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The objective of the current study was to identify the primary volatile organic compounds (VOCs) in the passenger cabin of selected sedan automobiles under static (parked, unventilated) and specified conditions of operation (*i.e.*, driving the vehicle using air conditioning alone, vent mode alone, or driver's window half open). Data was collected on five different passenger sedan vehicles from three major automobile manufacturers. Airborne concentrations were assessed using 90 minute time weighted average samples under USEPA Method IP-1B to assess individual VOC compounds and total VOCs (TVOCs) calibrated to toluene. Static vehicle testing demonstrated TVOC levels of approximately 400 to 800 $\mu\text{g}/\text{m}^3$ at warm interior vehicle temperatures (approx. 80°F), whereas TVOCs at least 5-fold higher were observed under extreme heat conditions (*e.g.*, up to 145°F). The profile of most prevalent individual VOC compounds varied considerably according to vehicle brand, age, and interior temperature tested, with predominant compounds including styrene, toluene, and 8- to 12-carbon VOCs. TVOC levels under varied operating conditions (and ventilation) were generally 4- to 8-fold lower (at approx. 50 to 160 $\mu\text{g}/\text{m}^3$) than the static vehicle measurements under warm conditions, with the lowest measured levels generally observed in the trials with the driver's window half open. These data indicate that while relatively high concentrations of certain VOCs can be measured inside static vehicles under extreme heat conditions, normal modes of operation rapidly reduce the inside vehicle VOC concentrations even when the air conditioning is set on recirculation mode. Due to the relatively low magnitude of individual VOC concentrations and the short exposure period expected for breathing static vehicle inside air at higher interior temperatures, the study results do not suggest any appreciable safety hazard associated with VOCs in the passenger compartment of the automobiles tested.

A PILOT STUDY ASSESSING PHTHALATE EXPOSURE AFTER PERSONAL HYGIENE PRODUCT USAGE.

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Phthalates are ubiquitous plasticizers used to give certain plastics their flexibility and used as a solvent in cosmetic and personal hygiene products. Administration of high doses and administration of chronic doses of diethylhexyl phthalate (DEHP), mono-2-ethylhexyl phthalate (MEHP), di-n-butyl phthalate (DBP), and mono-butyl phthalate (MPB) can produce fetal toxicity and reproductive tract disorders in both male and female rodents. In the third National Health and Nutrition Examination Survey (NHANES III), mean urinary excretions of mono-ethyl phthalate (MEP), MBP, and MBzP, the monoester of benzyl butyl phthalate, were 345 $\mu\text{g}/\text{g}$ creatinine, 20.2 $\mu\text{g}/\text{g}$ creatinine, and 36.9 $\mu\text{g}/\text{g}$ creatinine, respectively. All three phthalates are used extensively in the production of cosmetics and personal hygiene products. We report the results of a pilot study designed to assess whether exposure to commercial products such as cologne, soap, and shampoo could be measured by urinary excretion of phthalate metabolites, specifically phthalate monoesters. We recruited 20 female volunteers from the Centers for Disease Control and Prevention/National Center for Environmental Health to participate. Five groups comprising four women each were asked to use different commercially available shampoos, soaps, and perfumes. They provided 2 urine samples a day over the 3 days of the study, a first morning void and one hour after showering or applying cologne. Urinary levels of monoethyl, butyl, cyclohexyl, ethylhexyl, octyl, benzyl, isononyl, and isodecyl phthalate were measured by for all five groups. After solid phase extraction of the phthalate monoesters, samples were analyzed using a HPLC coupled with a triple quadrupole mass spectrometer equipped with an APCI interface. This technique avoids contamination from the ubiquitous phthalate diester. We will present results utilizing this novel analytical technique to measure phthalate exposures following personal hygiene product usage.

BREATHING RATES FOR INFANTS 0-6 MONTHS OF AGE FOR USE IN EXPOSURE ASSESSMENT.

