

Appendix H: Chemicals

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This appendix presents basic facts about chemicals. The information is intended to be a basis for understanding the dose or relative toxicity assessment associated with possible releases from the Oak Ridge Reservation (ORR), not a comprehensive discussion of chemicals and their effects on the environment and biological systems.

PERSPECTIVE ON CHEMICALS

The lives of modern humans have been greatly improved by the development of chemicals such as pharmaceuticals, building materials, housewares, pesticides, and industrial chemicals. Through the use of chemicals, we can increase food production, cure diseases, build more efficient houses, and send people to the moon. At the same time, we must be cautious to ensure that our own existence is not endangered by uncontrolled and overexpanded use of chemicals (Chan et al. 1982).

Just as all humans are exposed to radiation in the normal daily routine, humans are also exposed to chemicals. Some potentially hazardous chemicals exist in the natural environment. In many areas of the country, soils contain naturally elevated concentrations of metals such as selenium, arsenic, or molybdenum, which may be hazardous to humans or animals. Even some of the foods we eat contain natural toxins. Aflatoxin is a known toxin found in peanuts and cyanide is found in apple seeds. However, exposures to many more hazardous chemicals result from the direct or indirect actions of humans. Building materials used for the construction of homes may contain chemicals such as formaldehyde (in some insulation materials), asbestos (formerly used in insulations and ceiling tiles), and lead (formerly used in paints and gasoline). Some chemicals are present as a result of application of pesticides and fertilizers to soil. Other chemicals may have been transported long distances through the atmosphere from industrial sources before being deposited on soil or water.

PATHWAYS OF CHEMICALS FROM THE ORR TO THE PUBLIC

Pathways refer to the route or way in which a person can come in contact with a chemical substance. Chemicals released to the air may remain suspended for long periods of time, or they may be rapidly deposited on plants, soil, and water. Chemicals may also be released as liquid wastes called effluents, which can enter streams and rivers.

People are exposed to chemicals by inhalation (breathing air), ingestion (eating exposed plants and animals or drinking water), or by direct contact (touching the soil or swimming in water). For example, fish that live in a river that receives effluents may take in some of the chemicals present. People eating the fish would then be exposed to the chemical. Less likely would be exposure by directly drinking from the stream or river.

The public is not normally exposed to chemicals on the ORR because access to the reservation is limited. However, chemicals released as a result of ORR operations can move through the environment to off-site locations, resulting in potential exposure to the public.

DEFINITIONS

Toxicity

Chemicals have varying types of effects. Generally, when considering human health, chemicals are divided into two broad categories: chemicals that cause adverse or toxic health effects but do not cause cancer (noncarcinogens) and chemicals that cause cancer (carcinogens). Sometimes a chemical can have both a toxic and a carcinogenic effect. The toxic effect can be acute (short-term severe health effect) or chronic (longer-term persistent health effect). Toxicity is often evident in a shorter length of time than the carcinogenic effect. The potential health effects of noncarcinogens range from skin irritation to life-shortening. Carcinogens cause or increase the incidence of malignant neoplasms or cancers.

Toxicity refers to an adverse effect of a chemical on human health. Not all chemicals are toxic: Every day we ingest chemicals in the form of food, water, and sometimes medications. Even those chemicals that are usually considered toxic are usually nontoxic or harmless below a certain concentration.

Concentration limits or advisories are set by government agencies for some chemicals that are known or are thought to have an adverse effect on human health. These concentration limits can be used to calculate a chemical dose that would not harm even individuals who are particularly sensitive to the chemical.

Dose Terms for Noncarcinogens

Reference Dose

A reference dose (RfD) is an estimate (with uncertainty spanning an order of magnitude or greater) of a daily exposure level for the human population, including sensitive subpopulations, that is likely to be without an appreciable risk of deleterious effects during a lifetime. Units are expressed as milligrams of chemical per kilogram of an adult's body weight per day ($\text{mg kg}^{-1} \text{ day}^{-1}$). These values are given in Table H.1.

