimated from a regression equation if the octanol-water partitioning coefficient,  $K_{ow}$ , for the compound is known (Karickhoff, Brown, and Scott, 1979). If  $K_{ow}$  is not known, then  $K_{oc}$  can be estimated using the solubility of the compound in water (Chiou et al., 1977).

### 2.3.1.2 Concentration in Soil

Material which infiltrates into soil after deposition from the atmosphere is assumed to be uniformly concentrated within some depth  $d_{\text{soil}}$  of the surface. Consequently, for a steady deposition of a material onto the ground from the atmosphere, the net concentration of the material in the region below the surface can be given by

$$C_{\text{soil}} = \frac{R_d \times r}{(\lambda_{\text{surf}} + r)} \frac{1}{\lambda_{\text{soil}}} \frac{1}{d_{\text{soil}}} \frac{1}{P}, \quad (2-14)$$

where

$C_{\text{soil}}$  = concentration of the material in soil ( $\mu\text{g}/\text{kg}$ ),

$R_d$  = areal rate of atmospheric deposition on soil ( $\mu\text{g}/\text{m}^2 \cdot \text{s}$ ),

$r$  = fractional rate of infiltration into the root zone of the soil ( $\text{s}^{-1}$ ),

$\lambda_{\text{surf}}$  = net degradation constant for material very close to the surface of the soil ( $\text{s}^{-1}$ ),

$\lambda_{\text{soil}}$  = net degradation constant in soil ( $\text{s}^{-1}$ ),

$d_{\text{soil}}$  = depth in which infiltrated material is concentrated (m), and

$P$  = soil density ( $\text{kg}/\text{m}^3$ ).

### 2.3.1.3 Degradation of Organics in Soils

A number of interrelating factors govern persistence of organic molecules in soils. Chief among these are chemical structure and stability (Edwards, 1966). These characteristics control such physical processes as volatilization and photodecomposition (Merkle, 1972; Hamaker, 1972) and such biological activities as transfer across microbial cell membranes and induction of microfloral enzymes responsible for chemical transformation. The second most important determinant of degradation of organics is soil type, with its inherent characteristics of structure and sand/silt/clay content (Edwards, 1966). Soil organic matter is the main soil characteristic controlling degradation. Soil moisture and temperature also influence degradation, although less so than chemical structure and soil type.

The principal source of data describing degradation of organic chemicals in soils is the extensive literature produced on the fate of agricultural pesticides (Goring and Hamaker, 1972; Edwards, 1966; Upchurch, 1966). Focus on synfuel products has occurred only recently, and much new work is in progress (Ward, 1981; Strayer, 1981). It is expected that the mechanisms of soil degradation for potential synfuel releases will be similar to those already described for organic agricultural materials; however, reaction rates will depend on the specific molecule in question.

The most common function used to describe reaction kinetics of chemicals in soils is the "power rate model" (Hamaker, 1972):

$$\lambda_{\text{soil}} = - \frac{dc_{\text{soil}}}{dt} = kc_{\text{soil}}^n \quad , \quad (2-15)$$

where

$\lambda_{\text{soil}}$  = net degradation constant in soil ( $s^{-1}$ )

$c_{\text{soil}}$  = concentration of the material in soil ( $\mu\text{g}/\text{kg}$ ),

$k$  = rate constant, and

$n$  = order of the reaction.

This model assumes a homogeneous soil solution, where concentration of the reactants is the primary factor governing reaction. Estimates of  $n$  derived from experimental data range between 0.45 to 3.8, with most values  $>1.0$  (Hamaker, 1972). However, statistical reliability is considered too low for distinguishing these values from first order (Hamaker, 1972). Thus, the power rate model, with  $n = 1$ , will be used to estimate soil degradation. No generalized method for predicting the rate of degradation of organics in soil is currently available. Degradation rates for agricultural pesticides will be used as a guide.

#### 2.3.1.4 Transport from Localized Releases

A subsurface waterbody is modeled as a homogeneous medium of uniform depth  $d$ . Therefore, for a steady release  $b$  of a material into an aquifer or other subsurface waterbody, the concentration of the

material at a given location downstream (x,y) can be approximated (Bateman, 1954) by

$$c_{\text{water}} = \frac{b}{4\pi\sqrt{D_x D_y} a \epsilon d} e^{\frac{xu}{2D_x a}} K_0 \left[ \left( \frac{x^2}{D_x} + \frac{y^2}{D_y} \right)^{1/2} \left( \frac{u^2}{4D_x a} + \lambda \right) \right], \quad (2-16)$$

where  $D_x$  and  $D_y$  are the x- and y-components of the dispersion coefficient, respectively; u is the groundwater speed; a is the retardation factor of the compound relative to the groundwater movement (specifically,  $a \equiv [1 + (\rho/\epsilon) K_d]$ , where  $(\rho/\epsilon)$  is the ratio of the bulk density and the porosity of the soil);  $K_0[z]$  represents the modified Bessel function of the third kind for argument z; and  $\lambda$  is the decay constant of the compound in soil.

Of the parameters needed to estimate the concentration in the groundwater, only the distribution coefficients and the decay constants depend on the compound under consideration. As was previously indicated,  $K_d$ 's (and  $K_{oc}$ 's) describe the net effect of sorption and other related physicochemical processes. The decay constant,  $\lambda$ , describes the net effect of processes such as microbial degradation and chemical decomposition; it is not often available and is not generally predictable (Mill, 1978). Therefore, it will be included only for those few compounds for which specific data exist.\*

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\*Most of the limited data which are available are applicable only to regions near the ground surface.

### 2.3.2 Surface Water

Synfuels technologies will result in the release of a variety of contaminants into surface water. Since surface water transport of these pollutants may be an important pathway of exposure to the general public, (either through drinking water or aquatic food ingestion), it is necessary to estimate the extent that transport affects concentrations reaching human populations.

#### 2.3.2.1 Model Description

Concentrations of synfuels-derived contaminants in surface water are estimated using a simple steady-state model similar in concept to the EXAMS model (Baughman and Lassiter, 1978), but simpler in terms of process chemistry and environmental detail. It is analogous to the radionuclide transport model described by Niemczyk, Adams, and Murfin (1980). As in the EXAMS model, a river is represented as a series of completely mixed reaches. Within each reach, steady-state contaminant concentrations are estimated based on dilution and physical/chemical removal of contaminants from the water column. Figure 2.2 presents a schematic diagram of model compartments, transport pathways, and degradation processes associated with a typical river reach. The removal processes incorporated are volatilization, net adsorption, net settling, photolysis, and microbial degradation. If no reliable literature information is available for any of the removal processes for a particular contaminant, that removal rate is set to zero. If all removal processes are set to zero, the approach degenerates to a simple dilution model.

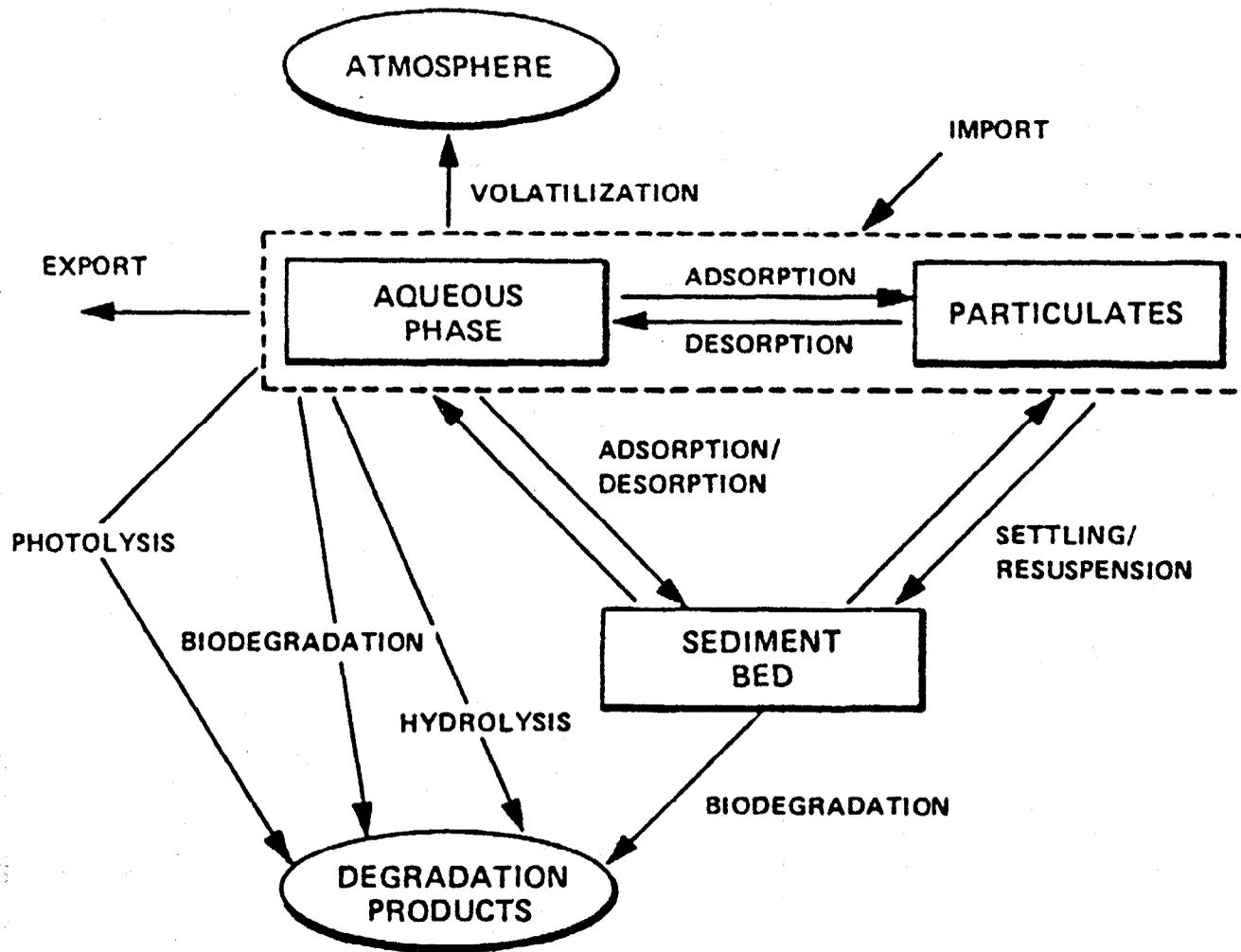


Figure 2-2. Compartments, exchanges, transformations, and sinks affecting contaminant fate in aquatic systems.