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Breathing rates normalized to body weight (L/kg-day) for infants 0-6 months of age were estimated for use in exposure assessment. Data were compiled from the literature on directly measured minute ventilation rates (ml/kg-min), energy intake and energy expenditure. The energy data were used to derive breathing rates from the metabolic balance equation, $V_e = H \cdot VQ \cdot E$, of Layton (1993). For this equation, V_e is ventilation rate (vol/kg-time), E is energy expenditure or intake (kcal/kg-time),

and H (kcal/L O₂) and VQ (unitless) are empirically derived values relating oxygen consumption to energy and volume of inhaled air, respectively. Energy expenditure (EE) was measured with indirect calorimetry or the doubly labeled water method. Energy intake (EI) was estimated by multiplying breast milk or formula intake (g/kg-day) by caloric content (kcal/g) and adding the energy intake of supplemented foods or liquids. EI measures incorporate 24-hour energy for basal metabolism as well as energy for active movements while sleeping and awake, food-induced thermogenesis, and tissue growth, and may assume 100% digestibility. On the other hand, the doubly labeled water method did not measure energy for tissue growth and indirect calorimetry did not measure energy for tissue growth or activity. Directly measured ventilation rates did not incorporate the increased breathing rates of physical activity. To derive representative daily breathing rates the following adjustments were made: (1) EI measures were multiplied by a digestibility constant of 92%, (2) ventilation rates and energy associated with physical activity were added to direct measurement and indirect calorimetry estimates, respectively, and (3) tissue growth energy was added to doubly labeled water and indirect calorimetry measures. The studies were combined to give estimated daily breathing rates of 549, 595, 582, 569, 512, 471, 437, and 498 L/kg-day at approximate ages of 0.0-0.5, 1.0, 1.5, 2.0, 3.0, 4.0, 5.0, and 6.0 months, respectively.

ASSESSMENT OF SENSITIZATION RISK TO CONSUMERS USING A LAUNDRY PRESPOTTER PRODUCT CONTAINING PROTEASE.

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When proteolytic enzymes were first introduced to common laundry detergents over 30 years ago, their ability to cause hypersensitivity due to exposure by inhalation was soon recognized as a problem, especially for production workers. Subsequently formulations and manufacturing methods were developed to minimize exposure to enzymes *via* inhaled dust particles. Although detergents containing proteases are now considered safe for consumers, the experience with laundry prespotter products is not as extensive. The study purpose was to examine the risk of sensitization to protease used in a trigger-spray laundry prespotter product. Exposure to the commercial prespotter was measured by simulating a heavy-use scenario in a controlled environment cubical chamber (14.5 m³). The product was applied to a series of fabric targets held vertically over a standard washing machine. Eight replicates of the experiment were done, using 30 sprays for each replicate. Airborne particle distributions in the breathing zone were characterized using a TSI particle analyzer. Enzyme concentrations in air were measured using PTFE membrane filters that were frozen until analyzed by an ELISA procedure. Aerosol concentrations returned to baseline within 10 minutes, during which the average enzyme concentration in air was 17 (s.d. 5) and 12 (s.d. 2.6) ng/m³ using low- and high-volume samplers, respectively. The corresponding amount of enzyme inhaled is significantly less than allowed in occupational situations. Recent prospective clinical data and consumer surveillance confirm that no sensitization is expected.

CHARACTERIZATION OF AN ASPHALT FUME GENERATION SYSTEM AND DETERMINATION OF FUME COMPOSITIONS AT SIMULATED ROAD PAVING CONDITIONS.

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A highly sensitive, selective, and reliable analytical method has been developed and validated for characterization of asphalt fume generated under road paving conditions. A new approach was developed utilizing a microflow liquid chromatogram (LC) coupled to atmospheric pressure chemical ionization (APCI) of quadrupole/time-of-flight mass spectrometry (Q-TOF MS). A dynamic asphalt fume generation system was modified to provide consistent test atmospheres at simulated road asphalt paving conditions. Characterization of the asphalt fume test atmospheres included (1) determination of the uniformity of the aerosol distribution within the generator and exposure chamber; (2) quantitative detection of total extractable asphalt fume content by electron ionization of isotope dilution GC-MS; (3) use of a photo ionization detector (PID) for on-line monitoring; and (4) identification of individual priority polycyclic aromatic hydrocarbons (PAHs) in the asphalt fume by selected ion monitoring GC-MS, and further clarification of important PAH by coupling microflow LC to Q-TOF MS. Total extractable asphalt fume components were quantified over the 5 day exposure. Sixteen individual priority