Values for RfDs are derived from doses of chemicals that result in no adverse effect or the lowest dose that showed an adverse effect on humans or laboratory animals. Uncertainty factors are typically used in deriving RfDs. Uncertainty adjustments may be made if animal toxicity data is extrapolated to humans, to account for human sensitivity, extrapolation from subchronic to chronic no-observed-adverse-effect-levels (NOAELs), extrapolation from lowest-observed-adverse-effect-levels (LOAELs) to NOAELs, and to account for data base deficiencies. The use of uncertainty factors in deriving RfDs is thought to protect the sensitive human populations. The EPA maintains the Integrated Risk Information System (IRIS) data base, which contains verified RfDs and up-to-date health risk and EPA regulatory information for numerous chemicals.

Primary and secondary maximum contaminant level

For chemicals for which RfDs are not available in IRIS, national primary drinking water maximum contaminant levels (MCLs) and secondary drinking water regulation concentrations [secondary MCLs (SMCLs)], expressed in milligrams of chemical per liter of drinking water, are converted to RfD values by multiplying by 2 liters (L) (the average daily adult water intake) and dividing by 70 kg (the reference adult body weight). The result is a "derived" reference dose expressed in milligrams per kilogram per day ($\text{mg kg}^{-1} \text{ day}^{-1}$). These values are given in Table H.1.

Table H.1. Chemical reference doses and slope factors used in drinking water and fish intake analysis

Chemical	Reference dose or slope factor ^a	Reference ^b
Aluminum	5.7E-03	SMCL ^c
Aroclor-1016	7.0E-5	RfD ^d
Aroclor-1248	7.0E-5	RfD ^d
Aroclor-1254	2.0E-5	RfD ^d
Aroclor-1260	2.0E-5	RfD ^d
Barium	7.0E-02	RfD
Beryllium	2.0E-03	RfD
Beta-BHC	4.0E-6	TN WQC
4,4'-DDE	3.4E-01	SF
Iron	8.6E-03	SMCL
Manganese	4.7E-02	RfD
Mercury	1.0E-04	RfD ^e
PCBs (mixed)	2.0E+00	SF ^f
1,1,1-Trichloroethane	5.7E-03	MCL
Toluene	2E-01	RfD
Zinc	3.0E-01	RfD

^aRfD: reference dose (mg kg⁻¹ day⁻¹); SF: slope factor (risk per mg kg⁻¹ day⁻¹).

^bThe maximum contaminant level (MCL), secondary maximum contaminant level (SMCL), and Tennessee Water Quality Criteria (TN WQC) are in units of mg/L. To convert the concentration to a RfD (mg kg⁻¹ day⁻¹), multiply by the consumption rate (2 L/day), and divide by the mass of a reference man, 70 kg.

^cBased on the TN SMCL of 0.2 mg/L; the federal SMCL is a range of 0.05–0.2 mg/L.

^dThe RfD for Aroclor-1016 is also used for Aroclor-1248. The RfD for Aroclor-1254 is also used for Aroclor-1260.

^eInterim Reference Dose.

^fThe cancer potency of PCB mixtures is determined using a three-tiered approach. This value is the upper bound slope factor for the High Risk and Persistence Tier.

Dose Term for Carcinogens

Slope Factor

A slope factor (SF) is a plausible upper-bound estimate of the probability of a response per unit intake of a chemical during a lifetime. The SF is used to estimate an upper-bound probability of an individual developing cancer as a result of a lifetime exposure to a particular level of a potential carcinogen. Units are expressed as risk per dose (mg kg⁻¹ day⁻¹). These values are given in Table H.1.

The SF converts the estimated daily intake averaged over a lifetime exposure to the incremental risk of an individual developing cancer. Because it is unknown for most chemicals whether a threshold (a dose below which no adverse effect occurs) exists for carcinogens, units for carcinogens are set in terms of risk factors. Acceptable risk levels for carcinogens range from 10⁻⁴ (risk of developing cancer over a human lifetime of 1 in 10,000) to 10⁻⁶ (risk of developing cancer over a human lifetime is 1 in 1,000,000). In this

assessment, the risk level of 10^{-5} (risk of developing cancer over a human lifetime of 1 in 100,000) was used to establish acceptable levels of exposure. In other words, a certain chemical concentration in food or water could cause a risk of one additional cancer case for every 100,000 exposed persons.