Reference values for environmental parameters employed in the model are presented in Chapter 3. Contaminant properties employed include molecular or atomic mass, aqueous solubility, octanol-water partition coefficient, quantum yield of direct photolysis, and microbial degradation rate. These properties are chemical-specific and are not presented in this report.

The steady-state contaminant concentration ( $C_{w,n}$ ) in the  $n^{\text{th}}$  reach downstream of a continuous discharge is given by

$$C_{w,n} = (I/V_n) / [(Q_n/V_n) + k_{t,n}] \quad (2-17)$$

where

$I$  = contaminant input rate (kg/s),

$V_n$  = volume of reach  $n$  ( $m^3$ ),

$Q_n$  = streamflow leaving reach  $n$  ( $m^3/s$ ), and

$k_{t,n}$  = total removal rate ( $s^{-1}$ ).

The overall or total removal rate ( $k_{t,n}$ ) is equal to the sum of removal rates due to volatilization ( $k_v$ ), adsorption to the sediment surface ( $k_a$ ), settling ( $k_s$ ), and direct photolysis ( $k_p$ ). Models used to calculate these rate constants are described in the following sections.

#### 2.3.2.2 Volatilization

The rate of removal of a contaminant due to volatilization from the water-column of a stream at the air-water interface is given by

$$k_v = k_m F_d / D_w \quad (2-18)$$

where

$k_v$  = the rate constant for volatilization ( $s^{-1}$ ),

$k_m$  = the overall mass transfer rate (m/s),

$F_d$  = the fraction of contaminant dissolved in the water column (unitless), and

$D_w$  = the depth of stream channel (m).

The mass transfer rate,  $k_m$ , can be estimated (Southworth, 1979) using

$$k_m = H_c k_g k_l / (H_c k_g + k_l) \quad , \quad (2-19)$$

where

$H_c$  = The Henry's Law coefficient (unitless),

$k_g$  = the gas phase mass transfer rate (m/s), and

$k_l$  = the liquid phase mass transfer rate (m/s).

These parameters must either be supplied from scientific literature or be approximated. Henry's Law constant,  $H_c$ , can be approximated using the method of Dilling (1977), and the transfer rates  $k_g$ , and  $k_l$ , can be computed using the method of Southworth (1979). These formulae are

$$H_c = 16.04 P_v M / T_w S_w \quad , \quad (2-20)$$

$$k_g = 1137.5 (V_w + V_c) (18/M)^{1/2} \quad , \quad (2-21)$$

$$k_l = 23.51 (V_c^{0.969} / D_w^{0.673}) (32/M)^{1/2} \quad . \quad (2-22)$$

where

$P_v$  = the vapor pressure of the contaminant (mm Hg),

$M$  = the molecular weight of the contaminant (g/mole),

$T_w$  = the temperature of stream water ( $^{\circ}K$ ),

$S_w$  = the solubility of the contaminant ( $\mu g/L$ ),

$V_w$  = wind velocity immediately above the water (m/s), and

$V_c$  = stream current velocity (m/s).

The fraction of contaminant dissolved in the water-column ( $F_d$ ) is

$$F_d = 1/(K_d C_{ss} + 1) \quad (2-23)$$

where

$K_d$  = the soil distribution coefficient (L/g), and

$C_{ss}$  = the suspended solids load (g/L).

The fraction of the total contaminant load adsorbed to suspended particles ( $F_a$ ) is given by

$$F_a = 1 - F_d = K_d C_{ss} / (K_d C_{ss} + 1) \quad (2-24)$$

### 2.3.2.3 Adsorption

The extent of sorption of hydrophobic solutes in water at solid-liquid interfaces is inversely proportional to the solute's water solubility: Low water solubility results in high sorption potential.

If the adsorption distribution coefficient,  $K_d$ , is not known, it may be estimated by use of the octanol-water distribution coefficient for the solute. The partitioning of contaminant between aqueous solution and particulate surface is a function of the hydrophobicity of the contaminant as indicated by its octanol-water partition coefficient,  $K_{ow}$ , and the fraction of organic carbon in particulates,  $F_{oc}$ . The distribution coefficient,  $K_d$ , may be estimated for organic contaminants using the method of Karickhoff, Brown, and Scott (1979):

$$K_d = 0.63 K_{ow} F_{oc} \quad (2-24)$$

The adsorption of contaminant to sediment is analogous to mass transfer at the air-water interface. A first-order rate expression for this mass transfer is

$$-dC_w/dt = (k_l D_w) / [1 - (C_{sed} P_w / K_d C_w F_d)] C_w F_d \quad (2-25)$$

where

- $C_w$  = the concentration of contaminant in the water column (g/L),
- $k_l$  = the liquid phase mass transfer rate (m/s),
- $D_w$  = Depth of stream channel (m),
- $C_{sed}$  = the concentration of the contaminant in sediment (g/g),
- $P_w$  = the density of water (g/m<sup>3</sup>),
- $K_d$  = the soil distribution coefficient (g/m<sup>3</sup>), and
- $F_d$  = the fraction of contaminant dissolved.

In absence of contaminant biodegradation in sediment, the steady-state removal rate of the contaminant would be zero (Southworth, 1979). If microbial degradation occurs, the degradation rate ( $\text{g}\cdot\text{cm}^{-2}\cdot\text{s}^{-1}$ ) per  $1\text{ cm}^2$  of interface is

$$\text{degradation rate} = k_b C_{\text{sed}} P_s D_s \quad (2-26)$$

where

$k_b$  = the rate constant for biological degradation by microbial activity ( $\text{s}^{-1}$ ),

$P_s$  = the density of sediment ( $\text{g}/\text{cm}^3$ ), and

$D_s$  = the depth of biologically active sediment (cm).

Adsorption rate per  $1\text{ cm}^2$  interface is

$$\text{adsorption rate} = k_1 [1 - (C_{\text{sed}}/K_d C_w F_d)] C_w F_d P_w \quad (2-27)$$

where

$k_1$  = the mass transfer rate of contaminant in the liquid phase (m/s), and

$P_w$  = the density of water ( $\text{g}/\text{cm}^3$ ).

At steady state, the degradation rate equals the adsorption rate; therefore,

$$C_{\text{sed}} = K_d k_1 C_w F_d / (K_d k_b D_s P_s + k_1 P_w) \quad (2-28)$$

Substituting this expression for  $C_{sed}$  into Eq. (2-25) yields

$$-dC_w/dt = (k_1/D_w)[1 - k_1 P_w / (k_1 P_w + K_d k_b D_s P_s)] C_w F_d \quad (2-29)$$

The removal rate constant for adsorption to sediment  $k_a (s^{-1})$  is thus

$$k_a = (k_1/D_w)[1 - k_1 P_w / (k_1 P_w + K_d k_b D_s P_s)] F_d \quad (2-30)$$

#### 2.3.2.4 Settling

Removal of contaminant from the water-column by sedimentation of particulates containing adsorbed contaminant is a function of settling and resuspension velocities of particulates ( $V_s$  and  $V_r$ , respectively), and of the contaminant load on particulates. Change in water-column contaminant concentration due only to settling (resuspension of particulates not considered) is

$$-dC_w/dt = C_w F_a V_s / D_w \quad (2-31)$$

Settling velocity,  $V_s$ , is calculated from Stoke's Law:

$$V_s = 2gr^2(P_s - P_w)/9\eta \quad (2-32)$$

where

$g$  = the gravitational acceleration constant ( $cm.s^{-2}$ ),

$r$  = the radius of suspended particles (cm), and

$\eta$  = the coefficient of viscosity of water ( $dyne.s.cm^{-2}$ ).

Resuspension of particulates increases the concentration of contaminant in the water-column, with the rate of change given by

$$-dC_w/dt = -C_w F_r V_r / D_w \quad (2-33)$$

where

$F_r$  = the fraction of contaminant adsorbed to resuspended particles (unitless).

Thus, the equation for the net settling removal rate constant  $k_s$  ( $s^{-1}$ ) is

$$k_s = (F_a V_s - F_r V_r) / D_w \quad (2-34)$$

Estimates of resuspension velocities are difficult to obtain. However, investigation of two scenarios provides limits of net settling rate:

(a) no resuspension ( $V_r = 0$ ); and (b) no net sedimentation ( $V_s F_a = V_r F_r$ ).

For settling scenario 1, Eq. (2-34) simplifies to

$$k_s = F_a V_s / D_w \quad (2-35)$$

For the second scenario,  $k_s = 0$ .

#### 2.3.2.5 Direct Photolysis

The rate of direct photolysis of a contaminant in an aqueous solution is a function of effective incident radiation, quantum yield of reaction, and the absorption spectrum of the contaminant. In natural waters

attenuation of incident solar radiation by materials in water reduces effective incident radiation. Light attenuation is a function of the concentration and absorptive characteristics of dissolved and suspended substances, the suspended solids load in the water-column, and the depth of the column.

The method used to estimate direct photolysis is based on the model developed by Zepp and Cline (1977), as modified by Southworth (1979). The rate of decrease of water-column contaminant concentration due to direct photolysis is

$$-dC_w/dt = \Phi k'_p C_w F_d \quad (2-36)$$

where

$\Phi$  = the quantum yield of direct photolysis (%), and

$k'_p$  = the light absorption factor ( $s^{-1}$ ).

