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. Chemical health effects are divided into two broad categories: adverse or systemic effects (noncarcinogens) and 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 fatality. Carcinogens cause or increase the incidence of malignant neoplasms or cancers.

Toxicity refers to an adverse effect of a chemical on human health. Every day we ingest chemicals in the form of food, water, and sometimes medications. Even those chemicals 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 is an estimate 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 (mg/kg-day). These values are given in Table H.1.

Values for reference doses 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 reference doses. Uncertainty adjustments may be made if animal toxicity data are extrapolated to humans to account for human sensitivity, extrapolated from subchronic to chronic no-observed-adverse-effect-levels, extrapolated from lowest-observed-adverse-effect-levels to no-observed-adverse-effect-levels, and to account for database deficiencies. The use of uncertainty factors in deriving reference doses is thought to protect the sensitive human populations. The Environmental Protection Agency (EPA) maintains the Integrated Risk Information System data base, which contains verified reference doses and up-to-date health risk and EPA regulatory information for numerous chemicals.

Primary Maximum Contaminant Levels

For chemicals for which reference doses are not available in the Integrated Risk Information System, national primary drinking water maximum contaminant levels, expressed in milligrams of chemical per liter of drinking water, are converted to reference dose 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 (mg/kg-day). These values are given in Table H.1.

Dose Term for Carcinogens

Slope Factor

A slope factor is a plausible upper-bound estimate of the probability of a response per unit intake of a chemical during a lifetime. The slope factor 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-day). These values are given in Table G.1.

The slope factor 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 other words, a certain chemical concentration in food or water could cause a risk of one additional cancer for every 10,000 (10^{-4}) to 1,000,000 (10^{-6}) exposed persons, respectively.

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

Elements			Compounds		
Chemical	Factor	Reference[a]	Chemical	Factor	Reference[a]
Antimony	4.0E–04	RfD	Acetone	9.0E–01	RfD
Arsenic	3.0E–04	RfD	Aroclor-1254	2.0E–05	RfD
	1.5E+00	SF	Aroclor-1260	2.0E–05	RfD[b]
Barium	2.0E–01	RfD	Chlordane (alpha,beta)	5.0E–04	RfD
Beryllium	2.0E–03	RfD		3.5E–01	SF
Boron	2.0E–01	RfD	4,4′-DDD	2.4E-01	SF
Cadmium	5.0E–04	RfD	4,4′-DDE	3.4E–01	SF
Chromium VI	3.0E–03	RfD	PCBs (mixed)	2.0E+00	SF[f]
Lead	1.4E–04	*c,d*	Toluene	8.0E–02	RfD
Manganese	1.4E–01	RfD			
Mercury	3.0E–04	RfD[e]			
Molybdenum	5.0E–03	RfD			
Nickel	2.0E–02	RfD			
Selenium	5.0E–03	RfD			
Silver	5.0E–03	RfD			
Strontium	6.0E–01	RfD			
Thallium	5.7E–05	*c,g*			
Uranium	3.0E–03	RfD			
Vanadium	7.0E–03	RfD			
Zinc	3.0E–01	RfD			

[a]RfD: reference dose (mg kg^{-1} day^{-1}); SF: slope factor (risk per mg/kg-day).

[b]The RfD for Aroclor-1254 is also used for Aroclor-1260.

[c]The water quality criteria (WQC) are given in units of micrograms per liter. To convert the concentration to an RfD (mg kg^{-1} day^{-1}), divide by 1000 (to convert to milligrams per liter), multiply by the consumption rate (2 L/day), and divide by the mass of a reference man, 70 kg.

[d]This value is based on the 2004 Tennessee WQC for lead for domestic water supplies.

[e]An EPA-approved oral chronic RfD, SF, or other guideline for elemental mercury in water or aquatic organisms is not available. Most guidelines refer to "recoverable" or inorganic mercury. RfD values exist for several inorganic mercury salts. The EPA oral RfD for soluble mercuric chloride ($HgCl_2$) is 3.0E–04 mg/kg/day.

[f]The 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.

[g]This value is based on the 2004 Tennessee WQC for thallium for domestic water supplies, which reflects the maximum contaminant level value (2 µg/L).

Measuring Chemicals

Environmental samples are collected in areas surrounding the ORR and are analyzed for those chemical constituents 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 sensitive; however, they have limits below which they cannot detect the chemicals of interest. Concentrations 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 (~) or "J." The tilde indicates that estimated values were used in estimating the average concentration of a chemical. "J" indicates that the chemical concentration is detected below the reported analytical detection limits of the instruments and is recorded by the laboratory as an estimated value.

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 from the river (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 is determined. For chemicals, the dose to humans is measured as milligrams per kilogram-day (mg/ kg-day). 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:

$$I = \frac{CW \times IR \times EF \times ED}{BW \times AT},$$

where

I	=	intake (mg/kg-day)
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 for noncarcinogens (365 days/year × *ED*) or for carcinogens (365 days/year × 70 years)

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

$$I = \frac{CW \times IR \times EF \times ED}{BW \times AT},$$

where

I	=	intake (mg/kg-day)
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 for noncarcinogens (365 days/year × ED) or for carcinogens (365 days/year × 70 years)

Calculation Methodology

Current risk assessment methodologies use the term hazard quotient to evaluate noncarcinogenic health effects. Because intakes are calculated in milligrams per kilogram per day in the hazard quotient methodology, they are expressed in terms of dose. The hazard quotient is a ratio that compares the estimated exposure dose or intake (I) to the reference dose as follows:

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

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

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

To evaluate carcinogenic risk, slope factors are used instead of reference doses. In previous reports, the estimated dose from ingesting water or fish from rivers and streams surrounding the ORR is compared to the chronic daily intake I(10^{-5}) derived from assuming a human lifetime risk of developing cancer of 10^{-5} (1 in 100,000). However, as in typical human health risk assessments, risk levels are derived as follows:

$$R = I \times SF,$$

where
R = risk
I = estimated intake or (mg/kg-day),
SF = slope factor, oral (risk per mg/ kg-day).

To estimate the risk of inducing cancers from ingestion of water and fish, the estimated dose or intake (I) is multiplied by the slope factor (risk per mg/kg-day). As mentioned earlier, 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). The tilde (~) indicates that estimated values were used in estimating the average concentrations of a chemical.