SHEDS-Wood

Stochastic Human Exposure and Dose Simulation Model
for a
Wood Preservative Exposure Scenario

Technical Manual:
Using SHEDS-Wood for the Assessment of Children's Exposure and Dose from Treated Wood Preservatives on Playsets and Residential Decks

Prepared by

V.G. Zartarian, J. Xue, H. Özkaynak

U.S. Environmental Protection Agency
Office of Research and Development
National Exposure Research Laboratory

G. Glen, C.Stallings, L. Smith

ManTech Environmental Technology, Inc.

and

W. Dang, N. Cook, D. Aviado, S. Mostaghimi, J. Chen

U.S. Environmental Protection Agency
Office of Prevention, Pesticides and Toxic Substances
Office of Pesticide Programs, Antimicrobials Division

SHEDS-Wood Version 1.0

Table of Contents

List of Figures

List of Tables

List of Equations

Executive Summary

The U.S. Environmental Protection Agency's (EPA) Office of Research and Development (ORD), National Exposure Research Laboratory (NERL), in conjunction with the EPA's Office of Prevention, Pesticides, and Toxic Substances (OPPTS), Office of Pesticide Programs (OPP) has developed a modeling methodology to conduct a probabilistic exposure and dose assessment for chemicals in wood treatment preservatives, and applied this methodology to a hypothetical case study for demonstration purposes. Such a methodology could be applied to help determine the potential health risks to children from contact with treated wood in playsets and home decks and contaminated soil around these structures.

In October 2001, OPP presented a proposed deterministic exposure assessment approach, specific to Chromated Copper Arsenate (CCA), to the FIFRA (Federal Insecticide, Fungicide, and Rodenticide Act) Scientific Advisory Panel (SAP). One of the primary recommendations was to use a probabilistic model to predict variability of absorbed doses in a given population of interest. Following the SAP meeting, OPP requested assistance from ORD in addressing this recommendation by using NERL's physically-based, Monte Carlo, probabilistic SHEDS model (Stochastic Human Exposure and Dose Simulation model). The methodology and assessment presented in this document focuses only on exposures and absorbed doses (both average daily doses (ADDs) and lifetime average daily doses (LADDs)); it does not address risk estimates. Absorbed doses obtained via this methodology could be used by OPP to conduct separate risk analyses.

To demonstrate the methodology, SHEDS was applied to assess the exposure and dose of 1 to 6 year-old children to a hypothetical "Chemical X" and "Chemical Y" from a wood treatment preservative via contact with playsets and home decks. The Chemical X scenario corresponds to a "lower exposure" cold climate scenario; Chemical Y to a "higher exposure" warm climate scenario. Three exposure time periods were considered: short-term (one day to one month), intermediate-term (one month to six months), and lifetime (6 years over a 75 year lifetime). Dermal contact with and ingestion of the chemical in both soil and wood residues were considered for a population of children simulated using time-location-activity diaries from EPA's Consolidated Human Activity Database (CHAD). Model algorithms and input values used by SHEDS for the wood treatment preservative scenario were selected by OPP and ORD. Recommendations by the SAP were incorporated to the extent possible in the example assessment.

The primary outputs obtained using SHEDS for the two case studies and different time periods include the following: population cumulative density functions (CDFs) of total absorbed dose (ADD and LADD) and absorbed dose by each exposure pathway; sensitivity analyses identifying critical input variables with respect to population variability; and uncertainty analyses identifying critical input variables with respect to uncertainty in percentiles of population distributions. Children contacting playsets only were considered as well as children who contact both playsets and home decks. For the chemical-specific model inputs, data were fabricated by OPP and ORD to correspond to a "lower exposure" and a "high exposure" scenario. Most of the inputs, however, such as activity-related inputs and exposure factors, are independent of the chemical being addressed. Thus, where possible, distributions were fit to the best available data sets. These data are presented in this report in addition to the general exposure assessment methodology.

Introduction

Wood treatment preservatives containing pesticidal compounds protect wood from deterioration and are predominantly used to pressure treat lumber intended for outdoor use in constructing a variety of residential landscape and building structures, as well as home, school, and community playground equipment. Children may potentially be exposed to the pesticide residues remaining on the surfaces of the treated wood structures as well as the residues leached into the surrounding soil. The EPA is aware of increased concerns raised by the general public and state regulatory agencies regarding the safety of treated wood for residential applications. The children's exposure and dose assessment presented herein evaluates exposure routes and pathways anticipated as realistic, considering activity patterns and behavior of young children near home playsets, non-home playsets, and home decks. Children's exposure may occur through touching treated wood and contaminated soil near treated wood structures, placing the hands in the mouth after touching treated wood, and ingesting contaminated soil. The Stochastic Human Exposure and Dose Simulation (SHEDS) model for pesticides developed by the U.S. EPA's Office of Research and Development (ORD), National Exposure Research Laboratory (NERL) was selected by the U.S. EPA's Office of Prevention, Pesticides, and Toxic Substances (OPPTS), Office of Pesticide Programs (OPP) to conduct the probabilistic children's exposure and dose assessment for CCA. Since the methodology for a generic treated wood exposure scenario is being considered here for review, the assessment focuses on a hypothetical "Chemical X" and "Chemical Y" whose assumed residues and soil concentrations are completely independent and different than those for CCA. The Chemical X scenario corresponds to a lower exposure scenario in a cold climate. The Chemical Y scenario corresponds to a higher exposure scenario in a warm climate.

SHEDS is a probabilistic, physically-based model that simulates aggregate exposures and doses for population cohorts and multi-media chemicals of interest. This model simulates individuals from the user-specified population cohort by selecting daily sequential time-location-activity diaries from surveys contained in EPA's CHAD (Consolidated Human Activity Database; McCurdy et al., 2000; http://www.epa.gov/chadnet1). SHEDS addresses the inhalation, dietary ingestion, dermal contact, and non-dietary ingestion (via both hand-mouth and object-mouth) routes. It includes the option of 1-stage or 2-stage Monte Carlo sampling to explicitly characterize both variability and uncertainty in model inputs and outputs. Prior to this wood treatment case study, SHEDS had been developed to address three other exposure scenarios of interest to OPP: indoor crack and crevice treatment, lawn treatment, and garden treatment. For these scenarios, SHEDS can be used to simulate one day post-application exposures to individuals from a single application event or daily, weekly, monthly, seasonal, or annual

average exposures from repeated pesticide applications over a year. At the request of OPP in November, 2001, NERL has incorporated a fourth exposure scenario to assess children's exposure to wood treatment preservatives. The algorithms and methods used for this scenario are discussed in this report.

SHEDS and SHEDS-related research has been in development since 1998 and has been presented within and outside of the Agency for the past three years. A paper presenting the first generation SHEDS-Pesticides model focusing on children's residential dermal and non-dietary ingestion exposure was published in Zartarian et al., 2000. A number of other technical presentations on this research have also been made at various specialty national and international conferences and workshops. These include:

"Assessing Residential Exposure Using the Stochastic Human Exposure and Dose Simulation (SHEDS) Model," International Society for Exposure Analysis (ISEA) Conference, Charleston, SC, November 2001.

"Quantifying Aggregate Chlorpyrifos Exposure and Dose to Children Using a Physically-Based Two-stage Monte Carlo Probabilistic Model," International Society for Exposure Analysis (ISEA) Conference, Charleston, SC, November 2001.

"SHEDS-Pesticides: Model Overview and Scenario Outputs for the Aggregate Residential Model Comparison Workshop," Aggregate Residential Exposure Model Comparison Workshop, Research Triangle Park, NC, October 10-11, 2001.

"Modeling Aggregate Chlorpyrifos Exposure and Dose to Children," International Society for Exposure Analysis (ISEA) Conference, Monterey, California, October 2000.

"Estimating Children's Exposures to Pesticides Using EPA's Residential SHEDS Model," Society for Risk Analysis (SRA), Atlanta, GA, December 1999.

"A Modeling Framework for Estimating Children's Residential Exposure and Dose to Chlorpyrifos via Dermal Residue Contact and Non-Dietary Ingestion," International Society for Exposure Analysis (ISEA) Conference, Athens, Greece, September 1999.

"The Stochastic Human Exposure and Dose Simulation Model for Pesticides," Aggregate Exposure Assessment Model Evaluation and Refinement Workshop, International Life Sciences Institute, Health and Environmental Sciences Institute, Baltimore, MD, October 19-21, 1999.

"Status of Advances in Probabilistic Pesticide Exposure and Dose Modeling by ORD/NERL," EPA Office of Pesticide Program's FIFRA Science Advisory Panel Meeting, Arlington, VA, September 21, 1999.

The SHEDS-Pesticides modeling framework, excluding the wood treatment scenario, has undergone external and internal review by ORD's University Partnership Agreement (UPA) peer review panel July 8-10, 2002.

Methods

OPP and ORD collaborated closely on the development and inclusion of the wood preservative scenario in the SHEDS model, including the algorithms, assumptions, and selected input values. The SAP recommendations in U.S. EPA (2001) were incorporated into this assessment to the extent possible and provided the justification for developing a probabilistic modeling assessment methodology for the wood preservative exposure scenario.

The next two sections ("General SHEDS Methodology" and "SHEDS Approach for the Treated Wood Case Study") describe the approach and algorithms used by the SHEDS model. As mentioned in the introduction, the SHEDS model for pesticides developed by NERL currently includes 3 exposure scenarios in addition to the wood preservative scenario (lawn, garden, indoor crack and crevice treatments). The "General SHEDS Methodology" section is included to give the reader an understanding of how SHEDS functions as an aggregate human exposure model. Not all of the routes described in this section (e.g., dietary) are relevant to the wood preservative scenario described in the rest of the technical report. The "SHEDS Approach for the Treated Wood Case Study" describes algorithms specific to the wood preservative scenario.

General SHEDS Methodology

The SHEDS model generates both exposure and dose time profiles for a population of simulated individuals. SHEDS is a two-stage Monte Carlo model. Each simulated person is assigned demographic properties and other characteristics that are generated randomly using specified input distributions, representing the first stage (variability) of random selection. A set of such individuals represents a random sample of the selected population. If run in its two-stage Monte Carlo mode, SHEDS also varies the input distributions themselves according to user-specified instructions, which constitutes the second stage (uncertainty) of random selection used in multiple iterations of the code. A more detailed explanation of variability and uncertainty is provided in subsequent sections of this report.

Exposure time profiles for individuals are the basis of the SHEDS exposure calculations. These are plots of instantaneous exposure (mass, concentration, or mass loading at the external human boundary) against time that preserve within-day peaks and variability as an individual moves throughout his or her day (Figure 1). These exposure profiles can yield toxicologically relevant dose profiles, and ultimately, improved risk estimates. They are constructed separately for each of the four exposure routes included in SHEDS: inhalation, dietary ingestion, dermal contact, and non-dietary ingestion (from both hand-to-mouth and object-to-mouth contact). The time step for these profiles is variable; it matches the duration of the CHAD diary location-activity events

which may range from one minute to one hour. Each diary event corresponds to one *macroactivity* for which the parameters relevant to exposure (e.g., the person's location and activity, the ambient chemical and surface residue concentration, and rate of contact) are assumed to remain constant. SHEDS currently includes a simple 3-compartment pharmacokinetic module which can be used to calculate time profiles for blood and urine dose on the same basis as for exposure.

To generate a daily inhalation exposure profile, SHEDS samples from indoor or outdoor air concentration distributions corresponding to locations occupied by the sampled individual's diary. The air concentrations are then combined with values for breathing volume, determined from basal metabolic rates and activity-specific energy expenditure distributions for the diary-reported activities.

Dermal exposure is modeled by combining dermal transfer coefficient information with surface residues and time spent touching surfaces. Residues and soil are assumed to remain on the skin until removed via absorption, bathing, hand washing, or hand mouthing. SHEDS assumes that a sampled individual bathes or showers at least once a day, even if a bathing event was not reported in the CHAD diary, based on the median of Table 8-9 of the Child-Specific Exposure Factors Handbook (USEPA, 2000). For bathing related locations and activities, a washing removal efficiency is applied to the profile to account for the reduction in dermal loading.

Non-dietary ingestion exposure from hand-to-mouth and object-to-mouth transfer is simulated by combining dermal hand loading or object residues with surface area of hands or objects inserted into the mouth, frequency of mouthing activities, and saliva removal efficiency. Because of this, non-dietary ingestion via hand-to-mouth contact is subtracted from the dermal hand exposure profiles.

The dietary module in SHEDS uses the latest USDA/EPA recipe files and 1994-1996, 1998 Continuing Survey of Food Intakes by Individuals (CSFII) consumption data, which includes about 10,000 food types and 21,660 person-days. CHAD individuals are currently matched with CSFII individuals by age and gender, and for each CSFII person, the reported consumption data are combined with sampled residue values in foods as eaten to yield a modeled mass of residue ingested by meal. To obtain residue values in foods as eaten, SHEDS applies the recipe files to the CSFII food types to break the food into raw agricultural commodities (RAC), and then combines the RAC residues with available use and processing factors.

To simulate one day post-application exposures for a population cohort, SHEDS samples a single diary and combines the sequential location-activity durations with sampled values from user-specified probability distributions for environmental media concentrations (either calculated from user-specified application rates or sampled from user-specified distributions of measured

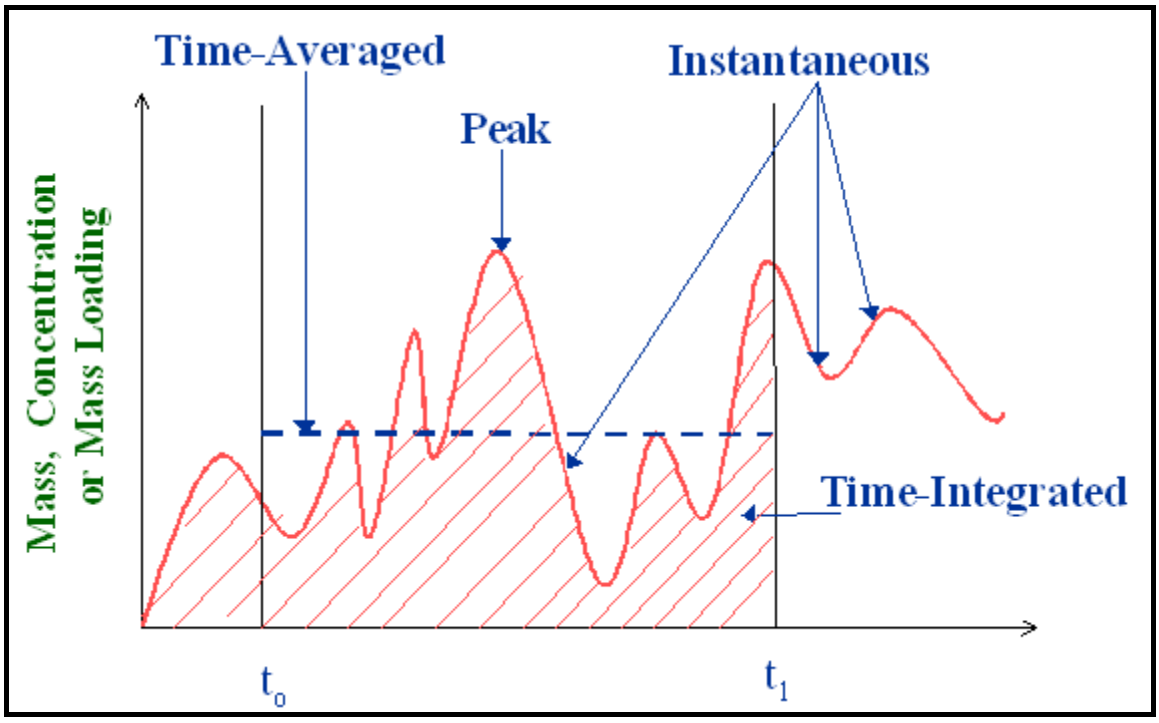

Figure 1. Hypothetical exposure profile for an individual.

values) and exposure factors (e.g., saliva and washing removal efficiency, skin surface area contacted, surface area of objects mouthed) into route-specific algorithms described above to construct daily exposure time profiles (Figure 2).