Thus, the first-order photolysis rate constant is given by

$$K_p = \Phi k'_p F_d \quad (2-37)$$

It is assumed that  $\Phi$  is independent of wavelength. Zepp and Cline (1977) developed two scenarios for calculating the light absorption factor,  $k'_p$ , depending on the depth and turbidity of the water body of interest. Because synfuel production facilities will likely be sited on large, turbid rivers, we have adopted Zepp and Cline's first scenario, which assumes that all sunlight is absorbed. Under this

assumption,  $k_p'$  is given by

$$k_p' = (\Sigma W_\lambda E_\lambda) / j D_w A \quad (2-38)$$

where

$W_\lambda$  = the intensity of light at wavelength  $\lambda$   
(photons  $\cdot$  cm $^{-2}$   $\cdot$  s $^{-1}$ ),

$E_\lambda$  = the molar extinction coefficient at  
wavelength  $\lambda$  (cm  $\cdot$  L  $\cdot$  moles $^{-1}$ ),

$j$  = the photo-intensity conversion factor  
(6.02E + 20 photons  $\cdot$  cm $^{-1}$   $\cdot$  L  $\cdot$  moles $^{-1}$ ), and

$A$  = the light attenuation coefficient (cm $^{-1}$ ).

The molar extinction coefficients,  $E_\lambda$ , are contaminant-specific and must be experimentally determined. The corresponding light intensity factors,  $W_\lambda$ , which are latitude- and season-dependent, can be obtained from Table II of Zepp and Cline (1977). The light attenuation coefficient,  $A$ , accounts for the absorption of light by suspended and dissolved material in the water body. Light attenuation varies with wavelength; we have adopted the procedure of Southworth (1979) of estimating  $A$  at the absorption peak of the contaminant being modeled. In the absence of empirical measurements of attenuation, we assume that  $A$  is inversely proportional to the suspended solids load ( $D_{SS}$ ). This assumption is consistent with data obtained by Southworth (1979) using suspensions of 2  $\mu$ m clay particles.

## 2.4 FOODCHAIN METHODOLOGY

### 2.4.1 Terrestrial Food Chains

After contaminants are released by synfuel technologies, they may enter terrestrial food chains and pose health risks to man via ingestion of contaminated foods. For our initial estimation of health risks associated with synfuel technologies, we will consider exposure pathways involving drinking water, agricultural produce, beef, and milk. These pathways include a substantial portion of the human diet (Rupp, 1980) and should provide a representative estimation of the health risks associated with synfuel compounds entering the food chain.

#### 2.4.1.1 Drinking Water

The concentration of a given pollutant in drinking water may be given as

$$C_{dw} = C_{sw} PF \quad , \quad (2-39)$$

where

$C_{dw}$  = the concentration of a compound in drinking water (g/L),

$C_{sw}$  = the concentration of a compound in the source water  
(ground or surface waters) (g/L), and

PF = the processing factor due to treatment of the  
source water (unitless).

For organic compounds, water treatment consists primarily of the removal of sediment (Niemczyk, Adams and Murfin, 1980). For inorganic compounds, treatment results in both sediment removal and ion exchange (Fletcher and Dotson, 1971; Denham and Soldat, 1975; Soldat, Robinson, and Baker, 1974; USNRC, 1977).

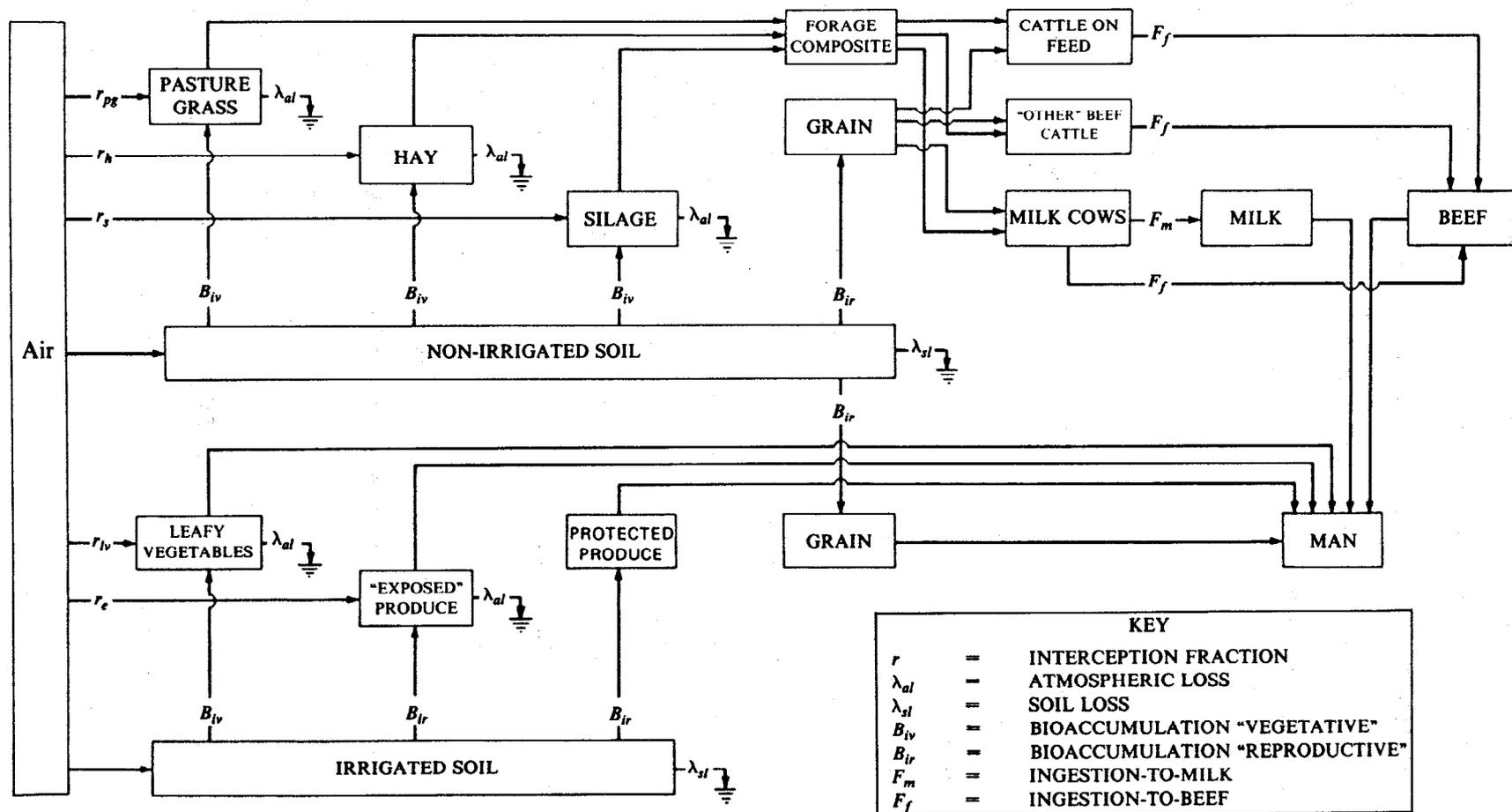
#### 2.4.1.2 Agricultural Foodchains

The assessment methodology for synfuels is derived from approaches previously used for assessment of radionuclides (USNRC, 1977; Baes et al., 1983a; Baes et al., 1983b), based on an analysis of agricultural practice in the United States (Shor, Baes, and Sharp, 1982). The methodology described below allows for a default data base of site-specific agricultural, meteorological, and land use parameters (Baes et al., 1983b) to be coupled with the basic transport equations. It should be stressed that the foodchain methodology presented here is preliminary.

The conceptual agricultural foodchain is summarized by Figure 2-3. Briefly, root uptake pathways for four food crop and four feed crop categories, direct deposition onto edible plant surfaces for two food crop and three feed crop categories, transport to three cattle types producing beef, and transport to cow's milk are considered. Also included are considerations for irrigated and nonirrigated soil, and differences in root uptake for "vegetative" (leafy) and "reproductive" (fruit) plant parts. The following sections discuss the relationships among compartment of the foodchain model.

Figure 2-3.

CONCEPTUAL GENERIC TERRESTRIAL FOODCHAIN



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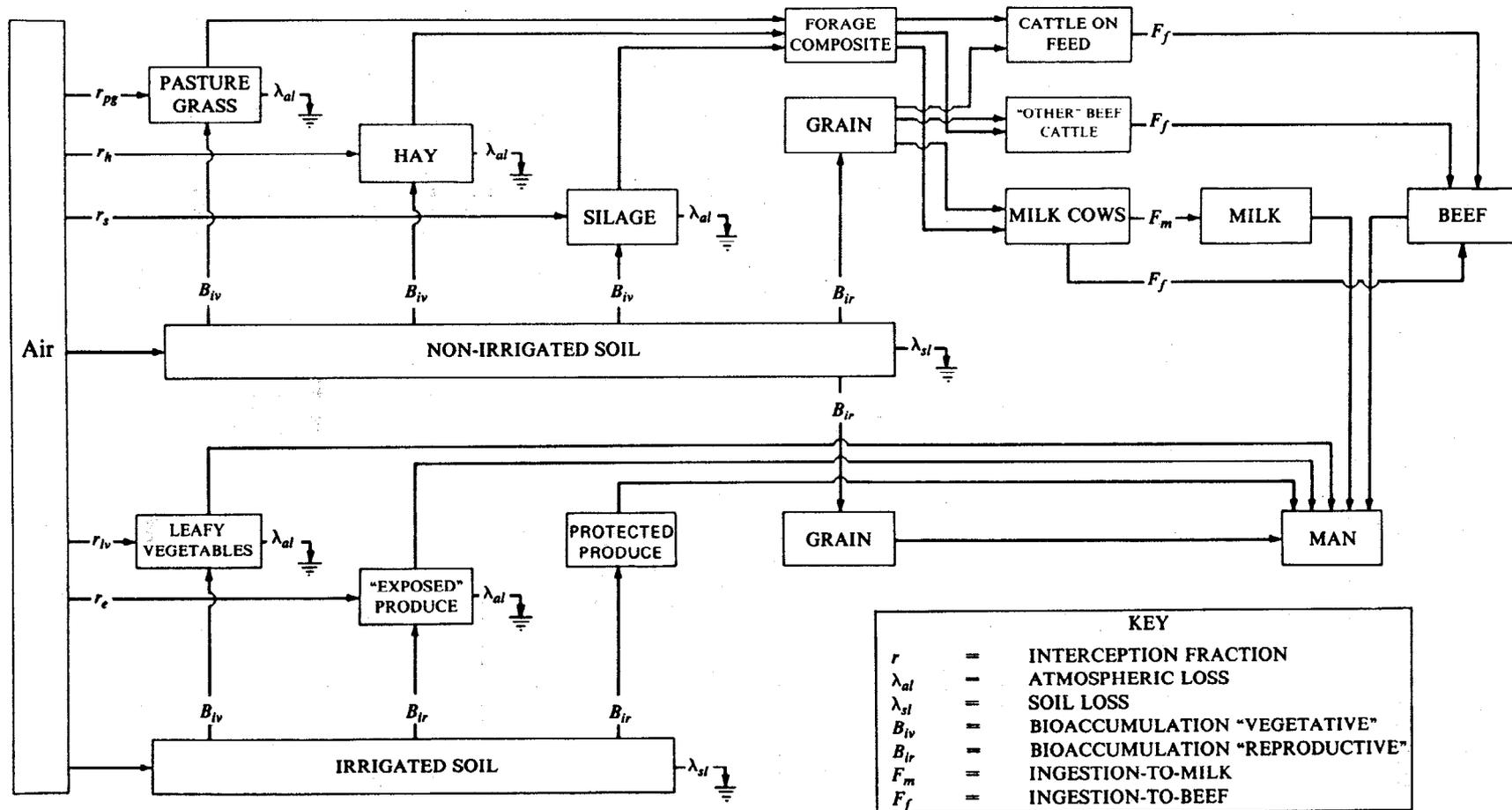
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Figure 2-3.