MEASURING CHEMICALS

Environmental samples are collected in areas surrounding the ORR and are analyzed for chemical constituents that are most likely to be released from the ORR. Typically, chemical concentrations in liquids are expressed in terms of milligrams or micrograms of chemical per liter of water; concentrations in solids (soil and fish tissue) are expressed in terms of milligrams or micrograms of chemical per gram or kilogram of sample material.

The instruments used to measure chemical concentrations are very sensitive; however, they have limits below which they cannot detect the chemicals of interest. Concentrations that are detected below the reported analytical detection limits of the instruments are recorded by the laboratory as estimated values, which have a greater uncertainty than those concentrations detected above the detection limits of the instruments. Health effect calculations using these estimated values are indicated with tildes (~). The tilde indicates that estimated values were used in estimating the average concentration of a chemical.

RISK ASSESSMENT METHODOLOGY

Exposure Assessment

To evaluate an individual's exposure by way of a specific exposure pathway, the intake amount of the chemical must be determined. For example, chemical exposure by drinking water and eating fish from the Clinch River is assessed in the following way. Clinch River surface water and fish samples are analyzed to estimate chemical contaminant concentrations. It is assumed that individuals drink 2 L (0.53 gal) of water per day directly from the river, which amounts to 730 L (193 gal) per year, and that they eat 0.06 kg of fish per day (21 kg per year). Estimated daily intakes or estimated doses to the public are calculated by multiplying measured (statistically significant) concentrations in water by 2 L or those in fish by 0.06 kg. This intake is first multiplied by the exposure duration (30 years) and exposure frequency (350 days/year), and then divided by an averaging time (30 years for noncarcinogens and 70 years for carcinogens). These assumptions are conservative, and in many cases they result in higher estimated intakes and doses than an actual individual would receive.

Dose Estimate

When the contaminant oral daily intake via exposure pathways has been estimated, the dose can be determined. For chemicals, the dose to humans is measured as milligrams per kilogram-day ($\text{mg kg}^{-1} \text{day}^{-1}$). In this case, the "kilogram" refers to the body weight of an adult individual. When a chemical dose is calculated, the length of time an individual is exposed to a certain concentration is important. To assess off-site doses, it is assumed that the exposure duration occurs over 30 years. Such exposures are called "chronic" in contrast to short-term exposures, which are called "acute."

The daily intake or dose from ingestion of water is estimated by the following equation:

$$\text{Intake (mg/kg-day)} = \frac{CW \times IR \times EF \times ED}{BW \times AT} ,$$

where

- CW* = Concentration in water (mg/L)
IR = Ingestion rate (2 L/day)
EF = Exposure frequency (350 days/year)
ED = Exposure duration (30 years)
BW = Body weight (70 kg)
AT = Averaging time (365 days/year × *ED*) noncarcinogens
 = Averaging time (365 days/year × 70 years) carcinogens

The daily intake rate or dose from consumption of fish obtained by recreational anglers is estimated by the following equation:

$$\text{Intake (mg/kg-day)} = \frac{CW \times IR \times EF \times ED}{BW \times AT},$$

where

- CW* = Concentration in fish tissue wet weight (mg/kg)
IR = Ingestion rate (0.06 kg/day)
EF = Exposure frequency (350 days/year)
ED = Exposure duration (30 years)
BW = Body weight (70 kg)
AT = Averaging time (365 days/year × *ED*) noncarcinogens
 = Averaging time (365 days/year × 70 years) carcinogens

Calculation Methodology

Prior to the 1998 annual environmental report, the “calculated daily intakes,” based on chemical concentrations in water or fish, were divided by the “acceptable daily intake,” which was based on the RfD. Both intakes were expressed in milligrams per day by multiplying by 70 kg for body weight. Current risk assessment methodologies use the term hazard quotient (HQ) to evaluate noncarcinogenic health effects. Therefore, since 1998 the HQ methodology has been used. Because intakes are calculated in milligrams per kilogram per day in the HQ methodology, they are expressed in terms of dose. The HQ is a ratio that compares the estimated exposure dose or intake (*I*) to the RfD as follows:

$$HQ = \frac{I}{RfD},$$

where

- HQ* = hazard quotient (unitless),
I = estimated intake or dose (mg kg⁻¹ day⁻¹),
RfD = reference dose (mg kg⁻¹ day⁻¹).