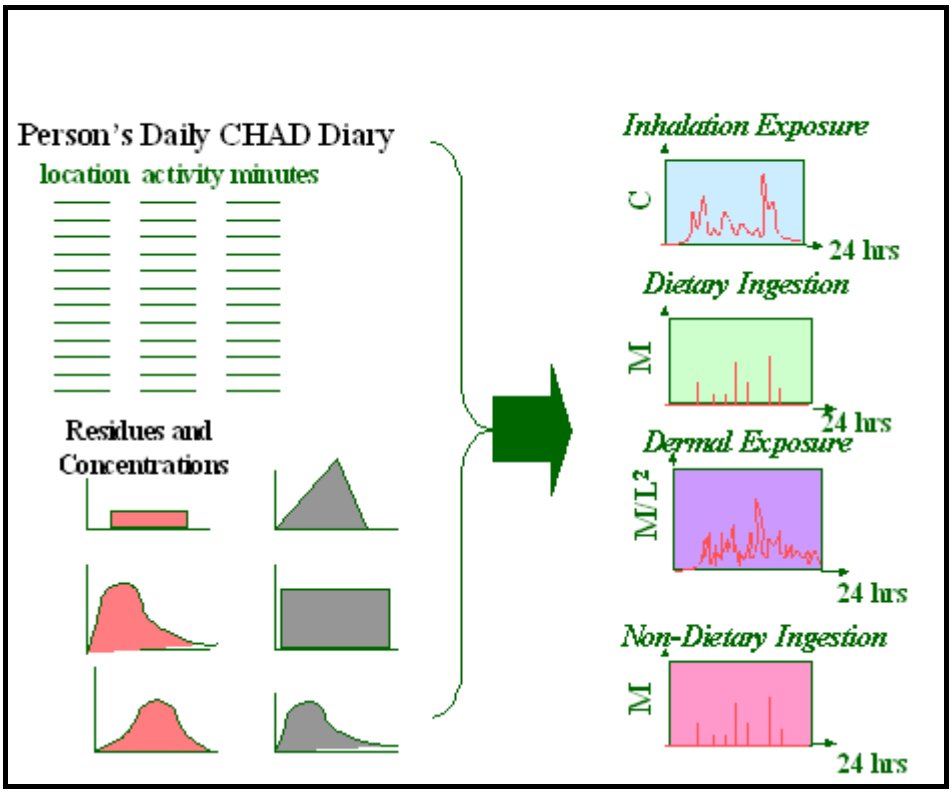

Figure 2. Calculation of exposure profiles in SHEDS.

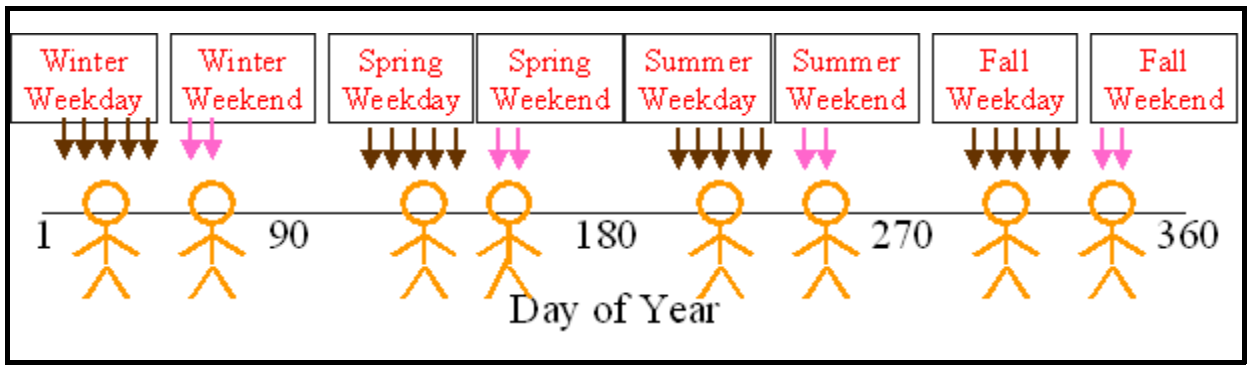

Figure 3. SHEDS approach for simulating one-year activity patterns.

SHEDS typically simulates exposures over a sequence of days rather than a single day. Most of the studies in CHAD are cross-sectional, representing snapshots of one day's activities in a person's life. This poses challenges for simulating longitudinal activity patterns. Two extreme options are to assume either an individual does the same activity pattern every day of the year or to assume independent activities over consecutive days. The alternate approach taken by SHEDS is intended to optimize intra- and inter- person variability (Figure 3). Eight CHAD diaries from the same age-gender cohort are used to simulate a child's year. These eight diaries consist of two from each of the four seasons, one sampled on a weekend and the other on a weekday (Monday-Friday). A composite activity dairy is assembled from these eight by concatenating copies according to the season and weekdays on the calendar. For simulation periods shorter than one year, the start date is selected at random, subject to the requirement that the stop date occur within the same year.

Along with the composite activity diary, SHEDS sets specific values for each person for a number of input parameters. Most parameters have fixed values over time for a given person but vary from one person to another, although some can vary over time even for one person (this is specified in the SHEDS input files). The parameters determine the presence or absence of potential sources such as decks and playsets, environmental media residues and concentrations, exposure factors (e.g., transfer coefficients, saliva and washing removal efficiency, skin surface area contacted, surface area of objects mouthed) and physiological parameters that affect dose (e.g., absorption and elimination rate constants, body mass, and basal metabolic rate).

The SHEDS model follows the simulated individual through time, using each activity diary event as a potential exposure event. Exposure is estimated differently for each of the three main routes (inhalation, dermal, ingestion). For the latter two, exposure persists over time until it is eventually absorbed or removed. This is not the case for inhalation because the rate constant for absorption is rapid compared to the duration of a diary event, and any mass not absorbed is

assumed to be exhaled, so exposure does not persist beyond the current event. The temporal sequence of events is central to the SHEDS methodology. For a fixed dermal exposure received at a given time, the absorbed dose will be much less if the person washes it off quickly as compared to leaving it on the skin for a long time.

Even if a given diary event does not result in additional (new) exposure, there will be changes to the existing exposure burden via absorption and (possibly) removal. Since absorption is ongoing, it can occur in locations far removed from the source of the exposure. Changes will also occur to the three measures of dose used in SHEDS: these are the absorbed dose, the blood dose, and the eliminated dose. The absorbed dose is the amount entering the body. It is a cumulative measure that is reset to zero at midnight on each simulation day. The blood dose measures the current amount present in the blood. This is an instantaneous measure like exposure, and each event starts at the same dose with which the previous event finished. Additions to blood dose come from absorption through the skin, the gastrointestinal (GI) tract and the lungs, and subtractions to the blood dose arise from elimination via urine. This last term constitutes the eliminated dose. Like the absorbed dose, it is measured cumulatively starting at zero each day at midnight.

The event-based time profiles for exposure and dose produce very large data sets. There are typically about 14,000 events per year and for each event there are numerous input and output exposure and dose variables to be evaluated. A variability run may consist of several thousand such profiles, and an uncertainty run will be larger still (typically over 100 replications of separate variability runs). For practical reasons SHEDS summarizes the data for each individual before proceeding to the next person. Measures such as average daily dose (ADD) or, if appropriate, lifetime average daily dose (LADD), are derived for each individual. Since SHEDS not only tracks the total dose but also tracks the route and pathway-specific portions of the total dose, summary statistics are derived for these variables as well. This permits the display of results such as the fraction of dose originating from the various SHEDS pathways.

Apart from using the built-in dose profile generation, the exposure profiles from SHEDS could be used as input to another pharmacokinetic model. A more elaborate model, such as NERL's Exposure-Related Dose Estimation Model (ERDEM), might include a number of target organs and multiple metabolic pathways. A simpler model might estimate dose using route-specific absorption fractions. For this latter approach, the event-based time profiles are unnecessarily detailed and the daily summary statistics provided by SHEDS would be sufficient to estimate dose. For a more sophisticated physically-based pharmacokinetic model (PBPK), the detailed SHEDS exposure information for each macroactivity within a day could be saved and exported rather than averaged.

The results from a SHEDS model run are presented differently for 1-stage and 2-stage Monte Carlo runs. For a single stage run (variability only), the process for obtaining information from individual exposure and dose profiles (described above) is repeated hundreds to thousands of times to construct a distribution over the simulated population for each selected exposure or dose variable (Figure 4). These distributions are characterized by the standard statistical parameters such as mean, standard deviation, minimum, maximum, median, and various percentiles. They can be graphed as boxplots or cumulative density functions (CDFs), or simply tabulated. Results

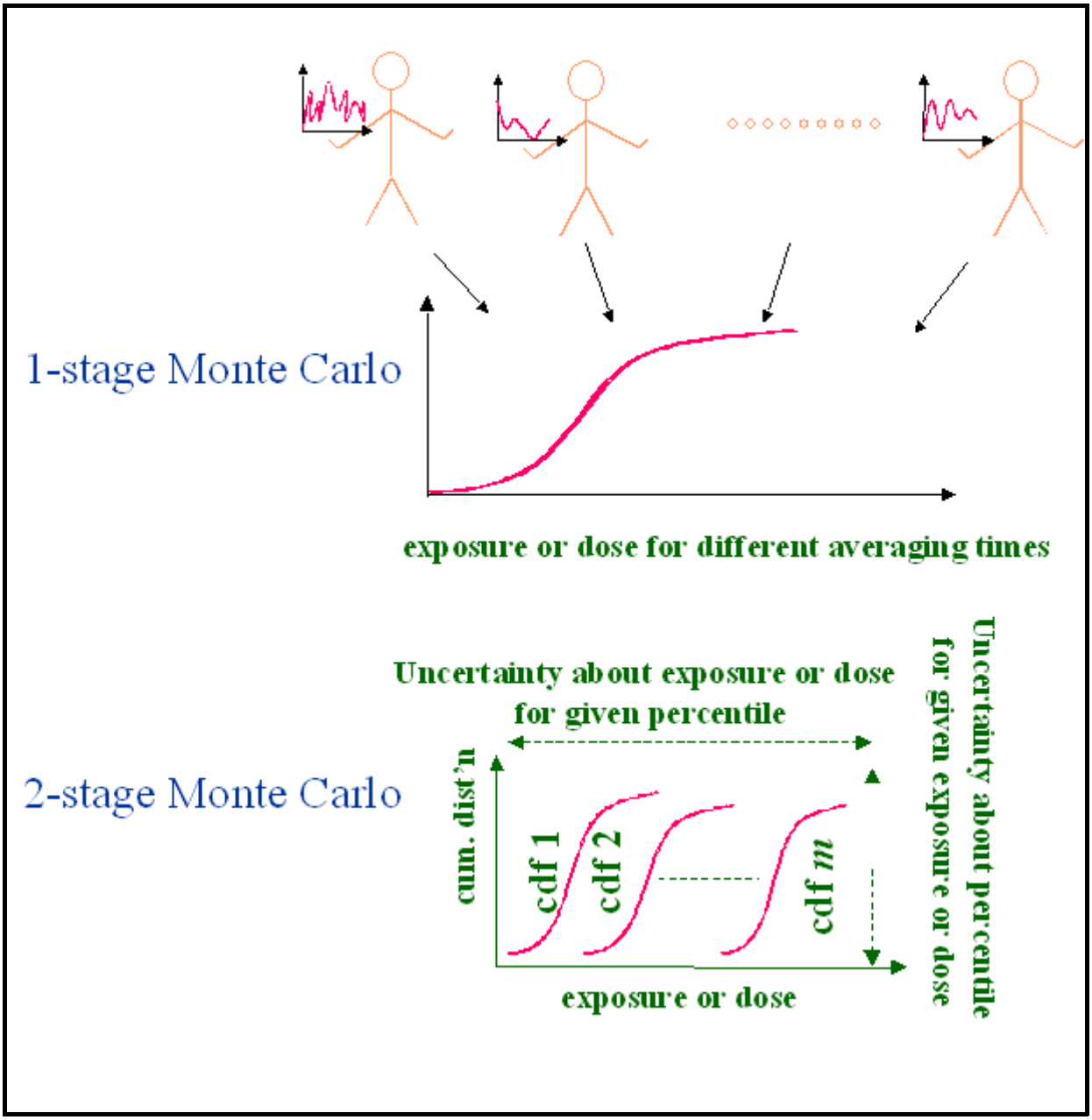

Figure 4. SHEDS computational sequence for estimating population aggregate dose.

may be over the entire simulation or presented separately for various time periods such as the number of days post-application. For a two-stage run (uncertainty), the results for specific individuals are not retained. Instead, on each iteration of the uncertainty loop, the results for each exposure or dose variable are summarized by selected statistical parameters before proceeding to the next iteration. Additionally, the specific values for each of the uncertain input parameters are noted. At the end of the model run, the relationship between input parameters and the output statistics can be examined using either regression or correlation methods. Details on SHEDS sensitivity analyses and uncertainty analyses are given in the next section.

SHEDS Approach for the Treated Wood Case Study

Figure 5 illustrates the SHEDS interface screen that allows the user to specify the population cohort and scenario of interest for the wood treatment preservative exposure scenario. Because the population of primary interest to OPP for this scenario is children ages 1 to 6 years who contact treated wood, and because the sample size in CHAD for children with reported time in playgrounds was too small for modeling, all CHAD diaries for children ages 1 to 6 years that reported some time outdoors (approximately 200 children in each age-gender cohort) were provided to SHEDS. The distribution of total time outdoors for 1 to 6 year-olds in CHAD was compared against total time outdoors for children 1 to 6 years who specified that they spent time outdoors in playgrounds (the assumption is that children who visit playgrounds represent children in the population of interest). These two distributions were very similar, which justifies the use of all diaries with reported time outdoors. It was then assumed that all children in the sampled population spend time at playgrounds playing

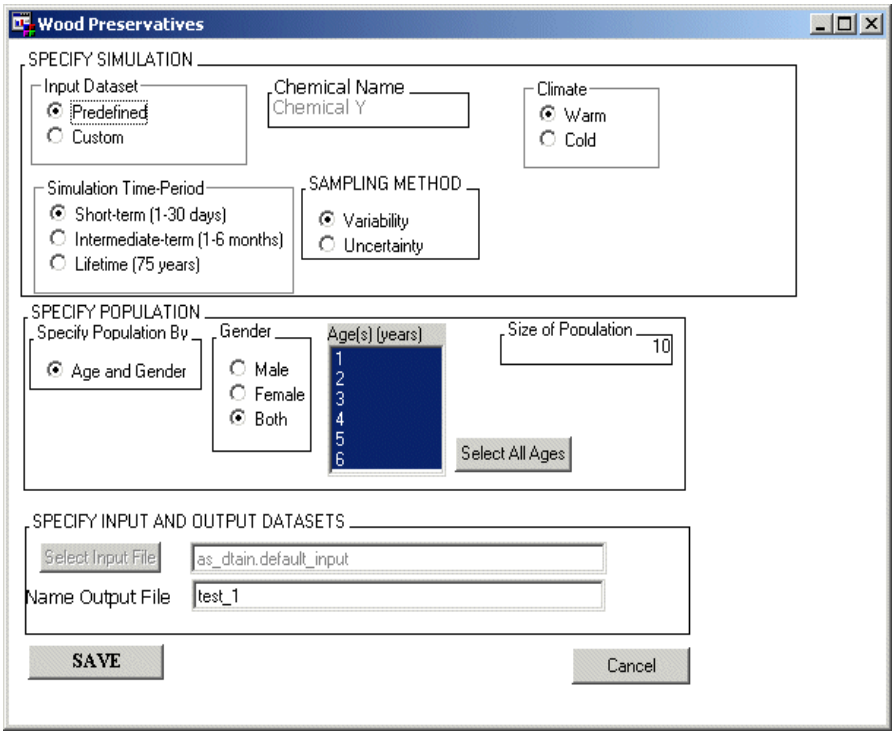

Figure 5. SHEDS interface screen for model scenario specification.

on treated playsets. These children may or may not also play on treated home playsets and/or treated home decks. Thus, the population of interest for this case study is 1 to 6 year-old children in the United States who contact treated wood on non-home playground playsets, at a minimum. A subset of these children also contacts treated wood on other non-home playsets (e.g., playsets at another child's home) and/or home playsets and/or home decks.