CONCEPTUAL GENERIC TERRESTRIAL FOODCHAIN



### Accumulation in Soil

The accumulation of synfuel compounds in soil is calculated for both irrigated and nonirrigated agricultural soils in preparation for calculation of root uptake by food and feed crops via

$$C_s = \frac{D[1 - \exp(-\lambda_s t_b)]}{10 \rho d \lambda_s}, \quad (2-40)$$

where

$C_s$  = the concentration of a compound in root zone soil  
( $\mu\text{g}/\text{kg}$ ,

$D$  = the ground-level deposition rate of a compound  
( $\mu\text{g}/\text{m}^2 \cdot \text{s}$ ),

$\lambda_s$  = the sum of all soil removal rate constants ( $\text{s}^{-1}$ ),

$t_b$  = the period of long-term buildup in soil, equal to the  
length of time that the source term is in operation (s),

$10$  = a conversion factor from  $\text{g}/\text{cm}^2$  to  $\text{kg}/\text{m}^2$  [ $(10,000 \text{ cm}^2/\text{m}^2)$   
( $1 \text{ kg}/1000 \text{ g}$ )],

$\rho$  = soil bulk density ( $\text{g}/\text{cm}^3$ ), and

$d$  = the depth of the root zone (cm).

The ground-level deposition rate,  $D$ , is output by either the short-range (<50 km) atmospheric dispersion code AIRDOS-EPA or the long-range (>250 km) atmospheric dispersion code RETADD-II. The time ( $t_b$ ) over which long-term buildup in the soil (equal to the time that the source term is in operation) occurs is currently assumed to be 35 y ( $1.08 \times 10^9$  s).

The removal rate constant,  $\lambda_s$ , is given by

$$\lambda_s = \lambda_l + \lambda_d + \lambda_r \quad , \quad (2-41)$$

where

$\lambda_l$  = loss constant due to leaching of material from the root zone ( $s^{-1}$ ),

$\lambda_d$  = loss constant due to degradation (biological, chemical, etc.) of material in soil ( $s^{-1}$ ), and

$\lambda_r$  = loss constant due to radiological decay ( $s^{-1}$ ).

The leaching removal rate constant is specified for either irrigated or nonirrigated soil. For irrigated agricultural soil the leaching constant,  $\lambda_l$  ( $s^{-1}$ ), is given by

$$\lambda_l = \frac{P + I - E}{\theta d [1 + (\frac{\rho}{\theta} K_d)] 3.16 \times 10^7} \quad , \quad (2-42)$$

where

P = annual average total precipitation (cm/y),

E = annual average evapotranspiration (cm/y),

I = annual average irrigation (cm/y),

d = soil depth from which leaching removal occurs (15 cm),

$K_d$  = the distribution coefficient (ml/g),

$\rho$  = soil bulk density ( $g/cm^3$ ),

$\theta$  = soil volumetric water content ( $ml/cm^3$ ),

$3.16 \times 10^7$  = the number of seconds in a year (s/y).

For nonirrigated soils, the numerator of Eq. (2-42) is (P - E). P, I, and E are read in from a data base (SITE) of site-specific information

(Baes et al., 1983b) in units of millimeters per year and converted to centimeters per year in Eq. (2-42).

### Accumulation in Plants

The food and feed plant categories shown in Fig. 2-3 are based on previous work by Shor, Baes, and Sharp (1982). Leafy vegetables present a broad, flat leaf surface for direct interception of depositing material. "Exposed" produce such as snap beans, tomatoes, and apples present edible surfaces for direct deposition pathways, but, in general, edible portions have reproductive functions and are associated with significantly different soil-plant uptake parameters than leafy or vegetative plant parts. "Protected" produce such as potatoes, peanuts, and citrus fruits do not have edible plant parts exposed to direct atmospheric deposition. Like "exposed" produce, edible portions are not vegetative in nature.

The general equation for contamination of plants by synfuels compounds is given by

$$C_p = \frac{Dr_p[1.0 - \exp(-\lambda_a t_e)]}{Y_p \lambda_a} + BC_s, \quad (2-43)$$

where

$C_p$  = the concentration of a compound in edible plant material  
( $\mu\text{g}/\text{kg}$ ),

$r_p$  = the fraction of depositing material initially intercepted  
by the plants (unitless),

$\lambda_a$  = the sum of all atmospheric loss constants ( $\text{s}^{-1}$ ),

$t_e$  = the time that above-ground plant parts are exposed to

depositing material (s),

$Y_p$  = the standing crop biomass or yield of the plant ( $\text{kg}/\text{m}^2$ ), and

$B$  = the soil/plant bioaccumulation factor ( $B_v$  or  $B_r$ , as described below) for root uptake pathways (unitless).

As shown in Fig. 2.3, leafy vegetables and "exposed" and "protected" produce are assumed to be grown on irrigated soils, and all other food and feed crops are assumed to be grown on nonirrigated soils. The respective soil concentrations, calculated via Eq. (2-40) are used to calculate the root uptake component of Eq. (2-43). The parameter  $B$  is either the vegetative plant part/soil ( $B_v$ ) or reproductive plant part/soil ( $B_r$ ) concentration factor (as described in Baes et al., 1983a), depending on the food or feed crop being simulated (fig. 2-3). The parameters  $B_v$  and  $B_r$  are given by

$$B_v = \frac{C_v}{C_s}, \quad (2-44)$$

and

$$B_r = \frac{C_r}{C_s}, \quad (2-45)$$

where

$C_v$  = the concentration of a compound in "vegetative" plant parts (leaves, straw, etc.) at edible maturity due to root uptake ( $\mu\text{g}/\text{kg}$ , dry weight), and

$C_r$  = the concentration of a compound in "reproductive" plant parts (fruits, seed, etc.) at edible maturity due to root uptake ( $\mu\text{g}/\text{kg}$ , dry weight).

For food crops  $C_p$  is converted to a fresh weight equivalent value using dry/fresh weight conversion factors for each food category after solving Eq. (2-43). Feed crop concentrations, however, are in dry weight.

The atmospheric loss constant,  $\lambda_a$ , is the sum of all losses due to weathering ( $\lambda_w$ ), degradation, including photodegradation ( $\lambda_{ad}$ ), or radiological decay ( $\lambda_r$ ). Thus,

$$\lambda_a = \lambda_w + \lambda_{ad} + \lambda_r \quad (2-46)$$

In Eq. (2-43), the interception fraction  $r_p$  modifies the ground-level deposition rate to account for the fraction of depositing material intercepted by the edible plant surface. Default crop category-specific interception fractions based on a theoretical analysis of field crop geometries (Baes et al., 1983b) are

$$r_{lv} = 1.0 - \exp(-0.0846 Y_{lv}) \quad (2-47)$$

$$r_e = 1.0 - \exp(-0.0260 Y_e) \quad (2-48)$$

$$r_s = 1.0 - \exp(-0.769 Y_s) \quad (2-49)$$

and

$$r_{pg \text{ or } h} = 1.0 - \exp(-2.88 Y_{pg \text{ or } h}) \quad (2-50)$$

where the subscripts lv, e, s, pg, and h refer to leafy vegetables, "exposed" produce, silage, pasture grasses, and hay, respectively.

The productivity value converts an input per square meter to a per kilogram basis. Productivity estimates for each crop category are obtained from the SITE data base.

### Accumulations in Milk and Beef

The transport of synfuels compounds to milk and beef may be calculated according to

$$C_m = \frac{(Q_g C_g + Q_f C_f) f_{tm} [1 - \exp(-\lambda_m t_m)]}{3.16 \times 10^7 \text{ mp } \lambda_m}, \quad (2-51)$$

$$C_b = \frac{(Q_g C_g + Q_f C_f) f_{tb} [1 - \exp(-\lambda_b t_b)]}{3.16 \times 10^7 \text{ bp } \lambda_b}, \quad (2-52)$$

where

$C_m$  and  $C_b$  = the concentration of a compound in milk and beef, respectively ( $\mu\text{g}/\text{kg}$ ),

$Q_g$  and  $Q_f$  = consumption rate of grain and forage, respectively, by a milk cow or beef cattle ( $\text{kg}/\text{y}$ ),

$C_g$  and  $C_f$  = the concentration of a compound in grain and forage, respectively, ( $\mu\text{g}/\text{kg}$ ),

$f_{tm}$  and  $f_{tb}$  = the fractional transfer of ingested compound to milk and beef, respectively (-),

$\lambda_m$  and  $\lambda_b$  = the metabolic turnover rate of a compound in milk and beef, respectively ( $\text{s}^{-1}$ ),

$t_m$  and  $t_b$  = the time at which milk and beef, respectively, are sampled (s), and

mp and bp = the quantity of milk or beef produced per milking or slaughter, respectively (kg).