HQ values of less than 1 indicate an unlikely potential for adverse health effects, whereas HQ values greater than 1 indicate a concern for adverse health effects or the need for further study.

To evaluate carcinogenic risk, SFs are used instead of RfDs. In this report, the estimated dose from ingesting water or fish from rivers and streams surrounding the ORR is compared to the chronic daily intake (CDI) derived from assuming a human lifetime risk of developing cancer of 10⁻⁵ (1 in 100,000). The CDI is estimated as follows:

$$CDI = \frac{1 \times 10^{-5}}{SF},$$

where

CDI = chronic daily intake (mg kg⁻¹ day⁻¹),
 SF = slope factor, oral (risk per mg kg⁻¹ day⁻¹).

In typical risk assessments, risks levels are generally derived; however, in this report 10⁻⁵ is assumed as the level of acceptable risk. To estimate the risk of inducing cancers, from ingestion of water and fish, relative to the risk of 10⁻⁵, the estimated dose or intake (I) is divided by the CDI. A ratio greater than one indicates a risk greater than 10⁻⁵ and a value less than one indicates a risk less than 10⁻⁵. The tilde (~) indicates that estimated values were used in estimating the average concentrations of a chemical.

RESULTS

For 1999, the estimated HQs and I/CDI ratios for consumption of drinking water collected from CRK 70 (upstream of ORR), CRK 32(downstream of ORNL), and CRK 16 (downstream from all DOE inputs) are summarized in Table H.2. See Sect. 7.4.2.2 for a discussion of the results. Table H.3 summarizes the estimated HQs and I/CDI ratios for the consumption of sunfish and catfish collected from CRK 70, 32, and 16. See Section 7.9.1.2 for a detailed discussion of the results.

Table H.2. 1999 chemical hazard quotients for drinking water^a

Chemical	Hazard quotient		
	CRK 70 ^b	CRK 23 ^c	CRK 16 ^d
<i>Metals</i>			
Aluminum	~1	~1	~3
Barium	0.01	0.01	0.02
Iron	0.6	0.8	2
Manganese	0.03	0.04	0.04
Zinc	~0.005		
<i>Volatile organics</i>			
1,1,1-Trichloroethane		~0.04	
Toluene		~0.001	

^aA tilde (~) indicates that estimated values and/or detection limits were used in the calculation, and a blank space indicates the parameter was undetected.

^bMelton Hill Reservoir above city of Oak Ridge input.

^cWater supply intake for the ETP.

^dClinch River downstream of all DOE inputs.

Table H.3. 1999 chemical hazard quotients (HQs) and estimated dose/chronic daily intake (I/CDIs) for carcinogens in fish^a

Parameters	Sunfish			Catfish		
	CRK 70 ^b	CRK 32 ^c	CRK 16 ^d	CRK 70 ^b	CRK 32 ^c	CRK 16 ^d
<i>HQs for metals</i>						
Mercury	0.3	0.4	0.8	1	2	3
Zinc	0.04	0.04	0.04	0.04	0.02	0.02
<i>HQs for pesticides and Aroclors</i>						
Aroclor-1016	~0.7		~0.8			
Aroclor-1248	~0.7		~0.8			
Aroclor-1254	~3		~3		13	7
Aroclor-1260	~3		~3		41	37
Beta-BHC	~4					
<i>I/CDIs for carcinogens</i>						
4,4'-DDE					0.7	0.3
PCBs (mixed) ^e	~31		~34		92	75

^aA tilde (~) indicates that estimated values were used in the calculation, and a blank space indicates that the parameter was undetected.

^bMelton Hill Reservoir, above Oak Ridge city input.

^cClinch River, downstream of ORNL.

^dClinch River, downstream of all DOE inputs.

^eMixed PCBs consists of the summation of Aroclors detected or estimated.