Playsets may be contacted at home, away from home, or both. Contacting both home and non-home playsets on the same day usually leads to higher maximum exposures than contacts on different days. The SHEDS input parameter labeled "#days/yr a child spends on both treated home and treated non-home playsets" (see Appendices 2 and 3) allows the user to specify the likelihood of such co-occurrence. Note that the term 'co-occurrence' here does not imply simultaneous contact; it means contact during different activity diary events on the same day.

For the treated wood case study, three exposure time periods were considered: short-term (one day to one month), intermediate-term (one month to six months), and lifetime (6 years of exposure over a 75 year lifetime). SHEDS simulates exposures for one individual at a time. To determine the lifetime exposure for each individual, activity diaries are matched by age, gender, and potential exposure for a six year span. To provide some consistency from year to year in the behavior of each child, each child is classified as a low-, middle-, or high- potentially exposed child, based on the amount of time spent in outdoor locations. In order to assemble a composite activity diary that represents the child, the diaries belonging to the same category as the child are preferentially selected. In this way, a child who spends a relatively long period of time outdoors (that is, potentially in contact with treated wood) at one age will also have a relatively high time outdoors at other ages, and vice versa.

This version of SHEDS does not separate CHAD diaries by warm and cold regions due to sample size considerations and small differences in time spent outdoors among geographic locations for CHAD diaries. The SHEDS user, however, can conduct warm weather and cold weather simulations by modifying input values for soil concentrations, wood surface residues, dermal transfer coefficients, and other parameters (as was done in the Chemical X and Chemical Y scenarios).

For lifetime simulations, even though a full six year activity diary could be processed at one pass, SHEDS breaks it into six one-year segments. The reason is that certain modeling parameters are age-dependent (e.g., body weight, frequency of hand-mouth activity) and their values are updated annually as the child ages. For each 1-year diary, the model steps through the sequence of events in chronological order, determining the additions or subtractions to exposure and dose at each

diary event. A one-year diary contains a variable number of events, usually between 12,000 and 15,000. The diaries indicate whether the child is indoors or outdoors and whether she or he is at home or away from home, but the diaries do not contain enough detail to determine when a child is specifically near a treated deck or playset. Thus, SHEDS includes a user-specified probability for the fraction of time outdoors at home (for home playsets and decks) or away from home (for non-home playsets) that the child spends on or around playsets and/or decks, and for the fraction of time contacting residues versus soil. For example, if a diary indicates that the child spent 2 hours on a given day outdoors away from home, and the fraction of time spent contacting treated non-home playsets was set to 0.5 in the SHEDS input file, then on that day the child is assumed to spend 1 hour contacting treated non-home playsets. If the outdoor time covers more than one diary event, then exposure contact occurs for the stated fraction (0.5 in this case) of the duration of each such event. Figure 6 indicates the SHEDS approach for simulating an exposure event. As indicated previously, once incurred, exposure remains with the child as he or she moves to other events. Gradually, absorption and removal processes will reduce exposure until a new exposure contact occurs. This means that the various dose measures might not peak until some later time when the child is no longer near a source of exposure.

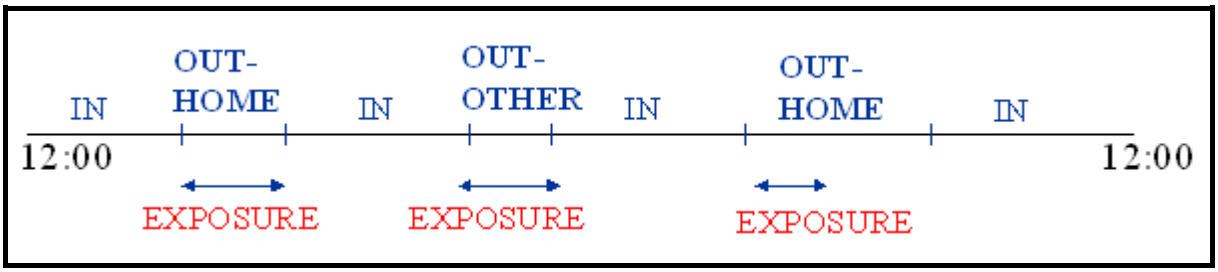

Figure 6. Schematic of SHEDS approach for simulating exposure events.

For each exposure for a given child, it is assumed that the same soil concentration and surface residues persist from day to day and from year to year (i.e., the child contacts the same playset and deck over 6 years, and the residues and soil concentrations for a given playsets or deck do not vary over time). This assumption was based on the facts that (1) typically, variability in environmental concentrations is much greater across geographic locations than across time for a given location, and (2) insufficient data are available for longitudinal concentration and residue information to vary these parameters for a given person in the assessment. However, if the concentration and residue parameters have variability distributions, then new values will be randomly generated by the model from one child to the next.

There are eight exposure pathways considered in SHEDS for the wood treatment assessment: dermal soil contact near decks; dermal residue contact from decks; soil ingestion near decks; residue ingestion from decks (via wood-to-hand-to-mouth pathway); dermal soil contact near playsets; dermal residue contact from playsets; soil ingestion near playsets; and residue ingestion from playsets (via wood-to-hand-to-mouth pathway). Soil ingestion includes the soil-to-hand-to-mouth pathway as well as direct ingestion of soil (e.g., pica behavior). To estimate the exposure, SHEDS simulates route-specific exposure time profiles over the child's year by combining the diaries with soil concentrations, residues, and exposure factors. The model samples input values (user-specified point estimates for deterministic sensitivity analyses, and values sampled from user-specified distributions for probabilistic analyses), and inserts them into route-specific algorithms presented in Appendix 1 to yield a 1-year exposure profile. The generation of exposure time profiles that preserves variability of an individual's exposure within a day allows for estimation of dose via pharmacokinetic or PBPK models. However, for this assessment OPP chose to apply route-specific absorption fractions to each route-specific exposure profile to obtain absorbed dose profiles. SHEDS converts daily absorption fractions to hourly absorption rate constants by dividing by 24. Example SHEDS-generated absorbed dose profiles are presented in Figure 7.

To obtain short-term absorbed dose estimates, SHEDS selects a random 15-day period within the given year and determines average exposure for that period. For intermediate-term estimates, SHEDS uses a random 90-day period. To determine lifetime average daily dose (LADD), SHEDS selects six single-year profiles (for a 1-yr-old, 2-yr-old, 3-yr-old, 4-yr-old, 5-yr-old, 6-yr-old) by correlating "high", "medium", and "low" potential exposure children (and also matching children by age and gender), assigning zero exposure for 7 to 75 years for that simulated child, then computing the LADD over the 75 years (Figure 8).

The steps described above are for estimating the absorbed dose for a single child. SHEDS then repeats this process as many times as requested (often more than a thousand iterations) to obtain population estimates. Statistical weights derived from the United States Census (U.S. Census Bureau, 2000) are applied so that population sampling is proportional by age and gender to reflect the U.S. population. The population CDFs reflect variability of doses due to differences in both the time children 1-6 years old spend contacting treated wood, residues and concentrations contacted by children, and exposure factors that affect how much of the chemical reaches and enters a child's body after contact. In addition to producing CDFs and summary statistics tables for ADD and LADD for the 2 chemicals (in 2 different climates) and 3 time periods, SHEDS computes the contribution to absorbed dose from each of the 8 different exposure pathways.

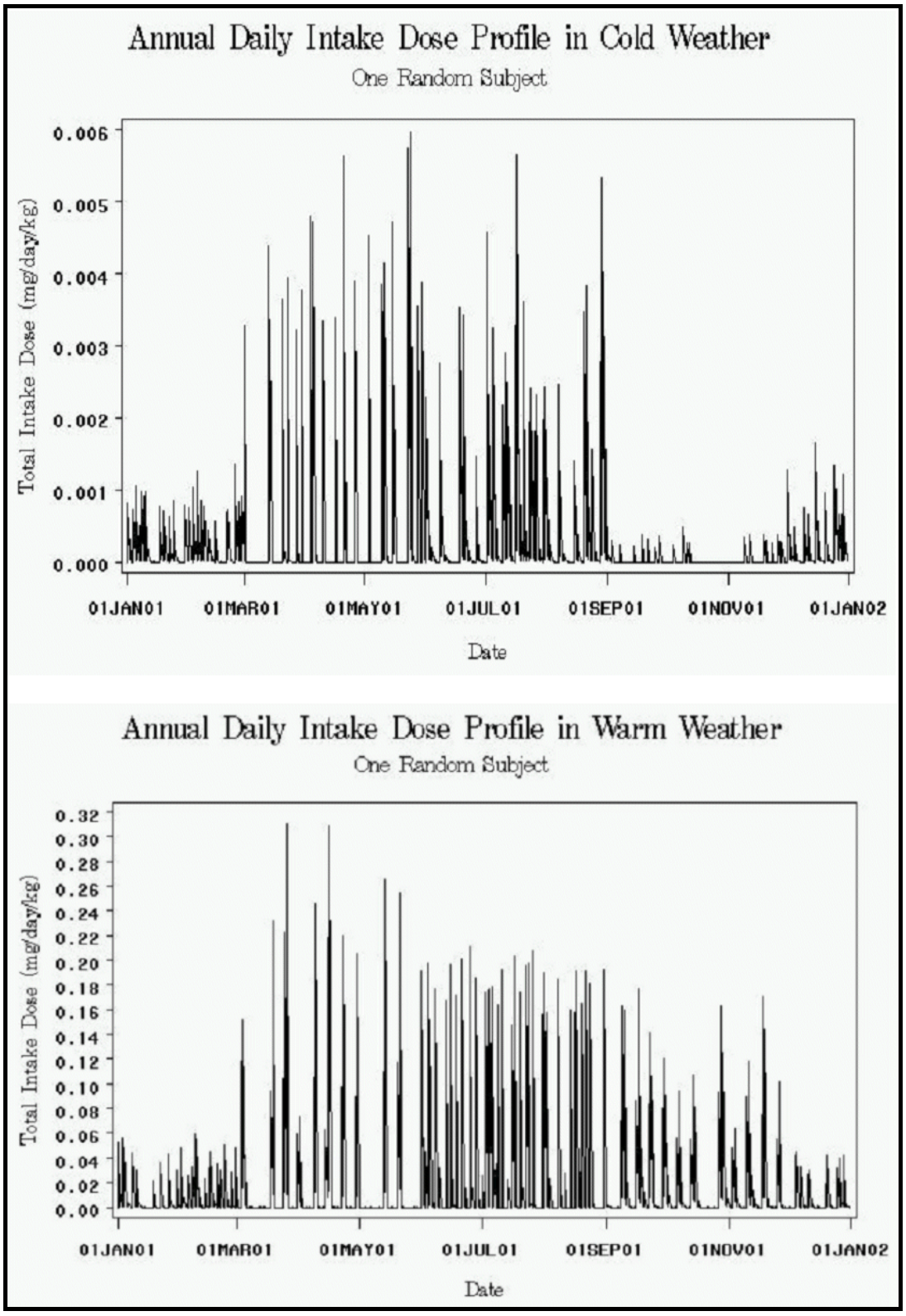

Figure 7. Example SHEDS annual daily dose profiles.

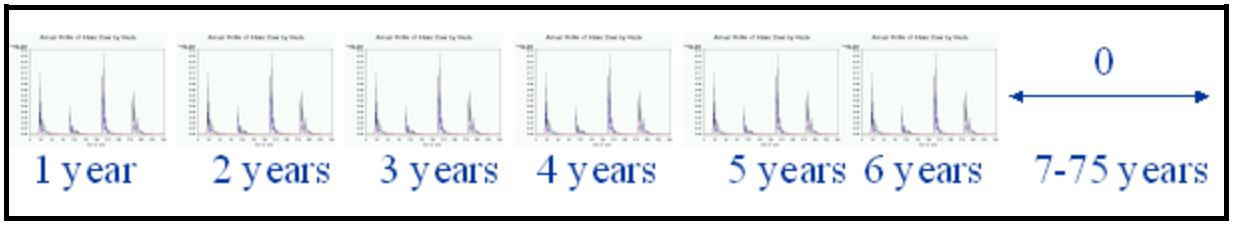

Figure 8. SHEDS algorithm for computing LADD.

Methods for Sensitivity Analyses

To demonstrate the SHEDS methodology for sensitivity analyses, these were conducted for the intermediate-term scenario for Chemical Y using 2 separate deterministic approaches. In the first approach, all independent variables were fixed as point estimates ("medium values"). For uniform and triangular model input distributions in the probabilistic analyses, the mean of the minimum and maximum values was used as the point estimate. For normal and lognormal distributions, the mean and geometric mean were used, respectively. Absorbed dose estimates were obtained with SHEDS by first increasing and then decreasing the medium values of model inputs by a factor of two (for "high" and "low" input values, respectively). With a total of 30 independent variables set to low, medium, and high values, and using 500 simulations per run, the total data size was 45,000 (30 variables * 3 values per variable * 500 simulations). The difference in predicted results between the low, medium, and high inputs was assessed by computing the ratio of medium to low, high to medium, and high to low absorbed doses. This provides information on the magnitude of sensitivity of each input to the LADD.

The second method of sensitivity analyses was to apply multivariate stepwise regression to all of the data generated with the first deterministic sensitivity analysis methodology (using all of the 45,000 data points). Unlike the first method, stepwise regression accounts for collinearities among independent variables. Using the multiple stepwise regression results the independent variables were ranked by their partial R^2 correlation coefficients to assess the relative importance of input variables based on contribution to population variance. Results from these two complementary approaches were analyzed to rank importance of inputs as a function of the sensitivity of predicted dose results on corresponding input variables.

Methods for Uncertainty Analyses

SHEDS uses 2-stage Monte Carlo sampling to conduct uncertainty estimates. Three statistical methods were used to analyze SHEDS model estimates of absorbed dose for the Chemical Y lifetime scenario: Spearman correlation, Pearson correlation, and multivariate stepwise regression. A user-specified number (M) of uncertainty runs (simulated populations) are

conducted, simulating N children per uncertainty run. For uncertainty analyses, SHEDS samples from the uncertainty distributions specified in the model input files (see Appendices 2 and 3). For example, suppose the model input for a particular parameter is a uniform distribution with minimum=a and maximum=b, and the uncertainty distributions for the minimum and maximum are uniform(a-c,a+c) and uniform(b-d,b+d), respectively (where c and d are values determined by the researcher). For M uncertainty runs with N people per population, SHEDS would sample M minimum values from uniform(a-c,a+c) and M maximum values from uniform(b-d,b+d) to obtain M different uniform distributions, representing M different populations. For each of those populations, N individuals are simulated using 1-stage Monte Carlo sampling (i.e., randomly sampling values from all SHEDS input distributions, inserting the sampled values into the SHEDS equations for absorbed dose, then repeating N times for population estimates for each set of input parameters). Thus, many different 1-stage Monte Carlo runs (in this case, M) for variability (in this case, N people per population) are simulated in 2-stage Monte Carlo sampling. This produces M different cumulative density functions of population estimates, each reflecting variability, and all considered collectively illustrating uncertainty in model inputs.