Because of the limitations of existing data on  $f_{tm}$  and  $f_{tb}$  and because equilibrium is assumed, the relationships given by

$$F_m = \frac{f_{tm}}{86,400 \text{ mp } \lambda_m} \quad (2-53)$$

and

$$F_f = \frac{f_{tb}}{86,400 \text{ bp } \lambda_b} \quad (2-54)$$

where

$F_m$  and  $F_f$  = the fraction of daily ingested compound which appears in milk and beef, respectively, at equilibrium (d/kg),  
and

86,400 = the number of seconds in a day (s/d),

are substituted into the equilibrium forms of Eqs. (2-51) and (2-52) to give

$$C_m = \frac{(Q_g C_g + Q_f C_f) F_m}{365.2422} \quad (2-55)$$

and

$$C_b = \frac{(Q_g C_g + Q_f C_f) F_f}{365.2422} \quad (2-56)$$

where 365.2422 is the number of days in a year (at equilibrium  $[(1 - \exp(-\lambda_m t_m))] = 1.0$ ).

The feed concentrations  $C_g$  and  $C_f$  are calculated via Eq. (2-43). The forage concentration is actually a weighted average of the concentrations calculated for hay, silage, and pasture (Fig. 2-3). The weighting factors are based on production of these forages at the given location. Hay and silage production are taken from the SITE data base and pasture production is calculated according to the method of Shor, Baes, and Sharp (1982) from inventories of cattle and sheep supplied from SITE.

#### 2.4.1.3 Parameters Estimation

For the heavy metals, the parameter values ( $K_d$ ,  $B_v$ ,  $B_r$ ,  $F_m$ ,  $F_f$ ) can be obtained from the review of transfer coefficients by Baes et al. (1983b). For all other compounds, values for these parameters are based on structure activity relationships. For the parameters  $K_d$  (Briggs, 1981),  $B_v$  (Baes, 1982), and  $F_m$  and  $F_f$  (Kenega, 1980), the relationships are

$$\log K_d = -0.99 + 0.53(\log K_{ow}) \quad , \quad (2-57)$$

$$\log B_v = 2.71 - 0.62(\log K_{ow}) \quad , \quad (2-58)$$

$$\log F_m = -6.12 + 0.50(\log K_{ow}) \quad , \quad (2-59)$$

and

$$\log F_f = -5.15 + 0.50(\log K_{ow}) \quad . \quad (2-60)$$

For  $F_m$  and  $F_f$ , the relationship between  $\log K_{ow}$  and the bioaccumulation factor for fat (BCF) was used. Using the fat contents of milk and beef (Spector, 1956), the relationships given in Eqs. (2-59) and (2-60) were derived. For the initial assessment, it was assumed that  $B_r = 0.1 B_v$  (Baes et al., 1983b).

#### 2.4.2 Aquatic Food Chains

The concentration of a compound in a product  $f_j$  derived from aquatic organism  $f_r$  can be written as a simple multiplicative chain:

$$c_{f_j} = (c_{\text{surface water}}) \times (CF)_{f_k} \times (PF)_{f_j/f_k}, \quad (2-61)$$

where

$(c_{\text{surface water}})$  = steady-state concentration of  
contaminant in surface water,

$(CF)_{f_k}$  = bioconcentration factor, defined as the ratio  
of the steady-state concentration of contaminant  
in the organism (whole body or reference organ)  
to the concentration in water, and

$(PF)_{f_j/f_k}$  = food processing factor, defined as the ratio of  
the concentration of contaminant in the  
food product to the whole-body or reference  
organ concentration.

Bioconcentration factors for organic compounds are estimated using empirical equations that relate the potential bioconcentration of a compound to its octanol-water partitioning coefficient (Kenaga and Goring, 1980; Mackay, 1982). Although these structure-activity relationships provide only crude approximations to measured values, they are useful for distinguishing between compounds with high and low potential for bioaccumulation (Trabalka and Garten, 1982).

Similar structure-activity relationships have not been developed for inorganic compounds. For radionuclides and other trace elements, bioconcentration factors are obtained from experimental measurements. Estimates suitable for use in risk analysis are available for arsenic (Sorensen, 1976), cadmium (Fulkerson and Goellar, 1973), lead (Killough and McKay, 1976; International Atomic Energy Agency, 1982), mercury (Huckabee et al., 1979), nickel (Killough and McKay, 1976; International Atomic Energy Agency, 1982), and radium (Killough and McKay, 1976; Blaylock, 1982; International Atomic Energy Agency, 1982; Stegnar and Kopal, 1982).

The processing factor for organic compounds can usually be estimated from a knowledge of the distribution of fat within the organism and/or its by-products. For any inorganic compounds, the processing factor is taken to be 1.

### 2.4.3 Estimation of Food Consumption Rates

To estimate risks to man via the food chain exposure pathway, intake rates for contaminants in the various food categories are calculated by

$$I_f = C_f R_f \quad , \quad (2-62)$$

where

$I_f$  = the intake rate of a compound ( $\mu\text{g}/\text{y}$ ) in food  $f$ ,

$C_f$  = the concentration of a compound in food  $f$  ( $\mu\text{g}/\text{kg}$ ), and

$R_f$  = the consumption rate of food  $f$  by the average individual ( $\text{kg}/\text{y}$ ).

For the initial synfuels risk assessment, food consumption rates developed by the Environmental Protection Agency's Office of Radiation Programs (EPA-ORP) for food categories corresponding to those used in the food chain exposure assessment were used (Nelson, 1982). These consumption rates are based on an analysis of a recent Department of Agriculture food consumption survey. The average consumption rates are given in Table 2-3.

Table 2-3. Annual-average individual food consumption rates

Item	Consumption rate (kg/y)	Item	Consumption rate (kg/y)
Total vegetables	178	Total meat	65
Leafy vegetables	14	Beef	33
"Exposed" produce	30	Pork	11
"Protected" produce	56	Poultry	11
Grain	75	Misc.	10
Total dairy	112	Fish	6.5
Total water	519	Eggs	10

### 3. REFERENCE SITES

#### 3.1 INTRODUCTION

In order to estimate the magnitudes of the potential impacts of synthetic fuels technologies it is necessary to have a description of the environment surrounding the facilities. Such a description should provide a range of parameters for input into the environmental transport methodologies described in Section 2.

The direct and indirect coal liquefaction technologies and the oil-shale synfuel technology will probably be developed in distinctly different regions of the United States. In particular, coal liquefaction plants are expected to be concentrated in the east, while oil shale plants will tend to be restricted to the west. This section will provide a generic characterization of both an eastern and a western synfuel site.

The reference environments discussed in this document do not correspond to specific locations. Instead, they are each based on consideration of large areas in which each of the technologies are most likely to be located. Thus, the reference environments represent composites of many possible sites, some of which may vary substantially in certain characteristics from the composites. The descriptions of the environments and the associated populations-at-risk have been based largely on consideration of the quantitative descriptions provided in Olson, Emerson, and Nungesser (1980); Shor, Baes, and Sharp (1982); and USDA (1980).

## 3.2 COMPONENTS OF REFERENCE ENVIRONMENTS

### 3.2.1 Introduction

The feasibility of siting a synfuels facility at a particular location is generally determined by availability of two important resources: an ample source of synfuels feed stock and a reliable supply of water. These factors were considered in the selection of the reference environments. In addition, sites recently suggested for construction of synfuels facilities were deemed particularly representative of future synfuels sites, and were included in our analysis of reference environments.

The characterization of generic environments is divided into three components: the physical environment, and the ecological and human populations at risk.

### 3.2.2 Physical Environment

Synfuel technologies will result in environmental release of a variety of particulate, gaseous, and aqueous pollutants. Dispersion of these pollutants through the environment will be influenced by the dominant physical characteristics of the environment. Important physical characteristics include terrain, meteorology, and surface and subsurface hydrologies. Specific parameters related to the physical environment will be discussed below for both the eastern and western synfuel sites.

### 3.2.3 Ecological Populations-at-Risk

Only biota that are relevant to the endpoints of the environmental risk assessment (fish production, nuisance algal blooms, forest production, agricultural production, and crop production) will be considered. Threatened and endangered species are not included because their occurrence and requirements must be evaluated specifically rather than generically. The descriptions of biota are based on discussions with local biologists, and data from environmental documents for proposed synfuels projects.

### 3.2.4 Human Populations-at-Risk

The near-field human populations-at-risk from synfuels contaminants include the following: people residing in the region (that is, those who might breathe near-field atmospheric contamination); people drinking water originating in the region; people ingesting foods derived from crops and animals grown in the region; and people ingesting foods derived from aquatic organisms residing in the region.

## 3.3 REFERENCE ENVIRONMENT FOR AN OIL SHALE TREATMENT SITE

### 3.3.1 Introduction

Most of the currently proposed oil shale facilities will be located in the Green River Formation of northwestern Colorado, southwestern Wyoming and northeastern Utah because of the rich deposits of oil shale

in those regions. The reference oil shale site is assumed to be located in the region of the Green River Formation, and characterization of the physical, ecological and human parameters is based on consideration of that region.

### 3.3.2 Physical Environment

The Western Site is located in a region of very rugged terrain, with steep valleys and numerous cliffs. It is basically a dissected plateau noted for its dramatic variations in relief over short distances.

The local meteorology is significantly affected by the topography, with air flows in many valleys being determined primarily by the local terrain and being essentially independent of the prevailing winds aloft. Because of this mountain-valley flow system, the frequent atmospheric inversions are often persistent. The climate of the region is arid to semiarid, with most of the precipitation occurring as snowfall. Because of both the topographical restrictions of air movement in the valleys and the limited amount of precipitation, pollution released into the valleys is sometimes dispersed relatively slowly. A summary of site climatological data is presented in Table 3-1. Meteorological data on wind speed, direction, and stability classes are too voluminous to include in this report. Instead we reference the appropriate National Oceanic and Atmospheric Administration (NOAA) data tapes. Meteorological data for the Western Site are taken from NOAA listings for Grand Junction, Colorado, 1960 through 1964 (NOAA, 1978).