PAHs were monitored and identified. These PHAs were detected at a trace level on filter fractions. By coupling microflow LC to APCI of Q-TOF MS, the new approach of collision-induced dissociation of fragmentation pathway leading to a characteristic fragmentation pattern for selected target analytes was used to further clarify the trace amount of PAHs present in simulated road paving asphalt fumes. These results demonstrate that asphalt fume compositions can be characterized and individual priority PAHs can be identified at trace levels using this developed method. Such a method is suitable for support of simulated occupational exposure for inhalation toxicity studies. (This research work was supported, in part, by NIEHS/NTP)

102 MEASUREMENT AND CHARACTERIZATION OF AEROSOLS FROM CONSUMER SPRAY CLEANER PRODUCTS WITH CONVENTIONAL AIR SAMPLERS AND A REAL TIME DEVICE.

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The objective of this investigation was to measure and characterize aerosols of spray cleaners in the breathing zone of a potential user with conventional air samplers and a real time device, i.e., an Aerodynamic Particle Sizer (APS). Real time devices allow to reflect more realistically consumer use while not requiring time consuming analytical programs. Sampler performance measuring consumer respiratory exposure was determined using the human use simulation model. In the model, the sprayer nozzle was targeted at the center of a vinyl tile, mounted vertically. Multistage samplers, an Andersen cascade impactor (ADS) and a Personal Dust Spectrometer (PIDS) as well as the sampling tube of an APS, were mounted next to each other on a ringstand at a defined distance from the tile. Sprayers were operated automatically according to sequence mimicking consumers' practices. Following each test, aerosol samples collected from the ADS and PIDS were recovered for assay. The model was shown to accurately simulate consumer exposure to aerosols generated by trigger sprayers. To evaluate the effectiveness of the samplers and the APS, aerosol mass levels and cumulative mass distribution d50 values were compared for particle size ranges (ISO definitions for health related sampling). The results, particularly for the APS, showed very low inter-run variability, with airborne aerosol concentrations in the range 0.5-6mg/m³. The performance of ADS, PIDS and the APS were equivalent for particles with an aerodynamic diameter (AD) of ≤10µm. PIDS and the APS produced similar results for aerosol particles of ≤15µm AD. The APS underestimated aerosol masses of particles >15µm AD. While conventional air sampling techniques are already well established for measuring water-based aerosols, this investigation lends support to the usefulness of the APS in assessing consumer exposure to sprayer aerosols.

103 APPLICATION OF QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP (QSAR) AND PHYSIOLOGICALLY BASED PHARMACOKINETIC (PBPK) MODELING TO PREDICT THE CONTRIBUTION OF SOIL EXPOSURE TO PCB LEVELS IN HUMAN SERUM.

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The major route of human exposure to polychlorinated biphenyls(PCBs) is through ingestion of contaminated food. Nationally, the average range of PCBs is 4-7µg/l in human serum. However, a much higher range of total PCBs levels (76.3 to 187.5 µg/l) was found in the serum of some residents living in a highly-contaminated residential area. Total PCB soils levels in this area ranged from 17.4 to 840 mg/kg. The purpose of this project was to estimate the contribution of exposure by soil ingestion to the levels of serum PCBs in this residential area. Physiologically based pharmacokinetic (PBPK) models are useful in relating environmental exposure to biological markers such as blood levels. Human PBPK models of the 25 most common PCB congeners were developed for the oral route. Parameters such as partition coefficients and metabolic constants used in the PBPK models were determined using quantitative structure activity relationships (QSAR). All simulations were run using a soil ingestion default rate of 50 mg/day for a life-time exposure scenario. To address exposure variability in the highly contaminated residential area, a probabilistic distribution model for contaminant levels was derived based on actual PCB soil measurements. This distribution was then applied to the 25 PBPK models to derive a distribution of total PCBs in blood for life-time exposure sce-

narios. The derived distribution of blood levels was superimposed on the actual distribution of measured serum levels estimated in the same community. The distribution of actual blood levels for 9 out of 10 persons falls within the modeled exposure range. This suggests that the PCBs from heavily contaminated soil in this residential area can significantly contribute to the overall elevated serum levels of PCBs.