To determine which model inputs contributed the most to uncertainty for the hypothetical Chemical Y lifetime scenario, the mean values of the 300 inputs and absorbed dose outputs were computed for each of 142 uncertainty runs. Thus, 142 numbers were obtained for each input (independent variable) and for absorbed dose (dependent variable). Spearman and correlation coefficients were computed between the dependent variable and each independent variable, and then these were ranked to identify the most important contributors to population uncertainty in model estimates. Multivariate stepwise regression was also applied to consider collinearties among independent variables, using the 142 numbers for each input and 142 absorbed dose estimates, to rank the inputs in order of relative importance by their partial R^2 correlation coefficients.

Two types of uncertainty plots can also be produced with SHEDS. In the first, a plot ("three selected population profiles" option in the SHEDS interface) appears of 3 uncertainty cumulative density functions (CDFs) for a representative low-dose population, a representative medium-dose population, and a representative high-dose population. For example, if SHEDS computes 1000 absorbed dose estimates for each of 100 uncertainty runs (i.e., "Size of Population" is 1000 and "Number of Populations" is 100 as specified by the user with the "Specify Model Scenario" button in the Main Window), there are 1000 numbers for each run, thus 100 medians that SHEDS orders. The "three selected population profiles" plot, then, is a plot of the three sets of 1000 numbers for each of the 5^{th}, 50^{th}, and 95^{th} percentiles from those ordered medians. This gives the user an idea of uncertainty for representative low-, medium-, and high-dose

populations, and also depicts the relative magnitude of variability versus uncertainty in population estimates. For each of the 3 populations, variability is the difference between the lower and upper percentiles of the individual CDFs, and uncertainty is seen as the vertical distance between the three CDFs at any of the percentiles along the x-axis.

For the second type of uncertainty plot ("all population profiles" option in the SHEDS interface), a 5^{th}, 50^{th}, and 95^{th} percentile is obtained from each of the 1000 numbers in the 100 runs, so the 3 CDF curves each represent 100 values. The uncertainty around the 5^{th}, 50^{th}, and 95^{th} percentiles is the difference between the lower and upper percentiles for the three respective curves. This second type of plot is particularly useful for regulatory decision making because it illustrates uncertainty for the entire population.

Model Inputs for Generic Wood Treatment Preservative Case Study

Appendices 2 and 3 contain a complete set of SHEDS model inputs used in the children's assessment for both variability and uncertainty analyses. In addition to distribution parameters selected, the justification for all values and sources of information are given in the notes column of these tables.

For fitting variability distributions, point estimates or uniform distributions were estimated where no data were available or where only a few data points (e.g., 5^{th} and 95^{th} percentiles) were available. Where more than a few data points were available, but not a robust data set, a triangular distribution was typically fit (e.g., frequency of hand-mouth activity outdoors). For more robust data sets, normal distributions (e.g., body surface areas used to estimate transfer coefficient) or lognormal distributions (e.g., soil ingestion rate, soil-skin adherence factor) were fit to the data. The method of moments or the maximum likelihood estimator was used to fit variability distributions other than uniform ones. Goodness-of-fit tests were applied to verify the selection.

For fitting uncertainty distributions, uniform distributions were applied to the minimum and maximum values of uniform variability distributions as well as to point estimates. The selection of minima and maxima were based on a subjective assessment of uncertainty. For the other distributions, a bootstrap method described in Frey et al. (2002) was applied. This involved (1) fitting a distribution to the original data set using the method of moments; (2) determining the parameters of interest from this distribution (e.g., geometric mean and geometric standard deviation; arithmetic mean and standard deviation; minimum, mode, and maximum); (3) sampling "B" data points from that distribution 100 different times; (4) for each of those 100 sets of "B" data points, computing the parameter values of interest; and (5) fitting distributions to the

uncertainty parameters of interest using those 100 sets of parameter values. For the Chemical X and Chemical Y case studies, the sample size "B" specified for the bootstrap resamples was based on both a subjective assessment of the uncertainty of the data set used to fit the variability distribution and on a quantitative evaluation of sensitivity of results to other sample size choices. A sample size of 3 was used for very small or highly uncertain datasets; 5 was used for slightly larger datasets; and 20 was used for even more robust or less uncertain datasets.

The use of the parametric bootstrap approach mentioned above provides the user with flexibility in selecting uncertainty distributions. This greater flexibility is of most benefit when the variability distribution is not well defined; this could result either from a paucity of data or a lack of knowledge about what kind of statistical distribution might arise from the underlying physical and biological processes. Alternatively, uncertainty distributions could be specified based on theoretical considerations. For example, if one is very confident based on a large sample of size N that the variability distribution is normal with a given mean (say, m) and standard deviation (say, s), then statistical theory may be used to assign the mean an uncertainty distribution as follows: normal with mean=m and standard deviation=$s / \sqrt{N}$. However, if one is unsure of the variability distribution, the outlined parametric bootstrap approach allows one to sample from distributions "around" this theoretically determined one.

Activity information specific to children contacting playsets and residential decks is not available. Thus, values for parameters such as days per year and minutes per day children spend on and around playsets and decks were estimated using the Child-Specific Exposure Factors Handbook (U.S. EPA, 2000) and SAP recommendations (U.S. EPA, 2001) (see Appendices 2 and 3).

For the purposes of demonstrating the SHEDS methodology, wood residues and soil concentrations for Chemical X and Chemical Y were fabricated by OPP and ORD to correspond to a "lower exposure" and "higher exposure" scenario, respectively. They do not represent actual chemicals. Lognormal distributions were used because these are typical of environmental concentrations and residues.

Distributions for the "fraction of hand with residue mouthed per mouthing event" and "frequency of hand-to-mouth activity per hour" were based on a small data set in Leckie et al. (2000) for 20 suburban children videotaped outdoors (Tables 2.5.1-2.5.39 for hand-in mouth immersion contacts). Methodologies and data in this report are still being reviewed and evaluated by the Agency. Leckie et al. (2000) estimated the "fraction of hand with residue mouthed per mouthing event" using the conservative assumption that all 5 fingers are involved in partial and total finger

immersion events, rather than weighting the surface area inserted by number of fingers mouthed. Thus, a fraction of 20% was applied to the Leckie et al. (2000) estimates to account for the facts that, typically, fewer than 5 fingers are inserted into the mouth, and that not all of the skin that enters the mouth is loaded with residue.

Input values for various other exposure factors used in the SHEDS exposure algorithms were taken from OPP's Residential Exposure Standard Operating Procedures (SOPs) (U.S. EPA, 1997a), recommendations by OPP's FIFRA Scientific Advisory Panel (U.S. EPA, 2001), EPA's Exposure Factor Handbook (U.S. EPA, 1997b), or peer-reviewed publications. To calculate children's body weight and surface area for this assessment, the Lifeline™ model approach was used (The Lifeline Group, Inc., 2000). This involves equations for body weight, height, and surface area that preserve correlations among those parameters between different ages for a given person.

The SAP recommended addressing exposure of children with pica in the population distributions. The EPA Exposure Factors Handbook (U.S. EPA, 1997b) proposed to use a value of 10 g soil ingestion/day, with low levels of confidence, for children with pica behavior for use in acute exposure assessments. EPA recommended the upper percentile soil ingestion rates for children as 400 mg/day and 200 mg/day for a conservative estimate of the mean. A lognormal distribution with geometric mean 40.9 and geometric standard deviation 3.6 was used in the SHEDS probabilistic scenarios (from Buck et al., 2001). This captures a soil ingestion rate of 10 g/day between the 95th and 99th percentiles. Thus, the upper tails of the SHEDS probability distributions do include pica children, assuming pica behavior of 10 g soil ingestion per day.

The Residential Exposure SOPs recommend values for dermal transfer coefficients (TC) of 2,600 to 5,200 cm^2/hr (short- to intermediate- term for ages 1-6 yrs) which were derived from adults performing 20 minutes of Jazzercise indoors on nylon carpet (U.S. EPA, 1997a). In this report, TC values differ from the SOPs because the wood treatment scenario is different than the indoor exposure scenario. In this assessment the TCs are based on different assumed clothing scenarios for warm and cold climates (the Chemical Y and Chemical X scenarios, respectively). For both warm and cold weather it was assumed that the hands are completely exposed. For warm weather it was assumed that the child wears a short sleeve shirt, short pants, shoes and socks, leaving the arms, lower legs, and hands exposed. For cold weather it was assumed that only the hands are exposed. It was also assumed that while playing on/around treated wood, the child's total bare skin surface area is covered by residue exactly once in an hour and that the surface to skin residue transfer efficiency is 90%. Hand skin surface areas were derived from Table 6-8 as well as Tables 6-6 and 6-7 of the Exposure Factors Handbook (U.S. EPA, 1997b), or Tables 8-1

and 8-2 of the Child-specific Exposure Factors Handbook (U.S. EPA, 2000). Total surface areas were calculated by averaging the values for males and females from Tables 6-6 and 6-7. Total surface areas are then multiplied by the age-specific hand fractions from Tables 6-8. Transfer coefficients for hands were estimated using an assumed fraction of the whole body transfer coefficient represented by the hands. These calculations provided means of normal transfer coefficient distributions for SHEDS inputs. To obtain the standard deviations, a coefficient of variation for indoor transfer coefficients for children from one of NERL's recent measurement studies was applied to the calculated means (U.S. EPA, 2002a).

Results

Variability Analyses

A summary of mean population values by exposure pathway for both Chemical X and Chemical Y scenarios and for the short-term, intermediate-term, and lifetime scenarios is given in Table 1 (for children both with and without decks who contact treated playsets). It shows that the short-term and intermediate-term estimates of absorbed dose are an order of magnitude higher than the lifetime estimates for both scenarios. Surface residue pathways contributed more to total absorbed dose than soil pathways by 1 to 3 orders of magnitude, and decks contributed more than playsets by a factor of 3 to 6. Chemical Y scenario estimates exceeded Chemical X scenario estimates by an order of magnitude. Details for each time frame are given below.

Lifetime Scenarios

Tables 2 and 3 present probabilistic estimates of lifetime average daily dose (LADD) for children exposed to dislodgeable residues and contaminated soil from treated wood for Chemical X in cold weather and Chemical Y in warm weather, respectively. These two tables separate results for the 30% of children assumed to not have residential decks (deck=0) and the 70% of children assumed to have residential decks (deck=1). Table 2 shows that (1) children with decks exposed to Chemical X in cold weather have higher absorbed doses than those children without decks (by a factor of about 9 based on mean and a factor of about 17 based on median), and (2) that for children with decks, the contribution to absorbed dose from decks is greater than from playsets (by a factor of about 8 based on the mean and a factor of about 11 based on median). Table 3 shows that (1) children with decks exposed to Chemical Y in warm weather have higher absorbed doses than those children without decks (by a factor of about 5 based on mean and a factor of about 10 based on median), and (2) that for children with decks, the contribution to absorbed dose from decks is greater than from playsets (by a factor of about 4 based on the mean and a factor of about 8 based on median). As expected, predicted total absorbed doses for probabilistic analyses are greater for the higher exposure scenario (Chemical Y in warm weather) than for the lower exposure scenario (Chemical X in cold weather), and residue pathways are consistently more important than soil pathways. Table 4 summarizes the results from Table 2 and 3 only for children who contact both playsets and residential decks. It includes means, medians, and 95th percentiles for lifetime Chemical X cold weather and Chemical Y warm weather probabilistic scenarios.

Table 1. Summary of Mean Population Values by Exposure Pathway for Chemical X and Chemical Y Scenarios and for the Short-term, Intermediate-term, and Lifetime Scenarios (mg/kg/day).

	Short-Term		Intermediate-Term		Lifetime	
Route	**Y Warm**	**X Cold**	**Y Warm**	**X Cold**	**Y Warm**	**X Cold**
Playset Surface Residue Dermal Dose	5.48e-05	8.69e-07	7.68e-05	9.49e-07	5.95e-06	6.71e-08
Playset Surface Residue Ingested Dose	5.29e-05	7.55e-06	7.15e-05	8.14e-06	5.36e-06	5.10e-07
Playset Soil Dermal Dose	2.05e-06	8.38e-10	1.66e-06	8.85e-10	1.37e-07	6.45e-11
Playset Soil Ingestion Dose	4.40e-06	2.54e-08	3.44e-06	1.97e-08	3.71e-07	1.68e-09
Deck Surface Residue Dermal Dose	1.77e-04	2.12e-06	1.80e-04	2.20e-06	1.42e-05	1.97e-07
Deck Surface Residue Ingested Dose	2.67e-04	3.74e-05	2.65e-04	3.58e-05	1.97e-05	3.31e-06
Deck Soil Dermal Dose	1.03e-06	1.61e-08	1.16e-06	1.55e-08	1.24e-07	1.55e-09
Deck Soil Ingestion Dose	2.93e-06	4.05e-07	3.64e-06	4.18e-07	3.28e-07	4.22e-08
Playset Total Dose	1.14e-04	8.44e-06	1.53e-04	9.11e-06	1.18e-05	5.79e-07
Deck Total Dose	4.47e-04	3.99e-05	4.50e-04	3.84e-05	3.44e-05	3.55e-06
Total Dose (Playset + Deck)	**5.62e-04**	**4.84e-05**	**6.03e-04**	**4.75e-05**	**4.62e-05**	**4.13e-06**

Table 2. Probabilistic Estimates of LADD (mg/kg/day) for Children Exposed to Chemical X Dislodgeable Residues and Contaminated Soil from Treated Wood Playsets and Residential Decks (separated by children with and without decks who contact treated playsets).

	Mean	Std. Dev	p50	p05	p25	p75	p95	Max
Route	**No Deck (N=416)**							
Total Dose	**5.83e-07**	**1.42e-06**	**1.44e-07**	**1.07e-08**	**5.32e-08**	**4.76e-07**	**2.98e-06**	**1.51e-05**
Playset Total Dose	5.83e-07	1.42e-06	1.44e-07	1.07e-08	5.32e-08	4.76e-07	2.98e-06	1.51e-05
Playset Surface Residue Ingestion Dose	5.14e-07	1.27e-06	1.24e-07	8.42e-09	4.51e-08	4.24e-07	2.60e-06	1.38e-05
Playset Surface Residue Dermal Dose	6.69e-08	1.52e-07	1.71e-08	1.32e-09	5.79e-09	5.73e-08	3.60e-07	1.27e-06
Playset Soil Ingestion Dose	2.05e-09	7.29e-09	5.81e-10	6.75e-11	2.46e-10	1.28e-09	7.68e-09	1.07e-07
Playset Soil Dermal Dose	6.79e-11	1.42e-10	2.87e-11	3.16e-12	1.22e-11	7.09e-11	2.74e-10	2.11e-09
	Has Deck (N= 1084)							
Total Dose	**5.49e-06**	**8.84e-06**	**2.43e-06**	**2.70e-07**	**1.07e-06**	**6.10e-06**	**2.05e-05**	**9.71e-05**
Deck Total Dose	4.91e-06	8.63e-06	1.87e-06	1.30e-07	6.79e-07	5.48e-06	1.89e-05	9.58e-05
Deck Surface Residue Ingestion Dose	4.58e-06	8.18e-06	1.72e-06	9.49e-08	5.76e-07	5.15e-06	1.78e-05	9.11e-05
Playset Total Dose	5.78e-07	1.73e-06	1.78e-07	1.37e-08	6.19e-08	4.75e-07	2.19e-06	3.39e-05
Playset Surface Residue Ingestion Dose	5.09e-07	1.53e-06	1.55e-07	1.07e-08	5.25e-08	4.23e-07	1.92e-06	2.95e-05
Deck Surface Residue Dermal Dose	2.72e-07	4.51e-07	1.05e-07	6.53e-09	3.61e-08	3.11e-07	1.09e-06	3.98e-06
Playset Surface Residue Dermal Dose	6.71e-08	2.03e-07	2.04e-08	1.46e-09	7.16e-09	5.54e-08	2.58e-07	4.43e-06
Deck Soil Ingestion Dose	5.84e-08	1.63e-07	1.47e-08	1.02e-09	5.08e-09	4.64e-08	2.44e-07	2.42e-06
Deck Soil Dermal Dose	2.15e-09	8.34e-09	5.56e-10	4.22e-11	1.98e-10	1.61e-09	7.05e-09	2.07e-07
Playset Soil Ingestion Dose	1.54e-09	3.01e-09	5.62e-10	6.15e-11	2.43e-10	1.45e-09	6.02e-09	2.95e-08
Playset Soil Dermal Dose	6.33e-11	1.09e-10	2.77e-11	3.15e-12	1.12e-11	6.65e-11	2.44e-10	1.38e-09

Table 3. Probabilistic Estimates of LADD (mg/kg/day) for Children Exposed to Chemical Y Dislodgeable Residues and Contaminated Soil from Treated Wood Playsets and Residential Decks (separated by children with and without decks who contact treated playsets).