Table 3-1. Climatological data

Month	Western Site <sup>a</sup>				Eastern Site <sup>b</sup>			
	Temperature (°C)	Precipitation <sup>c</sup> (mm)	Morning mixing height (m)	Afternoon mixing height (m)	Temperature (°C)	Precipitation <sup>c</sup> (mm)	Morning mixing height (m)	Afternoon mixing height (m)
January	-3.0	16.3			1.3	80.0		
February	0.9	15.5			2.3	73.7		
March	5.1	19.1			6.8	103.4		
April	10.9	20.2			13.2	82.8		
May	16.8	16.0			18.1	97.0		
June	21.8	14.0			22.4	85.6		
July	25.9	11.7			24.1	106.4		
August	24.1	26.7			23.3	84.8		
September	19.6	21.3			19.8	72.6		
October	12.7	23.6			13.9	53.1		
November	4.3	15.5			7.5	72.6		
December	-1.4	14.0			2.2	75.4		
Annual	11.5	213.6	344	2533	12.9	987.6	511	1490

<sup>a</sup>Based on climatological normals: 1941-1970, Grand Junction, Colorado.

<sup>b</sup>Based on climatological normals: 1941-1970, Huntington, West Virginia.

<sup>c</sup>Precipitation indicated by mm liquid water.

The rivers of this region tend to have large gradients and narrow floodplains. Inasmuch as most of the precipitation occurs in the winter, the largest stream flows occur during spring and early summer. Not only are the stream flows of the region seasonally variable, but they also vary on an annual basis due to varying climatic conditions from year to year.

Both large and small streams may be affected by oil shale retorting operations. Mining, retorting, and waste disposal will be conducted along small creeks exhibiting highly variable flows, temperatures, and sediment loads. Daily measurements of streamflow and temperature in Parachute Creek near Grand Valley, Colorado, were used to construct a creek scenario for the Western Site. Table 3-2 presents (for each month) a mean value, a minimum daily average, and a maximum daily average for both streamflow (Q) and temperature (T). Only irregular measurements of sediment load were available. Although insufficient for constructing a scenario, these data suggest that sediment loading in small, relatively undisturbed streams typical of western slope of the Rockies varies from <10 mg/l during the low flows to >1000 mg/l during spring snowmelt.

Rivers in the vicinity of oil shale retorting facilities may also be affected. Daily measurements of streamflow and temperature in the upper Colorado River were used to construct a river scenario for the Western Site. Table 3-3 presents (for each month) a mean value, a minimum daily average, and a maximum daily average for streamflow and temperature. Sediment loading in the upper Colorado resembles the pattern observed in smaller streams: 10 mg/l or less during low flows and up to 1000 mg/l during snowmelt.

Table 3-2. Mean, minimum daily, and maximum daily flows ( $m^3/s$ )<sup>a</sup> and daily temperatures ( $^{\circ}C$ )<sup>a</sup> for the western creek<sup>a</sup>

Month	$\bar{Q}$	$Q_{min}$	$Q_{max}$	$\bar{T}$	$T_{min}$	$T_{max}$
January	0.3	0.2	0.3	1	0	6
February	0.3	0.2	0.3	5	0	9
March	0.4	0.2	0.6	7	0	14
April	2.8	0.5	7.4	7	2	14
May	11.3	4.2	22.7	7	2	13
June	2.0	0.8	4.8	10	6	15
July	1.0	0.5	1.7	11	8	16
August	0.3	0.2	0.6	11	8	16
September	0.2	0.1	0.2	11	7	14
October	0.2	0.1	0.3	11	2	15
November	0.2	0.2	0.3	7	0	12
December	0.2	0.1	0.3	2	0	6

<sup>a</sup>From data for Parachute Creek, USGS Station No. 0903500, Water Year 1979 (USGS 1980).

Table 3-3. Mean, minimum daily, and maximum daily flows ( $m^3/s$ )<sup>a</sup> and daily temperatures ( $^{\circ}C$ )<sup>a</sup> for the western river<sup>a</sup>

Month	$\bar{Q}$	$Q_{min}$	$Q_{max}$	$\bar{T}$	$T_{min}$	$T_{max}$
January	40	30	40	1	0	2
February	40	30	40	2	0	4
March	50	40	60	6	3	10
April	70	60	70	10	5	14
May	280	110	590	13	8	18
June	420	340	570	15	10	18
July	240	110	450	19	15	23
August	80	60	110	21	17	25
September	60	50	70	19	16	22
October	50	40	60	11	7	16
November	50	50	60	6	2	10
December	40	30	60	2	0	3

<sup>a</sup>From data for the Colorado River, USGS Station No. 09093700, Water Year 1979 (USGS, 1980).

The remaining parameters for both the creek and the river are presented in Table 3-4. Stream width is assumed to be 5 m for the creek, and 20 m for the river. Current velocity is assumed to be 1.5 m/s for the creek and 0.5 m/s for the river. Site- or region-specific values could not be defined for sediment depth, solids density, fraction organic carbon, particle radius, or wind velocity. In the absence of empirical data, the values employed for these parameters can be found in Southworth (1979) and Karickhoff, Brown and Scott (1979), and are listed in Table 3-4.

### 3.3.3 Ecological Populations-at-Risk

The biota of the region are typical of the Colorado plateau. Streams that drain the canyons where the shale will be mined and retorted contain trout fisheries. The standing crop and harvest of brook trout and rainbow trout are listed in Table 3-5. Pollutants and water temperature changes could greatly impact this trout fishery. The larger rivers of the region contain a diverse fishery which would be much less affected by a synfuels facility than the stream fishery. This fishery includes the cold water populations of brook, rainbow, and brown trout (*Salmo trutta*), and introduced warm water populations of crappie (*Pomoxis spp.*), bluegill (*Lepomis macrochirus*), large-mouth bass (*Micropterus salmoides*), and walleye pike (*Stizostedion vitreum*).

Table 3-4. Values of parameters not obtained from USGS water resources data<sup>a</sup>

Parameter	Western Creek	Western River	Eastern River	Reference
Stream width (m)	5	20	30	--
Sediment depth (cm)	1.0	1.0	1.0	S <sup>b</sup>
Solids density (g/m <sup>3</sup> )	1.02	1.02	1.02	S
Fraction organic carbon	0.1	0.1	0.1	S, K&B <sup>c</sup>
Particle radius (cm)	0.005	0.005	0.005	S
Current velocity (m/s)	1.5	0.5	0.25	--
Wind velocity (m/s)	1.5	1.5	1.5	S

<sup>a</sup>Some of these parameters are not used for the health effects assessment.

<sup>b</sup>Southworth (1979).

<sup>c</sup>Karickhoff, Brown and Scott (1979).

Table 3-5. Western Site fish population parameters

	Standing crop (kg/km)	Harvest (kg/km/y)
Brook trout ( <i>Salvelinus fontinalis</i> )	30	10
Rainbow trout ( <i>Salmo gairdneri</i> )	20	7

Two percent of the reference environment site occurs at high elevations and contains Douglas fir (*Pseudotsuga menziesii*) in association with aspen (*Populus tremuloides*). Piñon pine (*Pinus monophylla*) and juniper (*Juniperus scopulorum* and *J. osteosperma*) woodlands occur at middle elevations. A narrow riparian forest of cottonwood (*Populus angustifolia*) borders on the creeks and rivers. Since these sparse woodland are not harvested, their production is not estimated. Range and native hay grasses include wheat grass (*Agropyron smithii*), cheat grass (*Bromus tectorum*), and mutton grass (*Poa fendleriana*). Browsed shrubs include mountain mahogany (*Cercocarpus montanus*), serviceberry (*Amelanchier alnifolia*), big sagebrush (*Artemisia tridentata*), and shadscale (*Atriplex confertifolia*). Range and agricultural production are presented in Table 3-6.

The predominant game species of the region is the mule deer. Elk and pronghorn antelope are present but are far less abundant. Small game species include the desert cottontail and the mourning dove. Numerous nongame species also exist in the region. (See Table 3-7).

Table 3-6. Plant production at the Western Site

	Production (kg/km <sup>2</sup> /y)
<u>Range</u>	
Grasses and forbes	20,000
Shrubs	100,000
<u>Agricultural</u>	
Hay	7,000
Alfalfa	4,000
Wheat	300
Oats	100
Barley	200

Table 3-7. Western Site wildlife parameters

	Density (no/km <sup>2</sup> )	Harvest (no/km <sup>2</sup> /y)
Mule deer ( <i>Odocoileus hemionus</i> )	30	1
Desert cottontain ( <i>Sylvilagus auduboni</i> )	200	5
Mourning dove ( <i>Zenaidura macroura</i> )	200	5
Nongame mammals	4000	-
Nongame birds	1500	-

### 3.3.4 Human Populations-at-Risk

The human population which would be affected directly by near-field atmospheric contamination would be relatively small and well dispersed. The area near the Western Site is sparsely populated, with few sizeable towns in the vicinity. Sixty percent of the population resides in rural areas, with about 6% of those rural inhabitants residing on farms and ranches. The other 40% of the total population resides in towns and small cities.

The near-field population-at-risk from contaminated drinking water would consist of both surface water (60%) and groundwater (40%) users. The majority of the "urban" residents live in municipalities located on rivers; most of these people use water obtained from nearby surface water sources. In contrast, people who live in cities near unreliable streams, as well as some of those located in rural areas, use water taken from groundwater sources.

The bulk of the crops produced in the region are grains and grasses intended for animal consumption. Some crops, namely a few grains and nonleafy vegetables, are also grown for human consumption. The primary farm animals raised in the region are cattle and sheep, with approximately equal numbers of the two being produced. The location of populations potentially affected by contamination of agricultural foods would be varied. Populations-at-risk for foods derived from animals and grains would tend to be remote from the site, whereas populations-at-risk for local vegetables would be close to the site. Parameters used in the food chain transport

calculations are obtained primarily from the SITE data base (Baes et al., 1983b) - see Section 2.4.1.2. Variables listed in the SITE database are given in Table 3.8.