104 SERUM PCB, PCDD, PCDF AND PESTICIDE LEVELS IN CONSUMERS AND NON-CONSUMERS OF LAKE ONTARIO WILDLIFE.

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Consumption of fish and wildlife from Lake Ontario represents a potential source of excess exposure to persistent halogenated aromatic hydrocarbons (HAHs), including dioxin-like polychlorinated dibenzo-p-dioxins (PCDDs), dibenzofurans (PCDFs), and coplanar polychlorinated biphenyls (PCBs). This study was designed to assess exposure to dioxin-like HAHs and non-coplanar PCBs and pesticides in anglers that consume Lake Ontario fish and wildlife (consumers, n=23) and an age and gender matched control group (non-consumers n = 16) with no history of consumption of Lake Ontario fish. Subjects who participated in this study are members of the New York State Angler Cohort (NYSAC) study that has been an ongoing investigation of fishing license holders, 18 to 40 years of age (as of 1991) who reside in the 16 upstate New York counties with close proximity to Lake Ontario. 2,3,7,8-TCDD, the most potent HAH, was detected at levels from <0.8 to 2.2 ppt (pg/g serum lipid) in non-consumers and at levels from 1.2 to 3.7 ppt in the serum lipid of consumers. 3,3',4,4',5-PentaCB (PCB 126), the most potent PCB, was detected in serum at levels ranging from 3.4 to 45.5 ppt in non-consumers and at levels from 4.2 to 151 ppt in consumers. In addition to these congeners, the serum levels of 1,2,3,7,8-PentaCDD, 1,2,3,7,8-PentaCDF and 2,3,4,7,8-PentaCDF, PCB 169, 20 non-coplanar PCBs, 3 pesticides (mirex, DDE and t-nonachlor) and total dioxin TEQs were significantly higher in consumers as compared to non-consumers. Serum mirex levels were increased about 8-fold in consumers, providing the best exposure marker for the consumption of Lake Ontario wildlife. These results show that consumption of Lake Ontario wildlife results in higher serum levels of persistent HAHs, that could have potential detrimental effects to certain biological functions. (Supported by ATSDR PN92594.)

105 A PROBABILISTIC ASSESSMENT OF HOUSEHOLD EXPOSURES TO MTBE FROM DRINKING WATER.

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The oxygenate methyl tertiary butyl ether (MTBE) has been added to reformulated gasoline in the United States to meet national ambient air quality standards. Although MTBE has provided significant health benefits in terms of reduced criteria and toxic air pollutants, detections of MTBE in some groundwater and drinking water sources have raised concerns about potential human exposures. In fact, a national program to phase out MTBE in gasoline has been proposed. Our analysis finds little scientific justification for this proposal, however, and little is known about potential health risks associated with MTBE alternatives. We examined the frequency and concentration of MTBE detections in drinking water sources in California from 1995 to 1999, and provide a preliminary analysis of the distribution of household exposures to MTBE from water-related activities. Using published data on the toxicity and possible cancer hazard, we estimate the likely cancer and non-cancer risk for the general population in California from past and potential future MTBE exposures. More highly exposed subgroups were also addressed. Our findings indicate that less than 2% of all sampled drinking water sources in California had detectable levels of MTBE in 1999, with average MTBE drinking water concentrations ranging from 0.09 to 4.9 ppb for this year. Both the detection rate for MTBE and average MTBE concentrations have remained relatively stable since 1995, despite increased sampling of drinking water sources in California. The probabilistic analysis suggests that ingestion, inhalation, and dermal exposures to MTBE in drinking water are unlikely to pose a significant health risk for the general population or more highly exposed individuals in California.

106 COMPARISON OF DISINFECTANT BYPRODUCTS CONCENTRATIONS FROM OZONATION AND CHLORINATION OF DRINKING WATER.

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Under the Safe Drinking Water Act, alternative disinfectants such as ozone is becoming popular in the disinfection of drinking water in the United States since the promulgation of the Stage 1 Disinfectant Byproducts (DBP) rule, which included



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Preface

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An alphabetical Author Index, cross referencing the corresponding abstract number(s), begins on page 451.

The issue also contains a Keyword Index (by subject or chemical) of all the presentations, beginning on page 479.

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