	Mean	Std Dev	p50	p05	p25	p75	p95	Max
Route	**No Deck (N=496)**							
Total Dose	**1.24e-05**	**2.09e-05**	**4.15e-06**	**3.83e-07**	**1.53e-06**	**1.28e-05**	**6.00e-05**	**1.53e-04**
Playset Total Dose	1.24e-05	2.09e-05	4.15e-06	3.83e-07	1.53e-06	1.28e-05	6.00e-05	1.53e-04
Playset Surface Residue Dermal Dose	6.44e-06	1.12e-05	2.06e-06	1.18e-07	6.41e-07	6.60e-06	2.97e-05	8.30e-05
Playset Surface Residue Ingested Dose	5.57e-06	9.83e-06	1.74e-06	9.57e-08	5.35e-07	5.77e-06	2.73e-05	7.02e-05
Playset Soil Ingestion Dose	2.79e-07	6.38e-07	8.14e-08	5.41e-09	3.40e-08	2.44e-07	1.08e-06	7.14e-06
Playset Soil Dermal Dose	1.17e-07	2.52e-07	4.15e-08	2.84e-09	1.42e-08	1.17e-07	4.77e-07	3.87e-06
	Has Deck (N=1004)							
Total Dose	**6.29e-05**	**5.78e-05**	**4.35e-05**	**6.47e-06**	**2.03e-05**	**8.97e-05**	**1.81e-04**	**4.15e-04**
Deck Total Dose	5.14e-05	5.32e-05	3.27e-05	3.05e-06	1.20e-05	7.46e-05	1.60e-04	4.03e-04
Deck Surface Residue Ingestion Dose	2.94e-05	3.26e-05	1.79e-05	1.41e-06	6.69e-06	4.13e-05	9.78e-05	2.82e-04
Deck Surface Residue Dermal Dose	2.12e-05	2.14e-05	1.31e-05	1.12e-06	4.82e-06	3.23e-05	6.39e-05	1.21e-04
Playset Total Dose	1.15e-05	2.22e-05	3.92e-06	4.00e-07	1.46e-06	1.12e-05	4.92e-05	2.33e-04
Playset Surface Residue Dermal Dose	5.71e-06	1.12e-05	1.75e-06	1.19e-07	6.20e-07	5.60e-06	2.46e-05	1.15e-04
Playset Surface Residue Ingested Dose	5.26e-06	1.10e-05	1.56e-06	1.11e-07	5.13e-07	4.61e-06	2.48e-05	1.18e-04
Deck Soil Ingestion Dose	4.90e-07	1.58e-06	1.19e-07	5.64e-09	3.36e-08	3.52e-07	1.75e-06	2.63e-05
Playset Soil Ingestion Dose	4.16e-07	1.45e-06	9.24e-08	6.62e-09	3.30e-08	2.47e-07	1.54e-06	2.31e-05
Deck Soil Dermal Dose	1.85e-07	7.64e-07	4.89e-08	3.31e-09	1.45e-08	1.41e-07	6.63e-07	2.11e-05
Playset Soil Dermal Dose	1.46e-07	3.35e-07	4.73e-08	3.48e-09	1.55e-08	1.18e-07	6.39e-07	5.13e-06

Table 4. Probabilistic Estimates of LADD (mg/kg/day) for Children Exposed to Chemical X and Chemical Y Dislodgeable Residues and Contaminated Soil from Treated Wood Playground Structures and Residential Decks (for children who contact both playsets and residential decks; results for 2 chemicals separate).

	Mean		Median		P 95	
Route	**Y Warm**	**X Cold**	**Y Warm**	**X Cold**	**Y Warm**	**X cold**
Playset Surface Residue Dermal Dose	5.71e-06	6.71e-08	1.75e-06	2.04e-08	2.46e-05	2.58e-07
Playset Surface Residue Ingestion Dose	5.26e-06	5.09e-07	1.56e-06	1.55e-07	2.48e-05	1.92e-06
Playset Soil Dermal Dose	1.46e-07	6.33e-11	4.73e-08	2.77e-11	6.39e-07	2.44e-10
Playset Soil Ingestion Dose	4.16e-07	1.54e-09	9.24e-08	5.62e-10	1.54e-06	6.02e-09
Deck Surface Residue Dermal Dose	2.12e-05	2.72e-07	1.31e-05	1.05e-07	6.39e-05	1.09e-06
Deck Surface Residue Ingestion Dose	2.94e-05	4.58e-06	1.79e-05	1.72e-06	9.78e-05	1.78e-05
Deck Soil Dermal Dose	1.85e-07	2.15e-09	4.89e-08	5.56e-10	6.63e-07	7.05e-09
Deck Soil Ingestion Dose	4.90e-07	5.84e-08	1.19e-07	1.47e-08	1.75e-06	2.44e-07
Playset Total Dose	1.15e-05	5.78e-07	3.92e-06	1.78e-07	4.92e-05	2.19e-06
Deck Total Dose	5.14e-05	4.91e-06	3.27e-05	1.87e-06	1.60e-04	1.89e-05
Total Dose	**6.29e-05**	**5.49e-06**	**4.35e-05**	**2.43e-06**	**1.81e-04**	**2.05e-05**

Table 5 is similar to Table 4, except it contains probabilistic LADD Chemical X and Chemical Y estimates for ALL children in the simulated population – those with and without decks who also contact playsets. The total LADD of Chemical X in cold weather was 1.5 e-6 mg/kg/day (median); 4.1 e-6 mg/kg/day (mean); and 1.7 e-5 mg/kg/day(95^{th} percentile). The LADD of Chemical Y in warm weather was 2.6 e-5 mg/kg/day (median), 4.6 e-5 mg/kg/day (mean), and 1.6 e-4 mg/kg/day (95^{th} percentile). Figures 9 and 10 illustrate the CDFs for LADD Chemical X probabilistic estimates for cold weather and Chemical Y probabilistic estimates for warm weather, respectively, for the entire simulated population (those values in Table 5). Population distributions are shown for total absorbed dose and dose from each of four exposure pathways (soil dermal contact around decks and playsets; ingested soil around decks and playsets; wood surface residue dermal contact from playsets and decks; wood surface residues ingested from playsets and decks). These show the magnitude and order of relative pathway importance (surface residue pathways higher contributors to dose than soil pathways) and also that there were 2 to 3 orders of magnitude between lower and upper percentiles of total LADD due to variability in activity patterns, residues and concentrations contacted, and exposure factors. Figures 11 and 12 are pie charts showing the percent contribution by pathway to Chemical X and Chemical Y LADD, respectively, based on population means. The most important pathway for both scenarios was ingestion of wood surface residues from hand-to-mouth contact.

Table 5. Probabilistic Estimates of LADD (mg/kg/day)for Children Exposed to Chemical X and Chemical Y Dislodgeable Residues and Contaminated Soil from Treated Wood Playground Structures and Residential Decks (for children with and without decks who contact treated playsets).

	Mean		Median		P 95	
Route	**Y Warm**	**X Cold**	**Y Warm**	**X Cold**	**Y Warm**	**X Cold**
Playset Surface Residue Dermal Dose	5.95e-06	6.71e-08	1.86e-06	1.93e-08	2.65e-05	2.67e-07
Playset Surface Residue Ingestion Dose	5.36e-06	5.10e-07	1.62e-06	1.48e-07	2.55e-05	2.11e-06
Playset Soil Dermal Dose	1.37e-07	6.45e-11	4.46e-08	2.77e-11	5.85e-07	2.51e-10
Playset Soil Ingestion Dose	3.71e-07	1.68e-09	8.77e-08	5.73e-10	1.40e-06	6.36e-09
Deck Surface Residue Dermal Dose	1.42e-05	1.97e-07	4.91e-06	4.67e-08	5.67e-05	9.15e-07
Deck Surface Residue Ingestion Dose	1.97e-05	3.31e-06	6.75e-06	7.82e-07	8.20e-05	1.47e-05
Deck Soil Dermal Dose	1.24e-07	1.55e-09	1.50e-08	2.57e-10	5.07e-07	5.24e-09
Deck Soil Ingestion Dose	3.28e-07	4.22e-08	3.40e-08	6.53e-09	1.34e-06	1.74e-07
Playset Total Dose	1.18e-05	5.79e-07	3.99e-06	1.70e-07	5.50e-05	2.42e-06
Deck Total Dose	3.44e-05	3.55e-06	1.22e-05	8.95e-07	1.38e-04	1.57e-05
Total Dose	**4.62e-05**	**4.13e-06**	**2.64e-05**	**1.48e-06**	**1.58e-04**	**1.67e-05**

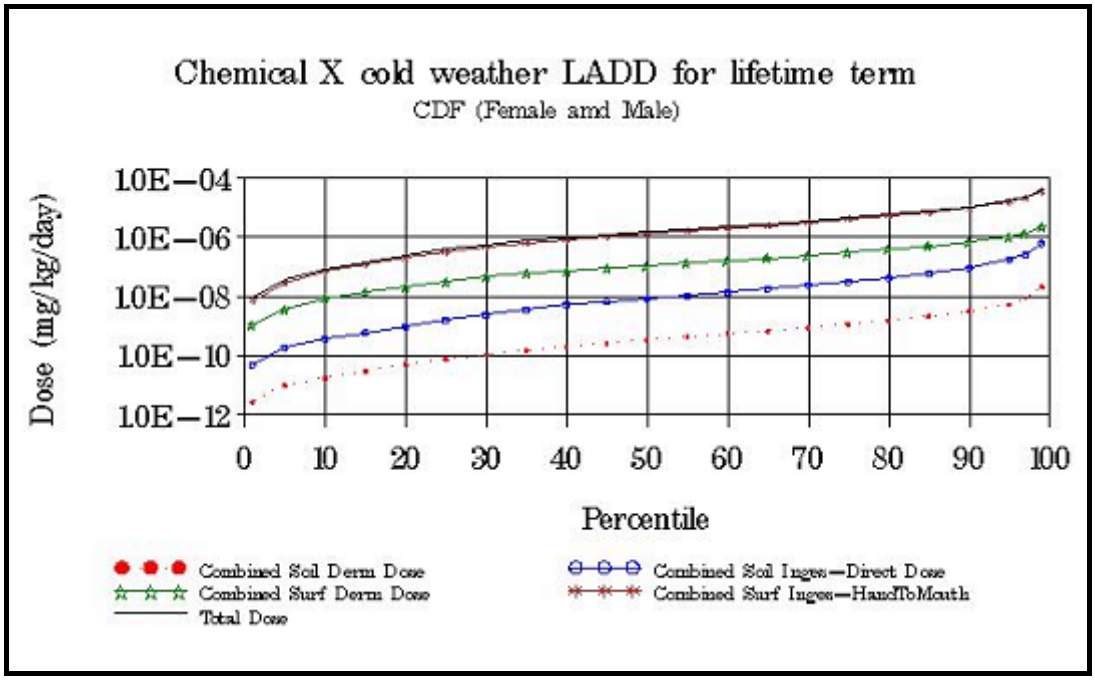

Figure 9. Cumulative Density Function of LADD for chemical X.

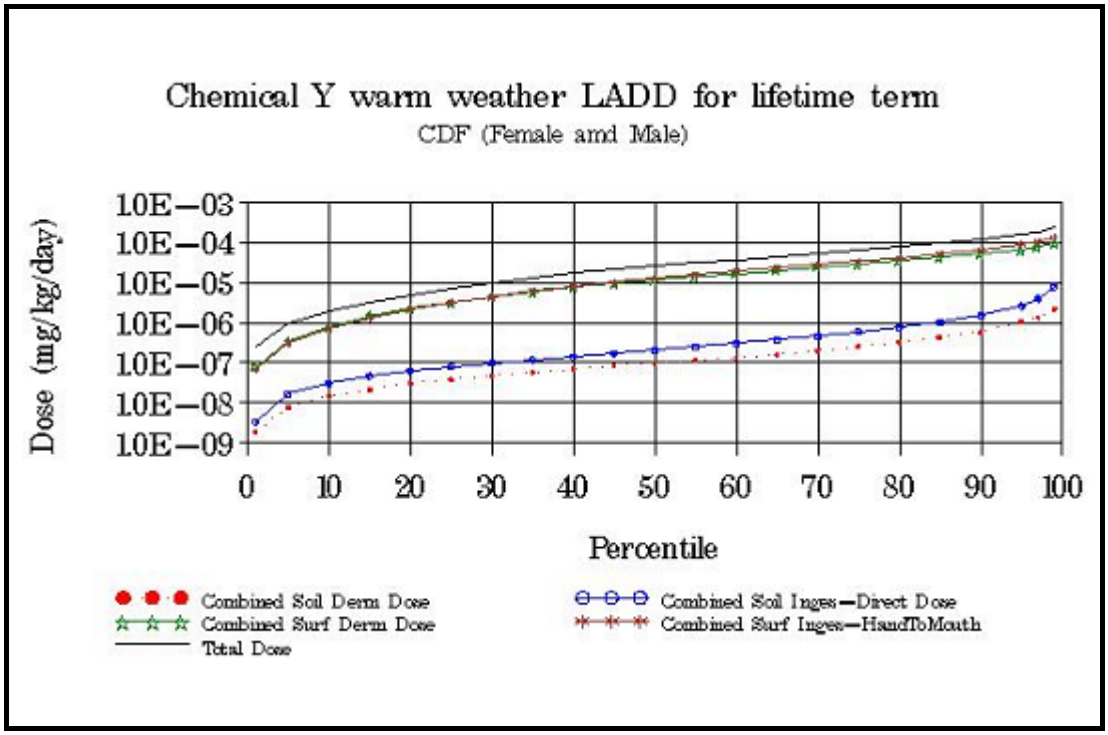

Figure 10. Cumulative Density Function of LADD for chemical Y.