The population-at-risk for aquatic foods contaminated in the near field would be comparatively small. The primary aquatic food pathway to humans would consist of finfish caught by recreational fishermen downstream from the facility. Thus, those fishers and their families and friends would tend to constitute the population-at-risk for fish caught near the facility. A comparison of parameters used for estimating human exposure in the Eastern and Western sites is listed in Table 3-9.

### 3.4 REFERENCE ENVIRONMENT FOR A COAL LIQUEFACTION SITE

#### 3.4.1 Introduction

Most proposed coal liquefaction facilities are to be located in the Appalachian Basin, in particular, eastern Kentucky and western West Virginia. Consequently, the reference coal liquefaction site is taken to be an eastern site located in the central portion of the Appalachian Basin.

Table 3-8. Variable names in the 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 <sup>2</sup>	yield of exposed produce
AYHF	kg(dry)/y/m <sup>2</sup>	areal yield of hay feed
YLV	kg(fresh)/m <sup>2</sup>	yield of leafy vegetables
YSF	kg(dry)/m <sup>2</sup>	yield of (corn and sorghum) silage feed
AREAP	m <sup>2</sup>	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
NUMSBP	head	number of sheep
PGF	kg	production of grain for feed
PBF	kg	production of hay feed
PSF	kg	production of (corn and sorghum) silage feed
HUMID	g/m <sup>3</sup>	average annual absolute humidity
AREAT	m <sup>2</sup>	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
PGB	kg	production of grain for human consumption
MNIXHT	m	morning mixing height
AMIXHT	m	afternoon mixing height
YPV	kg(fresh)/m <sup>2</sup>	yield of protected produce
YGF	kg(fresh)/m <sup>2</sup>	yield of grain food
YGH	kg(dry)/m <sup>2</sup>	yield of grain feed
FFDAYS	number	number of frost-free days in a year
NUMBC	head	number of beef cattle
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.
DOMLF	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 hay 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., 1983b.

Table 3-9. Comparison of the parameters chosen to model the near-field human populations of the reference sites<sup>a</sup>

	Western	Eastern
Human populations <sup>b</sup>		
Atmosphere <sup>c</sup>	2 people/km <sup>2</sup>	45 people/km <sup>2</sup>
Drinking water <sup>d</sup>	60% surface water	70% surface water
Fish harvests <sup>e</sup>	12 kg-finfish/km <sup>2</sup> (land)-y	34 kg-finfish/km <sup>2</sup> (land)-y
Crop production	Grains: 200 kg/km <sup>2</sup> for humans; 400 kg/km <sup>2</sup> for animals	Grains: 200 kg/km <sup>2</sup> for humans; 1000 kg/km <sup>2</sup> for animals; Leafy vegetables: 100 kg/km <sup>2</sup> ; Protected vegetables: 300 kg/km <sup>2</sup> ; Exposed vegetables: 150 kg/km <sup>2</sup>
Animal production	3 cows/km <sup>2</sup> /y; 2 sheep/km <sup>2</sup> /y	6 cows/km <sup>2</sup> /y; 6 hogs/km <sup>2</sup> /y

<sup>a</sup>The values presented in this table are based on consideration of the entire areas which might have synfuels facilities located in them and not on consideration of just specific regions within those areas.

<sup>b</sup>Except where noted otherwise, the affected populations important to the health assessment (namely, the humans, the crops, and the farm animals) are taken to be uniformly distributed throughout the near field. Thus, each of the populations given is averaged over the entire area of the near field. The parameters for these populations have been based primarily on consideration of Olson, Emerson, and Nungesser (1980), Shor, Baes, and Sharp (1982), and USDA (1980).

It should be noted that near the Western Site, the local increase in the human population associated with construction and operation of a synfuels facility could noticeably affect the overall distribution of that population and might even challenge the validity of the assumption of a uniform distribution of that population in the near-field region. The size of the effect would depend strongly upon the size of the facility. In contrast, near the Eastern Site, the local increase in the human population associated with a synfuels facility would not significantly affect the distribution of that population. Thus, the assumption of a uniform distribution would be unimportant for the near-field region of the Eastern Site.

<sup>c</sup>For atmospheric exposure, the near-field population is taken to consist of only residents of the region.

<sup>d</sup>For drinking water exposure, 50% of the near-field surface water drinkers are taken to be uniformly distributed along the surface water downstream from the facility. In contrast, the near-field groundwater drinkers are taken to be uniformly distributed throughout the entire region. It is assumed that there is no substantial human-related export of water from the region for human consumption.

<sup>e</sup>Recreational finfish harvest rates are based on national averages of 1580 kg/km<sup>2</sup> of surface water per year for streams and rivers, and 4740 kg/km<sup>2</sup> of surface water per year for reservoirs (Niemczyk et al., 1980). (The areas are yearly average surface water areas.) Commercial rates, where applicable, are taken to be equal to the recreational rates. The total surface water area in any region is taken to be twice the surface water area of all lakes greater than 40 acres and all streams greater than 1/8 mile wide in the region. The areas are based on Olson, Emerson, and Nungesser (1980).

### 3.4.2 Physical Environment

The Eastern Site is located in a region of wooded hills and narrow valleys. In comparison with the region surrounding the Western Site, the topography displays much less relief.

The local meteorology is somewhat affected by the topography, with the variations in the terrain frequently channeling the winds at the lower elevations. In general, the effect is not nearly as substantial in this region as it is in the region of the Western Site. At higher elevations, the wind direction is generally from the south. The climate is humid with a significant fraction of the precipitation occurring during thunderstorms. Because the topographical restrictions of the air movements are not as large as they are near the Western Site and because precipitation is abundant, pollution released to the valleys around the Eastern Site would often be dispersed much more rapidly than similar pollution released to the valleys around the Western Site. A summary of climatological parameters is presented in Table 3-1. Meteorological data is taken from NOAA listings for Huntington, West Virginia, 1974 (NOAA, 1978).

The larger rivers of this region tend to have moderate to low gradients and wide floodplains. In as much as monthly precipitation in this region is relatively uniform, stream flows tend to be much more constant than they are for the western region.

Direct and indirect coal liquefaction plants located in the Central Appalachian Coal Basin are likely to be sited on small rivers such as the Monongahela and Big Sandy Rivers. Relatively complete data on

streamflows and water quality are available for the rivers. Daily measurements of streamflow, temperature, and suspended sediment load in the Monongahela and Big Sandy were used to construct a 1-y scenario for use in risk assessment. Table 3-10 presents mean, minimum daily average, and maximum daily average values for each parameter for each of the 12 months of the year.

The remaining parameters for the Eastern Site stream are presented in Table 3-4. Stream width is assumed to be 30 m, and current velocity is assumed to be 0.25 m/s. The values of the other parameters are the same as those used for the Western Site.

The soil of the region is of varying fertility and abundance. Overall, this region is much more fertile than the region surrounding the Western Site. The vegetation is such that 55% of the region is forested, 30% is pasture and grazing land, and a tenth is crop land.

### 3.4.3 Ecological Populations-at-Risk

This region possesses a typical warm water riverine biota. The primary fish species of interest are carp, bigmouth buffalo, smallmouth buffalo, channel catfish, white bass, bluegill, green sunfish, black crappie, and largemouth bass. Most of the biomass consists of carp, catfish and buffalo. (Refer to Table 3-11 for details.)

Table 3-10. Mean, minimum, and maximum monthly flows ( $m^3/s$ ),<sup>a</sup> temperatures ( $^{\circ}C$ ),<sup>b</sup> and suspended sediment loads ( $mg/l$ )<sup>b</sup> for the eastern river

Month	$\bar{Q}$	$Q_{min}$	$Q_{max}$	$\bar{T}$	$T_{min}$	$T_{max}$	$\bar{SS}$	$SS_{min}$	$SS_{max}$
January	420	140	1900	2	0	4	50	5	105
February	230	110	620	2	0	3	55	15	340
March	510	80	1600	4	1	8	110	20	290
April	290	110	690	11	8	14	30	10	70
May	310	100	1100	14	13	18	25	5	80
June	130	50	420	22	18	26	25	10	70
July	230	70	1100	24	20	28	25	5	40
August	140	50	340	27	25	28	35	10	70
September	80	50	220	25	23	27	25	10	70
October	170	80	420	16	11	22	15	5	35
November	210	80	540	12	6	18	25	10	70
December	310	160	700	44	3	7	115	15	360

<sup>a</sup>Composite of data from the Big Sandy River, USGS Station No. 0321500, Water Year 1976 (USGS, 1977), and the Monongahela River, USGS Station No. 03085000, Water Year 1978 (USGS, 1979).

<sup>b</sup>From data for the Monongahela River, USGS Station No. 03085000, Water Year 1978 (USGS, 1979).

Table 3-11. Eastern Site fish population parameters

	Standing crop (kg/km)	Harvest (kg/km/y)
Carp	4000	1300
Bigmouth buffalo ( <i>Ictiobus cyprinellus</i> )	80	30
Smallmouth buffalo ( <i>I. bubalus</i> )	450	150
Channel catfish ( <i>Ictalurus punctatus</i> )	1500	500
White bass ( <i>Morone chrysops</i> )	50	10
Bluegill ( <i>Lepomis macrochirus</i> )	250	25
Green sunfish ( <i>L. cyanellus</i> )	50	5
Black crappie ( <i>Pomoxus nigromaculatus</i> )	150	30
Largemouth bass ( <i>Micropterus salmoides</i> )	300	100

The region contains mixed mesophytic forest, the dominant species of which are hardwoods such as yellow poplar, red maple, sugar maple, and black oak. In addition to the native forests, ten percent of the region is planted in loblolly pine plantations.

Pasture and hay fields, which are assumed to be planted in clover and fescue, occupy 30% of the region. The dominant crops are corn, soybeans, and tobacco. Production of forest and crop plants is presented in Table 3-12.

The only big game species of the region is the whitetail deer. Small game species include the eastern cottontail, eastern grey squirrel, bobwhite quail, and mourning dove. Numerous nongame species also reside in the region. (See Table 3-13.)