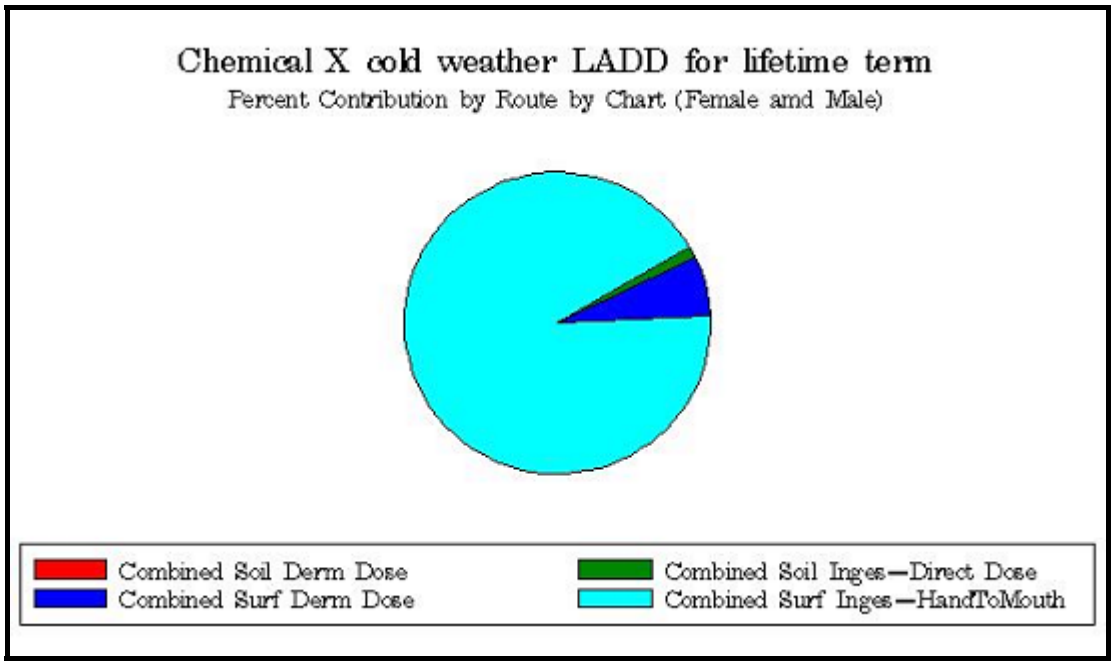

Figure 11. Pie chart of contribution to LADD by exposure route for chemical X (by mean).

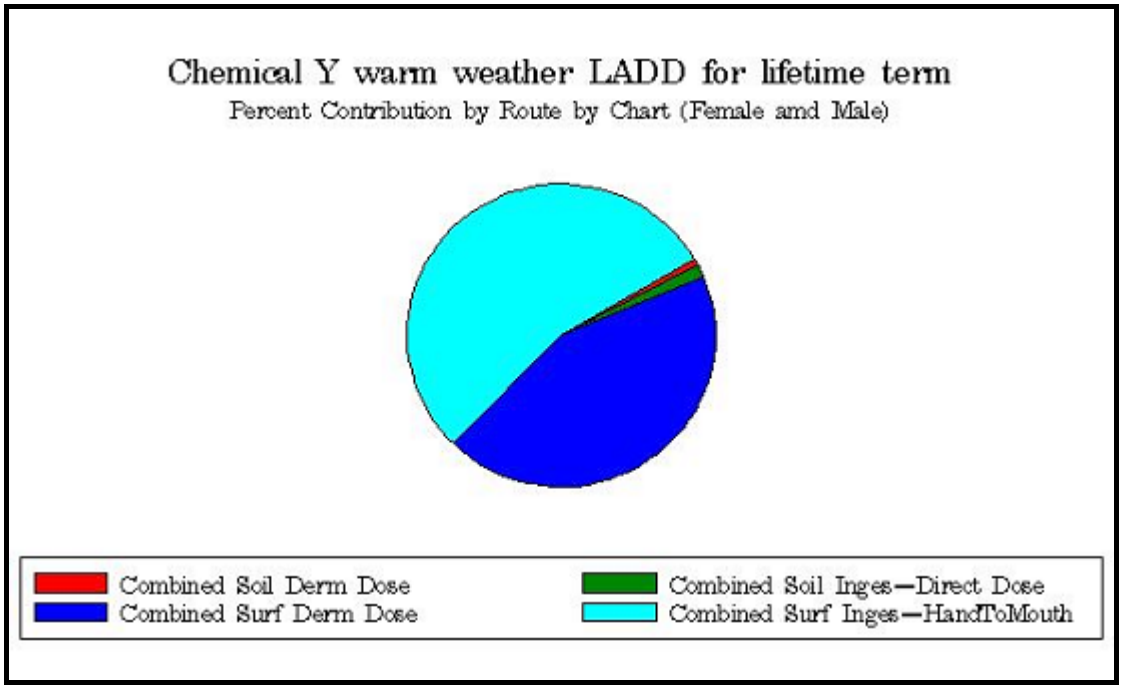

Figure 12. Pie chart of contribution to LADD by exposure route for chemical Y (by mean).

Short-Term and Intermediate-Term Scenarios

Table 6 presents mean, median, and 95th CDF percentiles of short- and intermediate-term Chemical X cold weather ADD and Chemical Y warm weather ADD for probabilistic simulations of children exposed to treated wood from playsets and home decks. As expected, predicted total absorbed doses are greater for the higher exposure scenario (Chemical Y in warm weather) than for the lower exposure scenario (Chemical X in cold weather), and residue pathways are more important than soil pathways. These values reflect all children in the simulated population, i.e., those with and without decks who also contact playsets. The mean, median, and 95th percentiles for total short-term Chemical X ADD in cold weather were 4.8 e-5 mg/kg/day , 6.8 e-6 mg/kg/day, and 1.8 e-4 mg/kg/day, respectively. The mean, median, and 95th percentiles for total short-term Chemical Y ADD in warm weather were 5.6 e-4 mg/kg/day, 1.7 e-4 mg/kg/day, and 2.4 e-3 mg/kg/day, respectively. The mean, median, and 95th percentiles for total intermediate-term Chemical X ADD in cold weather were 4.7 e-5 mg/kg/day, 8.6 e-6 mg/kg/day, and 2.1 e-4 mg/kg/day, respectively. The mean, median, and 95th percentiles for total intermediate-term Chemical Y ADD in warm weather were 6.0 e-4 mg/kg/day, 2.1 e-4 mg/kg/day, and 2.6 e-3 mg/kg/day, respectively. Figures 13, 14, 15, and 16 present the CDFs corresponding to Table 6 values. They illustrate the order of relative pathway importance and also that there were 4 to 5 orders of magnitude between lower and upper percentiles of total ADD due to variability in activity patterns, residues and concentrations contacted, and exposure factors.

Table 6. Probabilistic Estimates of Short- and Intermediate- Term ADD (mg/kg/day) for Children Exposed to Chemical X and Chemical Y Dislodgeable Residues and Contaminated Soil from Treated Wood Playground Structures and Residential Decks (for children with and without decks who contact treated playsets).

	Short-Term					
	Mean		Median		P 95	
Route	Y Warm	X Cold	Y Warm	X Cold	Y Warm	X Cold
Playset Surface Residue Dermal Dose	5.48e-05	8.69e-07	7.05e-06	7.62e-08	2.86e-04	3.95e-06
Playset Surface Residue Ingestion Dose	5.29e-05	7.55e-06	5.61e-06	4.76e-07	2.52e-04	2.92e-05
Playset Soil Dermal Dose	2.05e-06	8.38e-10	1.63e-07	8.68e-11	5.99e-06	3.90e-09
Playset Soil Ingestion Dose	4.40e-06	2.54e-08	2.09e-07	1.20e-09	1.59e-05	8.14e-08
Deck Surface Residue Dermal Dose	1.77e-04	2.12e-06	2.45e-05	9.96e-08	8.43e-04	1.09e-05
Deck Surface Residue Ingestion Dose	2.67e-04	3.74e-05	2.75e-05	1.30e-06	1.28e-03	1.48e-04
Deck Soil Dermal Dose	1.03e-06	1.61e-08	6.26e-08	4.30e-10	4.06e-06	6.54e-08
Deck Soil Ingestion Dose	2.93e-06	4.05e-07	8.48e-08	7.50e-09	9.90e-06	1.85e-06
Playset Total Dose	1.14e-04	8.44e-06	1.69e-05	5.92e-07	5.55e-04	3.42e-05
Deck Total Dose	4.47e-04	3.99e-05	6.12e-05	1.65e-06	2.18e-03	1.62e-04
Total Dose	**5.62e-04**	**4.84e-05**	**1.69e-04**	**6.79e-06**	**2.40e-03**	**1.81e-04**

	Intermediate-Term					
	Mean		Median		P 95	
Route	Y Warm	X Cold	Y Warm	X Cold	Y Warm	X Cold
Playset Surface Residue Dermal Dose	7.68e-05	9.49e-07	1.26e-05	1.14e-07	3.63e-04	3.46e-06
Playset Surface Residue Ingestion Dose	7.15e-05	8.14e-06	1.01e-05	7.85e-07	3.29e-04	2.59e-05
Playset Soil Dermal Dose	1.66e-06	8.85e-10	2.68e-07	1.55e-10	6.79e-06	3.42e-09
Playset Soil Ingestion Dose	3.44e-06	1.97e-08	3.80e-07	2.00e-09	1.36e-05	7.68e-08
Deck Surface Residue Dermal Dose	1.80e-04	2.20e-06	3.91e-05	1.75e-07	8.65e-04	1.07e-05
Deck Surface Residue Ingestion Dose	2.65e-04	3.58e-05	4.27e-05	2.67e-06	1.35e-03	1.69e-04
Deck Soil Dermal Dose	1.16e-06	1.55e-08	9.56e-08	9.42e-10	5.25e-06	6.14e-08
Deck Soil Ingestion Dose	3.64e-06	4.18e-07	1.28e-07	1.26e-08	1.36e-05	1.78e-06
Playset Total Dose	1.53e-04	9.11e-06	2.93e-05	9.74e-07	6.90e-04	2.78e-05
Deck Total Dose	4.50e-04	3.84e-05	8.84e-05	3.13e-06	2.21e-03	1.78e-04
Total Dose	**6.03e-04**	**4.75e-05**	**2.15e-04**	**8.62e-06**	**2.57e-03**	**2.08e-04**

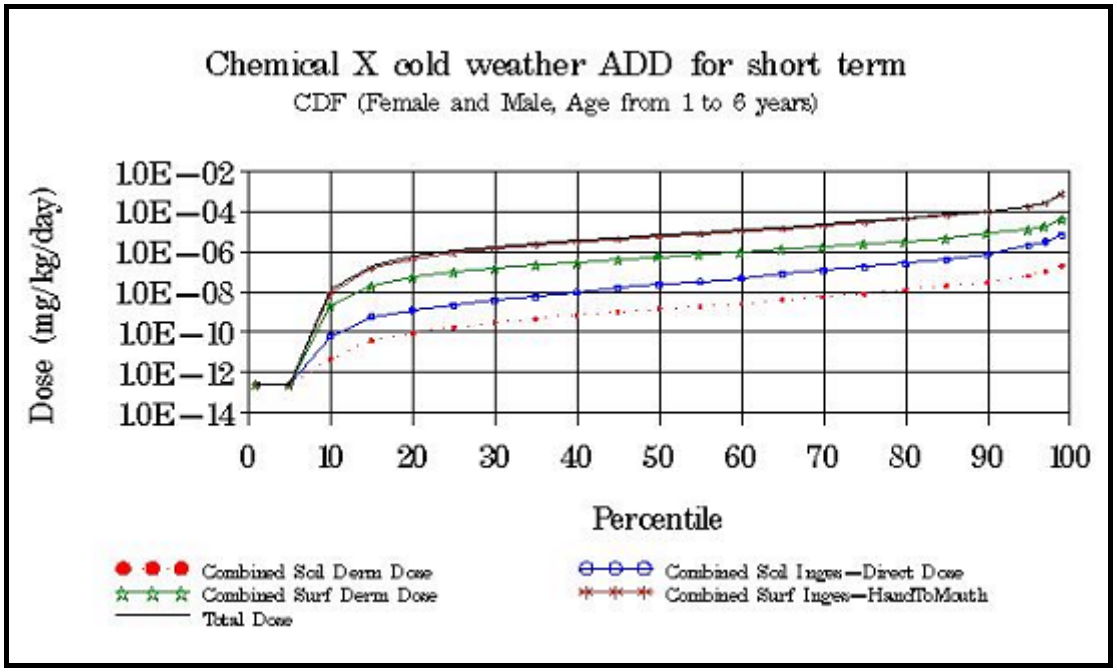

Figure 13. Cumulative density function of short-term ADD for chemical X.

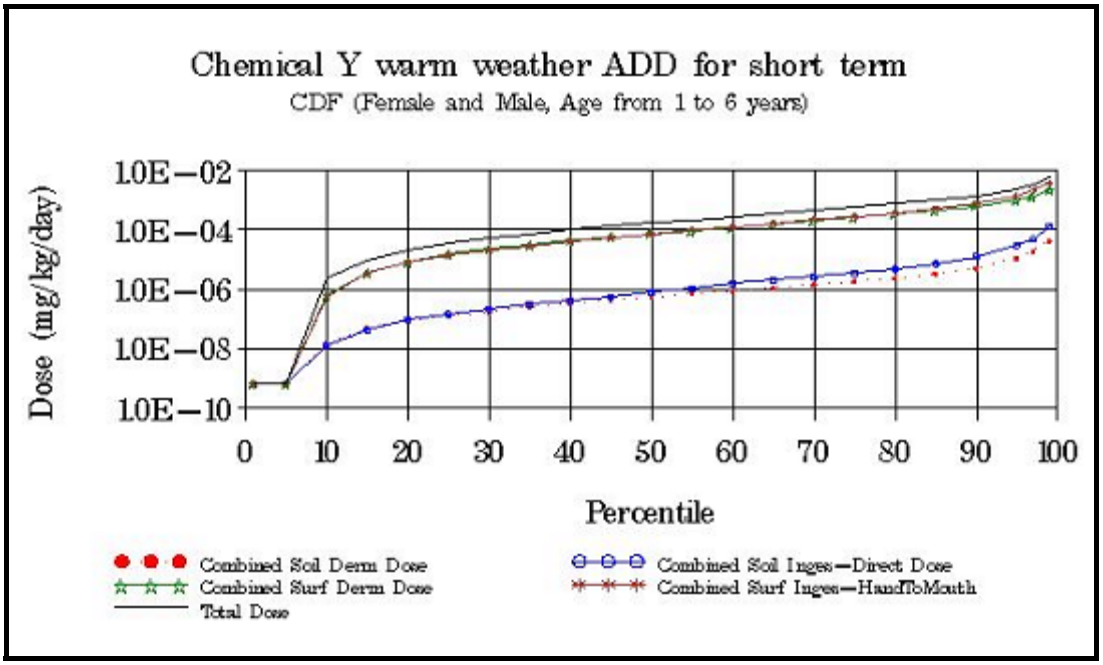

Figure 14. Cumulative density function of short-term ADD for chemical Y.

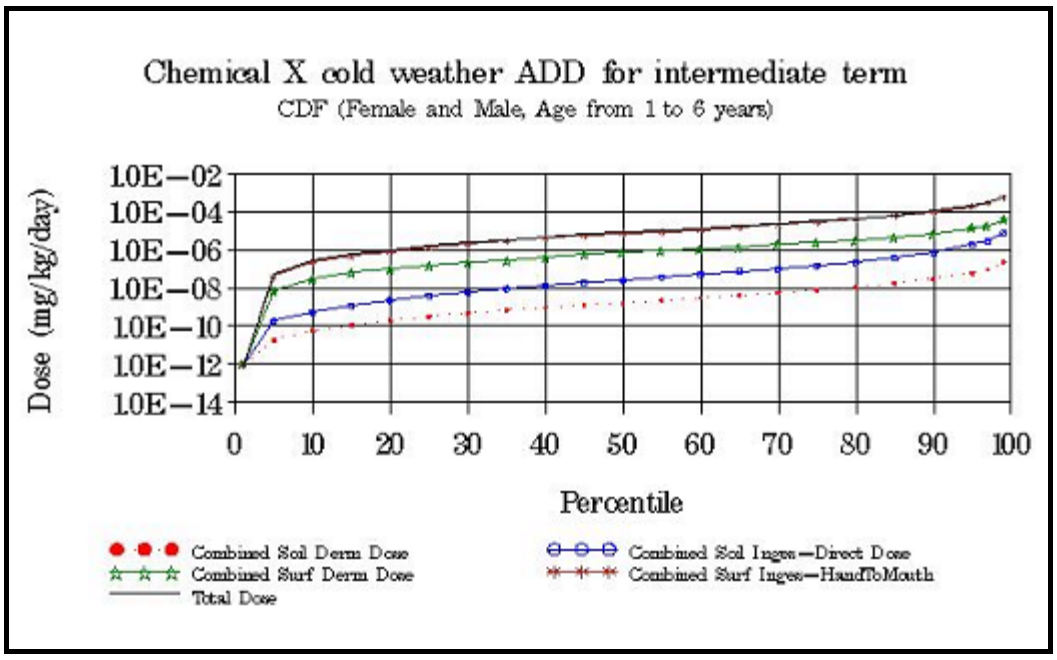

Figure 15. Cumulative density function of intermediate-term ADD for chemical X.