Table 3-12. Eastern Site vegetation parameters<sup>a</sup>

	Herbaceous production (MT/km <sup>2</sup> /y)	Stem mass (MT/km <sup>2</sup> )	Stem production (MT/km <sup>2</sup> /y)
<u>Crops</u>			
Corn	5		
Soybeans	2		
Tobacco	3		
<u>Pasture and Hay</u>			
Fescue ( <i>Fescuta arundinacea</i> )	100		
Clover ( <i>Trifolium repens</i> )	30		
<u>Hardwoods</u>			
Yellow poplar ( <i>Liriodendron tulipifera</i> )		2000	25
Red maple ( <i>Acer rubrum</i> )		1250	25
Sugar maple ( <i>Acer saccharum</i> )		250	10
Shagbark hickory ( <i>Carya ovata</i> )		100	5
Beech ( <i>Fagus grandifolia</i> )		100	5
White oak ( <i>Quercus alba</i> )		100	5
Black oak ( <i>Q. velutina</i> )		1000	25
Chestnut oak ( <i>Q. prinus</i> )		100	5
TOTAL		4900	130
<u>Softwoods</u>			
Loblolly pine ( <i>Pinus taeda</i> )		450	65

<sup>a</sup>Production is averaged over the entire region and not just the areas producing each vegetation type.

### 3.4.4. Human Populations-at-Risk

The region surrounding the Eastern Site is moderately populated (Table 3-9). Approximately two-thirds of the residents live in towns and small cities, with most of the other residents living in rural areas but not on farms.

The drinking-water population-at-risk for the Eastern Site would consist primarily of surface water users inasmuch as most communities in the region use water taken from nearby rivers or reservoirs.

Table 3-13. Eastern Site wildlife parameters

	Density (no/km <sup>2</sup> )	Harvest (no/km <sup>2</sup> /y)
Whitetail deer ( <i>Odocoileus virginianus</i> )	20	5
Eastern cottontail ( <i>Sylvilagus floridanus</i> )	500	200
Eastern grey squirrel ( <i>Sciurus carolinensis</i> )	500	200
Mourning dove ( <i>Zenaidura macrura</i> )	800	400
Bobwhite quail ( <i>Colinus virginianus</i> )	500	200
Nongame mammals	6000	-
Nongame birds	2000	-

Most of the crops produced in the eastern region are grains and grasses intended for animal consumption. Some grains and row crops (such as soybeans) are produced for human consumption. The primary farm animals are cattle (for beef) and hogs, with approximately equal numbers of the two being produced. In general, foods derived from crops intended

for human consumption and those derived from animals grown in the region are consumed by populations located outside the region. Parameters used in the food chain transport calculations are obtained primarily from the SITE data base (Baes et al., 1983b). Variables listed in the SITE data base are given in Table 3.8, and typical values of terrestrial transport and food chain parameters for the Eastern Site are given in Tables 3.14 and 3.15.

The population-at-risk for aquatic foods contaminated in the area would consist of only finfish consumers. Although most of the fishing in the region is done by recreational fishers, some fish are harvested commercially. Thus, the total catch is relatively small and tends to be consumed locally.

Table 3-14. Parameters used in terrestrial transport calculations for the Eastern Site

Parameter	Value	Definition
<b>Time constants:</b>		
$t_e$		Time of exposure to depositing material
leafy vegetables "exposed"	100 d	
produce	100 d	
silage	150 d	
hay	60 d	
pasture	30 d	
$t_b$	$1.08 \times 10^9$ s (35 y)	Time of long-term buildup in soil
<b>Soil constants:</b>		
$\rho$	1.35 g/cm <sup>3</sup>	Soil bulk density
$\theta$	0.485 ml/cm <sup>3</sup>	Volumetric water content of soil
$d$	15 cm	Depth of root zone
<b>Cattle feed consumption constants:</b>		
$Q_g$		Consumption rate of grain
Milk cows	2600 kg/y	
Feedlot cattle	1820 kg/y	
"Other"		
beef cattle	150 kg/y	
$Q_f$		Consumption rate of forage
Milk cows	4010 kg/y	
Feedlot cattle	970 kg/y	
"Other"		
beef cattle	3030 kg/y	

Table 3-15. Parameters for the initial food chain transport calculations

Category	Log K <sub>ow</sub>	$\lambda_{ad}$		$\lambda_d$	K <sub>d</sub>	B <sub>iv</sub>	B <sub>ir</sub>	F <sub>m</sub>	F <sub>f</sub>
		IL <sup>a</sup>	UR <sup>b</sup>						
Vol. carboxylic acids	-0.36	2.7x10 <sup>-6</sup>	1.9x10 <sup>-6</sup>	1.9x10 <sup>-6</sup>	0.067	840	84	5.0x10 <sup>-7</sup>	4.7x10 <sup>-6</sup>
Vol. O&S heterocyclics	2.00	1.7x10 <sup>-5</sup>	1.2x10 <sup>-5</sup>	1.2x10 <sup>-5</sup>	1.2	29	2.9	7.6x10 <sup>-6</sup>	7.1x10 <sup>-5</sup>
Vol. N-heterocyclics	-1.00	9.9x10 <sup>-6</sup>	6.8x10 <sup>-6</sup>	6.8x10 <sup>-6</sup>	0.031	2100	210	2.4x10 <sup>-7</sup>	2.2x10 <sup>-6</sup>
Benzene	2.09		1.2x10 <sup>-6</sup>	1.2x10 <sup>-6</sup>	1.3	25	2.5	8.3x10 <sup>-6</sup>	7.9x10 <sup>-5</sup>
Aliphatic/alicyclic hydrocarbons	4.00	1.2x10 <sup>-5</sup>	8.4x10 <sup>-6</sup>	8.4x10 <sup>-6</sup>	14	1.6	0.16	7.5x10 <sup>-5</sup>	7.1x10 <sup>-4</sup>
Mono/diaromatic hydrocarbons	3.18	1.9x10 <sup>-5</sup>	1.3x10 <sup>-5</sup>	1.3x10 <sup>-5</sup>	5.0	5.3	0.53	7.4x10 <sup>-5</sup>	3.4x10 <sup>-4</sup>
Polycyclic aromatic hydrocarbons	5.28	1.8x10 <sup>-6</sup>	1.5x10 <sup>-6</sup>	5.4x10 <sup>-8</sup>	65	0.20	0.025	3.3x10 <sup>-4</sup>	3.1x10 <sup>-3</sup>
Aliphatic amines	0.57		2.9x10 <sup>-6</sup>	2.9x10 <sup>-6</sup>	0.21	220	22	1.5x10 <sup>-6</sup>	1.4x10 <sup>-5</sup>
Aromatic amines	1.19	7.7x10 <sup>-6</sup>	6.5x10 <sup>-6</sup>	6.5x10 <sup>-6</sup>	0.44	91	9.1	3.0x10 <sup>-6</sup>	2.8x10 <sup>-5</sup>
Alkaline nitrogens	2.65	5.5x10 <sup>-6</sup>	3.8x10 <sup>-6</sup>	3.8x10 <sup>-6</sup>	2.6	11	1.1	1.6x10 <sup>-5</sup>	1.5x10 <sup>-4</sup>
Neutral N, O, S	2.96	1.9x10 <sup>-5</sup>	1.3x10 <sup>-5</sup>	1.3x10 <sup>-5</sup>	3.8	7.2	0.72	2.3x10 <sup>-5</sup>	2.1x10 <sup>-4</sup>
Carboxylic acids	1.97	3.2x10 <sup>-6</sup>	2.2x10 <sup>-6</sup>	2.2x10 <sup>-6</sup>	1.2	30	3.0	7.3x10 <sup>-6</sup>	6.9x10 <sup>-5</sup>
Phenols	1.55	2.4x10 <sup>-5</sup>	2.0x10 <sup>-5</sup>	7.5x10 <sup>-8</sup>	0.68	55	5.5	4.5x10 <sup>-6</sup>	4.2x10 <sup>-5</sup>
Aldehydes and ketones	0.90		2.1x10 <sup>-5</sup>	2.1x10 <sup>-5</sup>	0.31	140	14	2.1x10 <sup>-6</sup>	2.0x10 <sup>-5</sup>
Non-heterocyclic organo sulfurs	2.52	5.8x10 <sup>-6</sup>	4.1x10 <sup>-6</sup>	4.1x10 <sup>-6</sup>	2.2	14	1.4	1.4x10 <sup>-5</sup>	1.3x10 <sup>-4</sup>
Alcohols	-0.50	4.3x10 <sup>-6</sup>	3.0x10 <sup>-6</sup>	3.0x10 <sup>-6</sup>	0.056	1000	100	4.2x10 <sup>-7</sup>	4.0x10 <sup>-6</sup>
Nitroaromatics	2.31		1.4x10 <sup>-6</sup>	1.4x10 <sup>-6</sup>	1.7	18	1.8	1.1x10 <sup>-5</sup>	1.0x10 <sup>-4</sup>
Amides	0.64		4.2x10 <sup>-6</sup>	4.2x10 <sup>-6</sup>	0.23	200	20	1.6x10 <sup>-6</sup>	1.5x10 <sup>-5</sup>
Nitriles	-0.92		2.9x10 <sup>-6</sup>	2.9x10 <sup>-6</sup>	0.034	1900	190	2.6x10 <sup>-7</sup>	2.5x10 <sup>-6</sup>
Arsenic		0	0	0	200	0.040	6.0x10 <sup>-3</sup>	6.0x10 <sup>-5</sup>	2.0x10 <sup>-3</sup>
Mercury		0	0	0	10	0.90	0.20	4.5x10 <sup>-4</sup>	0.25
Nickel		0	0	0	150	0.060	0.060	1.0x10 <sup>-3</sup>	6.0x10 <sup>-3</sup>
Cadmium		0	0	0	6.5	0.55	0.15	1.0x10 <sup>-3</sup>	5.5x10 <sup>-4</sup>
Lead		0	0	0	900	0.045	9.0x10 <sup>-3</sup>	2.5x10 <sup>-4</sup>	3.0x10 <sup>-4</sup>

<sup>a</sup> Indirect liquefaction assessment

<sup>b</sup> Unit release assessment

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