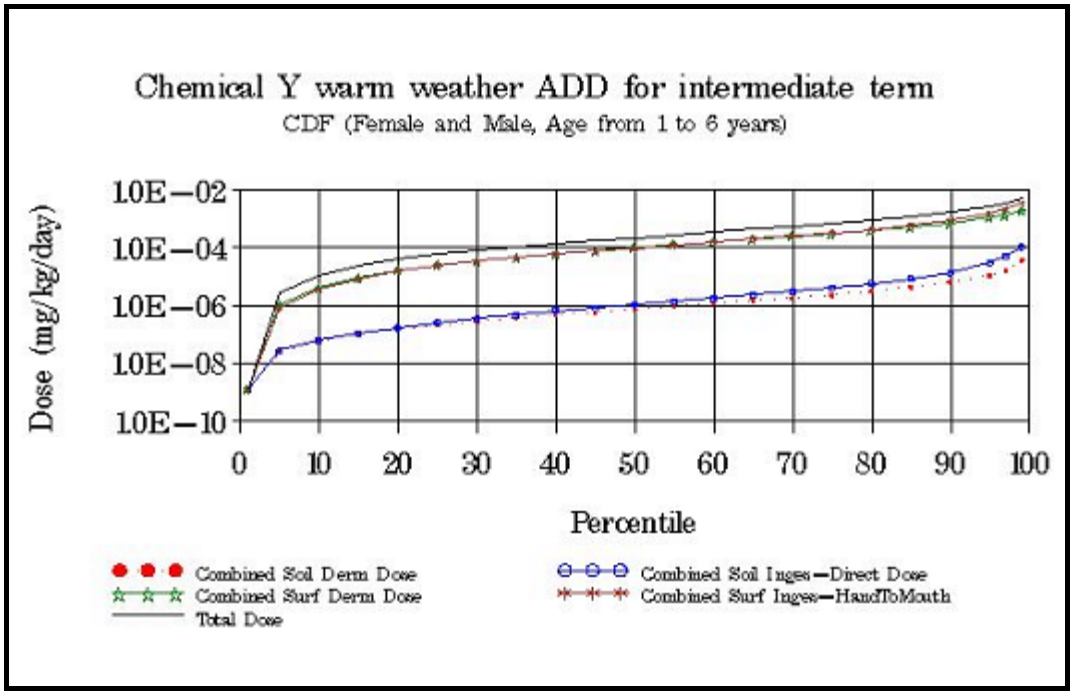

Figure 16. Cumulative density function of intermediate-term ADD for Chemical Y.

Sensitivity Analyses

Sensitivity analyses results for the intermediate-term deterministic Chemical Y warm weather scenario, based on mean and median values, are presented in Tables 7 and 8. The "stepwise_rank" column shows stepwise regression results and ranks with partial R^2 correlation coefficient values, and the 3 other columns show the effect of increasing and decreasing point estimate "medium values" (see Methods section above) of each input by a factor of 2 (mid:low is the unitless ratio of absorbed dose for the "medium" and "low" inputs; high:mid is the unitless ratio of absorbed dose for the "high" and "medium" inputs; and high:low is the unitless ratio of absorbed dose for the "high" and "low" inputs). Based on means, these analyses reveal that the most critical model inputs for variability in this case study were: fraction time a child (in the population of interest) outdoors at home with a treated deck is playing on/around deck; wood surface residues on deck; fraction time a child (in the population of interest) on/around a treated home deck contacts residues (vs. soil); #Days/Yr a child (in the population of interest) plays on/around a treated home deck; fraction children (in the population of interest) who have a treated home deck; hand dermal transfer coefficient; GI absorption fraction per day for residues; dermal absorption fraction per day; and bathing removal efficiency. The sensitivity analyses results from median statistics are similar except for a different sensitivity ranking for those input parameters. The stepwise regression results show the statistical importance for those input parameters, and indicate that 18 of the 30 variables were statistically significant with respect to variability in Chemical Y intermediate-term dose results.

Table 7. Sensitivity Analysis Comparison of Mean Total Chemical Y Intermediate-Term Dose in Warm Weather.

Input	Stepwise Rank	Mid:Low	High:Mid	High:Low
fraction time a child outdoors at home w/ treated deck is playing on/around deck	3	1.7	2.0	3.4
wood surface residues on deck	5	1.8	1.7	3.0
fraction time a child on/around treated home deck contacts residues (vs. soil)	4	1.6	1.9	3.0
#days/yr a child plays on/around treated home deck	6	1.6	1.8	2.8
fraction children who have a treated home deck		1.7	1.4	2.4
hand dermal transfer coefficient	2	1.4	1.6	2.2
GI absorption fraction per day for residues	8	1.5	1.4	2.0
dermal absorption fraction per day	10	1.3	1.5	2.0
fraction of hand with residue mouthed per mouthing event	9	1.2	1.5	1.9
saliva removal efficiency	11	1.3	1.5	1.9
body (non-hand) dermal transfer coefficient	12	1.4	1.3	1.8
frequency of hand-mouth activity per hour	1	1.3	1.2	1.6
fraction time a child on/around treated playset contacts residues (vs. soil)	14	1.1	1.2	1.3
#days/yr a child plays on/around treated playset away from home	13	1.1	1.1	1.3
fraction time a child* in non-home outdoor locations plays on/around treated non-home playsets	17	1.1	1.1	1.2
fraction time a child outdoors at home plays on/around treated playset	16	0.9	1.2	1.2
wood surface residues on playset		1.1	1.0	1.1
fraction children with treated home playset		1.0	1.1	1.1
maximum dermal loading for hands		1.2	1.0	1.1
soil-skin adherence factor		1.0	1.1	1.1
#days/yr a child plays on/around treated playset at home		1.1	1.0	1.0
GI absorption fraction per day for soil (BF)		1.0	1.0	1.0
soil concentrations near deck		1.1	1.0	1.0
daily soil ingestion rate		1.0	1.1	1.0
soil concentrations near playset		0.9	1.1	1.0
#days/yr a child spends on both treated home and treated non-home playsets		1.0	1.0	0.9
maximum dermal loading for body		0.8	1.1	0.9
hand washing events per day	18	0.9	1.0	0.9
hand washing removal efficiency	15	0.8	0.9	0.8
bathing removal efficiency	7	0.6	0.6	0.4

Table 8. Sensitivity Analysis Comparison of Median Total Chemical Y Intermediate-Term Dose in Warm Weather.

Input	Stepwise Rank	Mid:Low	High:Mid	High:Low
fraction children who have a treated home deck		3.2	1.6	5.3
fraction time a child outdoors at home w/ treated deck is playing on/around deck	3	1.7	1.9	3.2
fraction time a child on/around treated home deck contacts residues (vs. soil)	4	1.4	2.0	2.8
wood surface residues on deck	5	1.6	1.5	2.5
#days/yr a child plays on/around treated home deck	6	1.3	1.9	2.5
GI absorption fraction per day for residues	8	1.5	1.5	2.2
dermal absorption fraction per day	10	1.3	1.5	2.1
hand dermal transfer coefficient	2	1.4	1.4	2.0
body (non-hand) dermal transfer coefficient	12	1.5	1.3	1.9
saliva removal efficiency	11	1.4	1.4	1.9
fraction of hand with residue mouthed per mouthing event	9	1.3	1.4	1.8
fraction time a child on/around treated playset contacts residues (vs. soil)	14	1.2	1.3	1.6
#days/yr a child plays on/around treated playset away from home	13	1.2	1.3	1.6
frequency of hand-mouth activity per hour	1	1.2	1.3	1.5
wood surface residues on playset		1.2	1.1	1.3
fraction time a child in non-home outdoor locations plays on/around treated non-home playsets	17	1.1	1.2	1.3
fraction time a child outdoors at home plays on/around treated playset	16	1.1	1.1	1.3
fraction children with treated home playset		1.1	1.1	1.2
maximum dermal loading for hands		1.2	1.0	1.2
GI absorption fraction per day for soil (BF)		0.9	1.1	1.1
#days/yr a child plays on/around treated playset at home		1.1	0.9	1.0
soil concentrations near deck		1.0	1.0	1.0
daily soil ingestion rate		0.9	1.1	1.0
hand washing events per day	18	0.9	1.1	1.0
maximum dermal loading for body		0.8	1.1	1.0
#days/yr a child spends on both treated home and treated non-home playsets		1.0	0.9	0.9
soil-skin adherence factor		0.9	1.1	0.9
soil concentrations near playset		0.9	1.0	0.9
hand washing removal efficiency	15	0.8	0.9	0.7
bathing removal efficiency	7	0.4	0.6	0.3

Uncertainty Analyses

Uncertainty analyses were conducted using methods described in the Methods section above (with 142 uncertainty runs and 300 simulated individuals per uncertainty run), for the Chemical Y lifetime scenario example (Tables 9, 10, and 11). Results among the three statistical methods for the most important contributors to uncertainty in model predicted absorbed doses were similar. For at least two of the three analyses, the following inputs were important: surface residues and soil concentrations on and around decks and playsets; days per year a child plays on/around a treated home deck; fraction time a child outdoors at home with a treated deck plays on/around the treated deck; frequency of hand-mouth activity; hand dermal transfer coefficient; GI absorption fraction for residues; and daily soil ingestion rate.

Figures 17 and 18 depict uncertainty in model estimates as described in the Methods for Uncertainty Analysis section above. In Figure 17, three uncertainty CDFs for a representative low-dose population (5th percentile), a representative medium-dose population (50^{th} percentile), and a representative high-dose population (95^{th} percentile) are presented. There is an uncertainty factor of approximately 10 for all three populations (a factor of 8.4 between the median values of those 3 populations). This figure illustrates that the variability (difference between low and high x-axis percentiles on each CDF), approximately 3 orders of magnitude, is higher than uncertainty. Figure 18 shows uncertainties in selected percentiles of the entire population of interest: the uncertainty in the 5^{th} percentile absorbed dose ranges by a factor of 62; the uncertainty in the 50^{th} percentile absorbed dose ranges by a factor of 14; and the uncertainty in the 95^{th} percentile absorbed dose ranges by a factor of 8.

For comparison, an uncertainty analysis was also conducted for the Chemical Y short-term scenario. The uncertainty in the 50^{th} percentile absorbed dose ranged by a factor of 20, and the uncertainty in the 95^{th} percentile absorbed dose ranged by a factor of 8. Thus, the uncertainty results were quite similar for the short-term and lifetime scenarios.

Table 9. Uncertainty Analyses for Chemical Y LADD Using the Spearman Correlation Method.

Input	Spearman Correlation Coefficient[1]	
surface residues on deck(ug/cm2)	0.620	**
surface residues on the playset(ug/cm2)	0.366	**
#days/yr a child plays on/around treated home deck	0.232	**
GI absorption fraction per day for residues(1/day)	0.222	**
soil concentrations near playsets(mg/kg)	0.167	*
fraction time a child outdoors at home w/ treated deck plays on/around deck	0.159	
#days/yr a child plays on/around treated playset at home	0.147	
soil concentrations near deck(mg/kg)	0.144	
daily soil ingestion rate(mg/day)	0.127	
fraction time a child on/around treated deck contacts residues (vs. soil)	0.098	
GI absorption fraction per day for soil (BF)(1/day)	0.091	
body (non-hand) dermal transfer coefficient(cm2/hr)	0.090	
dermal absorption fraction per day(1/day)	0.087	
bathing removal efficiency	0.083	
saliva removal efficiency	0.065	
hand dermal transfer coefficient(cm2/hr)	0.063	
fraction time a child on/around treated playset contacts residues (vs. soil)	0.063	
maximum dermal loading for hand(ug/m2)	0.053	
maximum dermal loading for body(ug/m2)	0.042	
fraction time a child in non-home outdoor location plays on/around treated non-home playset	0.031	
hand washing events per day(events/day)	0.024	
frequency of hand-mouth activity per hour(events/hr)	0.013	
hand washing removal efficiency	0.004	
#days/yr a child spends on both treated home and treated non-home playsets	-0.001	
fraction time a child outdoors at home plays on treated playset	-0.029	
soil-skin adherence factor(mg/cm2)	-0.038	
#days/yr a child plays on treated playset away from home	-0.042	
fraction of hands mouthed per mouthing event	-0.044	
fraction time a child on/around treated playset contacts soil (vs. residues)	-0.063	
fraction time a child on/around treated deck contacts soil (vs. residues)	-0.098	

[1] A single asterisk indicates a P value of < 0.05, two indicate a P value of < 0.01.

Table 10. Uncertainty Analyses for Chemical Y LADD Using the Pearson Correlation Method.

Input	Pearson Correlation Coefficient[1]
surface residues on the playset(ug/cm2)	0.334 **
soil concentrations near deck(mg/kg)	0.314 **
daily soil ingestion rate(mg/day)	0.267 **
surface residues on deck(ug/cm2)	0.206 *
GI absorption fraction per day for residues(1/day)	0.179 *
#days/yr a child plays on/around treated home deck	0.151
fraction daily time a child outdoors at home w/ treated deck is playing on/around deck	0.127
#days/yr a child plays on/around treated playset at home	0.123
hand dermal transfer coefficient(cm2/hr)	0.113
GI absorption fraction per day for soil (BF)(1/day)	0.105
soil concentrations near playsets(mg/kg)	0.099
body (non-hand) dermal transfer coefficient(cm2/hr)	0.090
dermal absorption fraction per day(1/day)	0.077
saliva removal efficiency	0.069
bathing removal efficiency	0.067
fraction time a child on/around treated deck contacts residues (vs. soil)	0.066
maximum dermal loading for hand(ug/m2)	0.064
fraction time a child in non-home outdoor location plays on/around treated non-home playset	0.062
fraction time a child on/around treated playset contacts residues (vs. soil)	0.057
frequency of hand-mouth activity per hour(events/hr)	0.029
maximum dermal loading for body(ug/m2)	0.026
hand washing events per day(events/day)	0.025
#days/yr a child spends on both treated home and treated non-home playsets	0.024
soil-skin adherence factor(mg/cm2)	0.003
fraction of hands mouthed per mouthing event	-0.012
hand washing removal efficiency	-0.027
fraction time a child outdoors at home plays on treated playset	-0.042
fraction time a child on/around treated playset contacts soil (vs. residues)	-0.057
fraction time a child on/around treated deck contacts soil (vs. residues)	-0.066
#Days/Yr a child plays on treated playset away from home(days/yr)	-0.073

[1] A single asterisk indicates a P value of < 0.05, two indicate a P value of < 0.01.

Table 11. Uncertainty Analyses for Chemical Y LADD Using the Stepwise Regression Method.

Input	Step	Partial R^2	Model R^2	F (Probability)
surface residues on deck(ug/cm2)	1	0.069	0.069	0.000
#days/yr a child plays on/around treated home deck	2	0.027	0.096	0.000
surface residues on the playset(ug/cm2)	3	0.021	0.116	0.000
frequency of hand-mouth activity per hour(events/hr)	4	0.016	0.132	0.000
fraction time a child outdoors at home w/ treated deck is playing on/around deck	5	0.009	0.141	0.000
hand dermal transfer coefficient(cm2/hr)	6	0.008	0.149	0.000
maximum dermal loading for hand(ug/m2)	7	0.007	0.156	0.000
body (non-hand) dermal transfer coefficient(cm2/hr)	8	0.005	0.161	0.000
soil concentrations near deck(mg/kg)	9	0.004	0.166	0.000
maximum dermal loading for body(ug/m2)	10	0.003	0.169	0.000
daily soil ingestion rate(mg/day)	11	0.003	0.171	0.000
hand washing events per day(events/day)	12	0.002	0.173	0.000
#days/yr a child plays on treated playset away from home	13	0.002	0.175	0.000
fraction time a child in non-home outdoor location plays on/around treated non-home playset	14	0.001	0.176	0.000
soil concentrations near playsets(mg/kg)	15	0.001	0.178	0.000
#days/yr a child spends on both treated home and treated non-home playsets	16	0.000	0.178	0.000
#days/yr a child plays on/around treated playset at home	17	0.000	0.178	0.000
fraction daily time a child outdoors at home plays on treated playset only	18	0.000	0.178	0.000
GI absorption fraction per day for soil (BF)(1/day)	19	0.000	0.178	0.001
fraction time a child on/around treated deck contacts residues (vs. soil)	20	0.000	0.178	0.002
soil-skin adherence factor(mg/cm2)	21	0.000	0.178	0.020

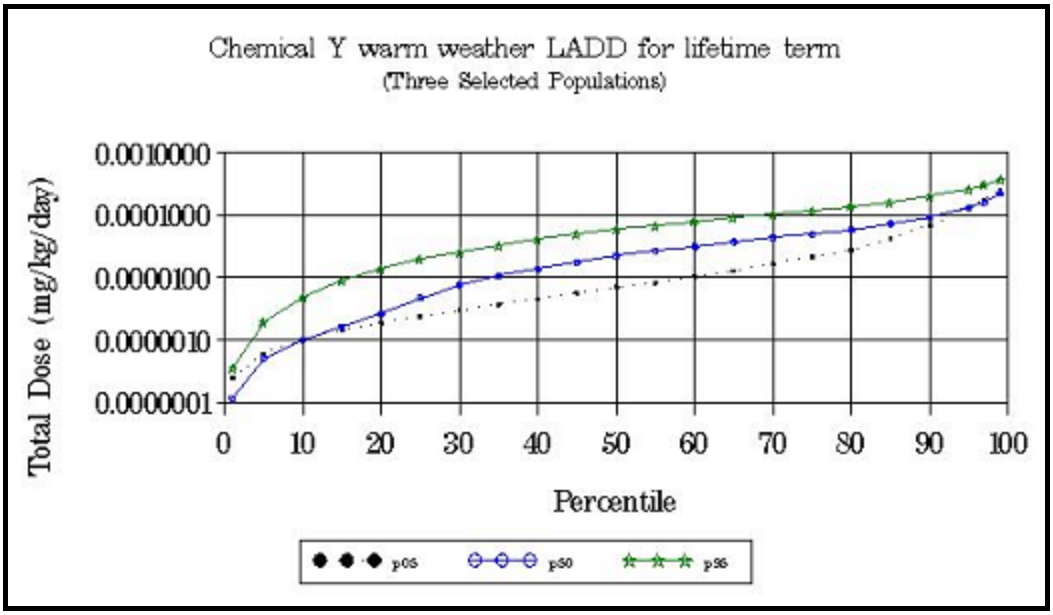

Figure 17. Uncertainty analysis CDFs for 3 selected populations: LADD for Chemical Y.

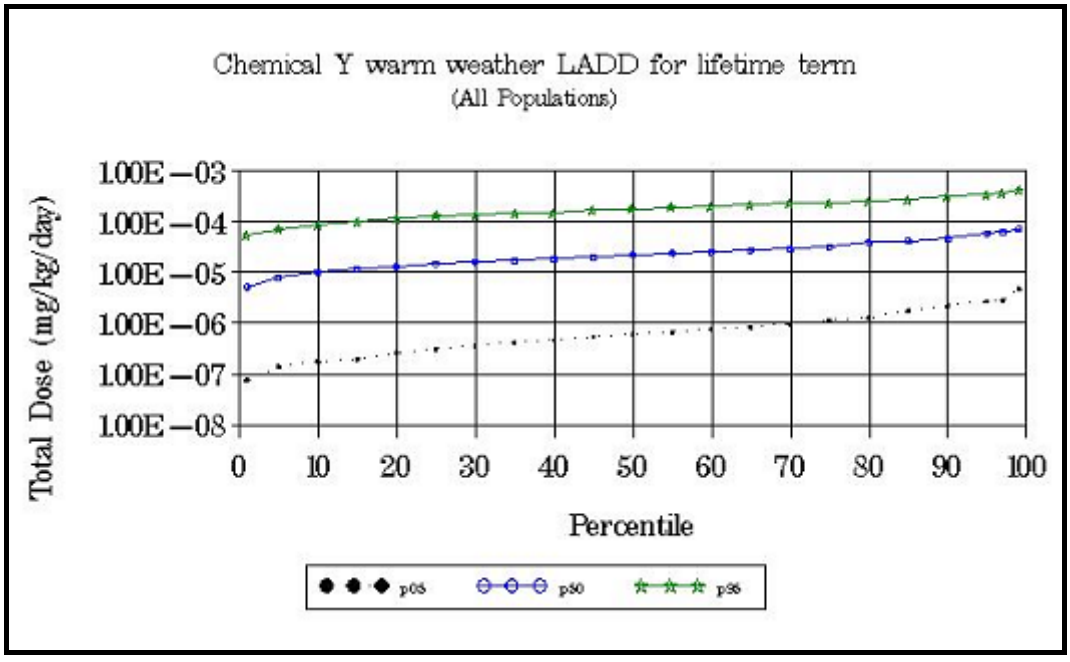

Figure 18. Uncertainty analysis CDFs for all populations: LADD for chemical Y.

Discussion

The October 2001 SAP recommended the use of probabilistic modeling to estimate children's exposure to wood preservatives from playsets and home decks (U.S. EPA, 2001). This report has described a methodology developed by ORD and OPP to do that using ORD's SHEDS model. The SHEDS methodology presented here meets the various conditions in the Guidance for Submission of Probabilistic Exposure Assessments to the OPP's Health Effects Division (U.S. EPA, 1998) which followed the Agency Policy Document (U.S. EPA, 1997c) for acceptance of probabilistic analyses techniques.

Sensitivity and uncertainty analyses conducted for the two hypothetical case studies suggest that more data are needed for a number of model inputs affecting variability and uncertainty in absorbed dose estimates. No data were available for dermal transfer coefficients and children's activity patterns (e.g., frequency of skin contact with treated vs. non-treated wood, or with contaminated vs. non-contaminated soil during typical outdoor play activity) specific to contact with treated wood on playsets and home decks. Thus, because many assumptions were made in developing these two critical model input values, this lack of information is an important source of uncertainty in the model results. More data for transfer coefficients and children's activity patterns (i.e., time spent on/around treated playsets and decks) would help reduce uncertainty in exposure and dose estimates. It is not clear, because of the lack of data, whether the assumed SHEDS input values for dermal transfer coefficients and time spent near treated wood are over-estimates or under-estimates.

Other exposure factors that were included in the SHEDS algorithms and appeared significant in the sensitivity analyses, such as hand-to-mouth frequency, saliva removal efficiency, and fraction of hands mouthed, also have limited data in the published literature. There are a number of ongoing and planned studies by EPA/ORD and outside of the Agency that will improve the databases for these parameters, and help reduce uncertainty in future assessments.

While the residues and concentrations in these case studies were hypothetical, information on spatial and temporal variability in wood surface residues and soil concentrations in general is also important. Modeling results may also be influenced by the methodology used to generate longitudinal diaries and estimate lifetime exposures. Thus, longitudinal activity data would help reduce uncertainty in model results.

Another area of future research pertaining to this assessment involves improved dose calculations. For this report the approach of applying route-specific absorption fractions to exposure profiles was applied. A more sophisticated option would be to link the SHEDS

exposure profiles with physically-based pharmacokinetic (PBPK) models (such as NERL's ERDEM model). More data related to uptake and distribution of wood treatment chemicals in the body would be useful, as would biomonitoring data to compare modeled results to actual human doses.

References

Buck, R.J., Özkaynak, H., Xue, J., Zartarian, V.G., Hammerstrom, K. (2001) Modeled Estimates of Chlorpyrifos Exposure and Dose for the Minnesota and Arizona NHEXAS Populations. Journal of Exposure Analysis and Environmental Epidemiology. 11(3): 253-268.

CINTRAFOR (Center for International Trade in Forest Products). (1996) Working paper abstract no. 56 (www.cintrafor.org/RESEARCH). "North American Residential Decking and Siding Markets" by Stephen R. Shook and Ivan L. Eastin.

Frey, C., Zheng, J., Zhao, Y., Li, S., Zhu, Y. (2002). Technical Documentation of the AuvTool Software Tool for Analysis of Variability and Uncertainty. Prepared for U.S. EPA Office of Research and Development, Research Triangle Park, NC under contract number IDC-S794-NTEX.

International Play Equipment Manufacturers Association (IPEMA). (2001) Personal communication with Bill Duffy, Administrator.

Leckie, J.O., Naylor, K.A., Canales, R.A., Ferguson, A.C., Cabrera, N.L., Hurtado, A.L., Lee, K., Yu-Chen Lin, A., Ramirez, J.D., Vieria, V.M.. (2000). Quantifying Children's Microlevel Activity Data from Existing Videotapes. Contract Report Submitted to U.S. EPA, ORD, NERL, Reference Number U2F112OT-RT-99-001182.

The Lifeline Group, Inc. (2000) Lifeline™ Version 1.0 Technical Manual.

McCurdy, T., Glen, G., Smith, L., Lakkadi, Y. (2000). The National Exposure Research Laboratory's Consolidated Human Activity Database. Journal of Exposure Analysis and Environmental Epidemiology, 10(6part1): 566-578.

Ross, J., Thongsinthusak, T., Fong, H.R., Margetich, S., Krieger, R. (1990). Measuring potential dermal transfer of surface pesticide residue generated from indoor fogger use: an interim report. Chemosphere 20(3/4): 349-360.

U.S. Census Bureau. (2000) GCT-P7. Households and Families (www.factfinder.census.gov/bf/.....).

U.S. EPA. (1997a). DRAFT Standard Operating Procedures (SOPs) for Residential Exposure Assessments. Contract No. 68-W6-0030. Work Assignment 3385.102. The Residential Exposure Assessment Workgroup.

U.S. EPA. (1997b). Exposure Factors Handbook. Volume I-III. Office of Research and Development. Washington, D.C. EPA/600/P-05/002Fa.

U.S. EPA. (1997c). Policy for Use of Probabilistic Analyses in Risk Assessment at the U.S. Environmental Protection Agency. May 15, 1997.

U.S. EPA. (1998). Guidance for Submission of Probabilistic Exposure Assessments to the Office of Pesticide Programs' Health Effects Division. Draft, 2/6/98. Office of Pesticide Programs, U.S. Environmental Protection Agency, Arlington, VA.

U.S. EPA. (2000). Child-Specific Exposure Factors Handbook. USEPA NCEA-W-0853. 01 June 2000. US Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Washington, DC.

U.S. EPA. (2001). SAP Report No. 2001-12. (December 12, 2001) FIFRA Scientific Advisory Panel Meeting, October 23-25, 2001, held at the Sheraton Crystal City Hotel, Arlington, Virginia, A Set of Scientific Issues Being Considered by the Environmental Protection Agency Regarding: "Preliminary Evaluation of the Non-dietary Hazard and Exposure to the Children from Contact with Chromated Copper Arsenate (CCA)-treated Wood Playground Structures and CCA-contaminated Soil." Office of Pesticide Programs, U.S. Environmental Protection Agency, Arlington, VA.

U.S. EPA Office of Research and Development, National Exposure Research Laboratory. (2002a). Personal communication with Nicolle Tulve.

U.S. EPA Office of Research and Development, National Exposure Research Laboratory. (2002b). Personal communication with Elaine Cohen Hubal.

Zartarian V.G., Özkaynak H., Burke J.M., Zufall M.J., Rigas M.L., and Furtaw Jr. E.J. (2000). A Modeling Framework for Estimating Children's Residential Exposure and Dose to Chlorpyrifos via Dermal Residue Contact and Non-Dietary Ingestion. Environmental Health Perspectives. 108(6): 505-514.

Appendix 1: Route-Specific Equations to Estimate Absorbed Dose

Notations

AD_e	Absorbed dose during macroactivity event "e" (ug/kg/event)
AF_{dermal}	Dermal absorption fraction (unitless)
BF	Bioavailability fraction (unitless)
$_{body}$	Specific to body, not hands
BW	Body weight (kg)
CF1	Conversion factor (kg/mg)
CF2	Conversion factor (ug/mg)
$_{dermal}$	Via the skin
$_{e}$	During macroactivity event "e"
ET	Time spent playing on or around playsets or decks (hr/event)
F	Fraction of time "ET" contacting wood residues or soil (unitless)
FQH	Frequency of hand-mouth activity (events/hr)
$_{hands}$	Specific to hands, not body
HF	Fraction of hands with residue going into mouth per event (unitless)
$IE_{dermal,hand,t}$	Time-integrated dermal hand loading during event "e" (ug)
IR_{soil}	Soil ingestion rate (mg/hr outside on day)
$_{residue}$	Specific to wood surface residue
$_{soil}$	Specific to soil
SR	Dislodgeable surface residue contacted (ug/cm^2)
SRE	Saliva removal efficiency (unitless)
TC	Dermal transfer coefficient (cm^2/hr)

Equation 1. Absorbed Dermal Dose from Hand-Residue Exposure

$$AD_{dermal,hands,residue,e} = (SR_e * TC_{hand,e} * ET_e * F_{residue,e} * AF_{dermal,e}) / BW$$

Equation 2. Absorbed Dermal Dose from Body-Residue Exposure

$$AD_{dermal,body,residue,e} = (SR_e * TC_{body,e} * ET_e * F_{residue,e} * AF_{dermal,e}) / BW$$

Equation 3. Absorbed Dermal Dose from Hand-Soil Exposure

$$AD_{dermal,hands,soil,e} = (C_{soil,e} * S_{adh,e} * TC_{hand,e} * CF1 * CF2 * ET_e * F_{soil} * AF_{dermal}) / BW$$

Equation 4. Absorbed Dermal Dose from Body-Soil Exposure

$$AD_{dermal,body,soil,e} = (C_{soil,e} * S_{adh,e} * TC_{body,e} * CF1 * CF2 * ET_e * F_{soil} * AF_{dermal}) / BW$$

Equation 5. Absorbed Non-Dietary Ingestion Dose from Hand-Residue-Mouth Exposure

$$AD_{ingestion,hand,residue,e} = (IE_{dermal,hand,e} * HF_e * FQH_e * ET_e * SRE_e * BF_{residue})/BW$$

Equation 6. Absorbed Non-Dietary Ingestion Dose from Soil Ingestion

$$AD_{ingestion,soil,e} = (C_{soil,e} * IR_{soil} * ET_e * CF1 * CF2 * BF_{soil,e}) / BW$$

Note: The above equations serve as the starting point for the SHEDS exposure and dose algorithms. In the detailed time-profile calculations, SHEDS does not determine the absorbed dose directly at the time of exposure contact, but instead spreads the absorption process over time. This more closely reflects the underlying physiological processes and permits the final absorbed dose resulting from each contact to be affected by subsequent behavior such as washing or bathing. This is achieved by calculating the incremental exposure for each contact, which is given by the above equations without the factors for absorption or bioavailability fractions. This exposure is then subject to competing processes including absorption (that is, it can become an absorbed dose), removal by washing, or transfer to the mouth. If these latter terms are small, then effectively the absorbed doses are given by the above set of equations.