

## **Appendix A**

### **List of Attendees**

**Voluntary Children's Chemical Evaluation Program (VCCEP)  
Peer Consultation on n-Alkanes**

**September 14, 2004**

**List of Attendees**

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## **Appendix B**

### **Meeting Materials**

#### **Agenda, Overview, Panel Charge, Panelist Biographical Sketches and Conflict of Interest/Bias Disclosures, and Presenter Biographical Sketches**

**Voluntary Children's Chemical Evaluation  
Program (VCCEP)  
Peer Consultations on  
n-Alkanes  
(Decane, Dodecane, and Undecane)**

**Meeting Materials**

**September 14, 2004**

**Kingsgate Conference Center, Salon A  
University of Cincinnati  
Cincinnati, Ohio**

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## Agenda for n-Alkanes

University of Cincinnati, Kingsgate Conference Center, Salon A

**Tuesday, September 14, 2004**

- 8:00 Registration and Check In**
- 8:30 Meeting Convened<sup>1</sup>**  
Welcome: Ms. Jacqueline Patterson, *TERA*  
Introductions and Disclosures, Panel  
Meeting Process: Dr. Michael Dourson, Chair
- 9:00 Sponsor Introduction**  
Mr. Andrew Jaques, ACC Consortium Manager
- Sponsor Presentation on Exposure Assessment**  
Dr. Ross MacDonald, Consortium Consultant
- Public Comments on Exposure Assessment**
- Panel Discussion**
- 11:30 Sponsor Presentation on Hazard Assessment**  
Dr. Ralph Gingell, Shell Chemicals LP
- Public Comments on Hazard Assessment**
- Panel Discussion**
- 12:00 Lunch**
- 1:00 Panel Discussion on Hazard Assessment (continued)**
- 2:00 Sponsor Presentation on Risk Characterization**  
Dr. Ross MacDonald, Consortium Consultant
- Public Comments on Risk Characterization**
- Panel Discussion on Risk Characterization**
- 3:00 Sponsor Presentation on Data Needs Assessment and Conclusion**  
Dr. David Penney, Sasol North America
- Public Comments on Data Needs**
- Panel Discussion on Data Needs**
- 4:30 Closing Remarks and Evaluation of Meeting**
- 5:00 Adjourn**

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<sup>1</sup> The Chair will call a 15-minute break each morning and afternoon.  
Voluntary Children's Chemical Evaluation Program (VCCEP)  
Peer Consultation Meeting Report on n-Alkanes

## **Overview of the Peer Consultation Process**

### **Introduction**

This peer consultation meeting has been organized by Toxicology Excellence for Risk Assessment (*TERA*). *TERA* is an independent non-profit organization with a mission to protect public health through the best use of toxicity and exposure information in the development of human health risk assessments. *TERA* has organized and conducted peer review and consultation meetings for private and public sponsors since 1996 (see <http://www.tera.org/peer> for information about the program and reports from meetings). As a part of this program, *TERA* is organizing peer consultation panel meetings for assessments developed under the Voluntary Children's Chemical Evaluation Program (VCCEP). This panel meeting will review the assessment on n-Alkanes, which was submitted by the American Chemistry Council (ACC) n-Alkane Consortium.

The VCCEP program is a voluntary pilot program and part of the Environmental Protection Agency's ([EPA Chemical Right-to-Know Initiative](#)). The goal of EPA's VCCEP program is to enable the public to better understand the potential health risk to children associated with certain chemical exposures. EPA has asked companies which manufacture and/or import 23 chemicals (that have been found in human tissues and the environment in various monitoring programs) to volunteer to sponsor their evaluation in Tier 1 of a pilot of the [VCCEP](#). Sponsorship requires the companies to collect or develop health effects and exposure information on their chemical(s) and then to integrate that information in a risk assessment and a "data needs" assessment. More information about the VCCEP is available in the December 26, 2000 Federal Register (65 FR 81700) (<http://www.epa.gov/oppt/chemrtk/ts00274d.htm>) and on EPA's VCCEP web site (<http://www.epa.gov/chemrtk/vccep/index.htm>).

The purpose of this meeting is to provide a science-based peer consultation on the data needs for n-Alkanes. The assessment developed by the sponsor is being considered by a panel of scientific experts using a peer consultation process developed by *TERA*. These experts have experience in toxicity testing, exposure evaluation, risk assessment, and children's health. *TERA* has selected Peer Consultation Panel members after careful consideration of nominations from the public, and is responsible for convening and chairing panel meetings to discuss the sponsors' submissions. *TERA* will prepare a report for the meeting and make this available to the public at <http://www.tera.org/peer/VCCEP/n-alkanes/n-alkanesWelcome.html>. The peer consultation meeting is open to the public.

### **Background on the Voluntary Children's Chemical Evaluation Program (VCCEP)**

The ACC n-Alkanes Consortium has volunteered to sponsor a Tier 1 assessment for n-Alkanes, including hazard, exposure, risk characterization, and data needs assessments, utilizing available data. The key question of the program and the peer consultation is whether the potential hazards, exposures, and risks to children have been adequately characterized and if not, what additional data are necessary.

The program was set up to use a tiered testing approach, which is explained in the December 26, 2000 Federal Register notice. For toxicity data, specific types of studies have been put into three

tiers. For exposure data, the depth of exposure information increases with each tier, with Tier 1 a screening level assessment and Tiers 2 and 3 more advanced assessments using exposure studies, monitoring data, and modeling. The Federal Register notes that the Tier 1 assessment should use all available data, and therefore some of the chemical assessment documents will include more than what is in the Tier 1 level.

The peer consultation is designed to be a forum for scientists and experts to exchange scientific views on the need for additional toxicity and exposure data and analysis. In selecting the panel, *TERA* has sought to involve stakeholders by considering their nominations for panel members, and has sought to have a range of perspectives on the panel. This is not a consensus based approach; rather the individual panel members will discuss their own views. In the meeting report, opinions of the individual panel members will be noted, along with areas of agreement and disagreement.

The VCCEP program is a voluntary program. The sponsor has volunteered to prepare the Tier 1 assessment. If data needs are identified through this process, the sponsor will choose whether or not to volunteer for Tier 2.

### **N-Alkanes Peer Consultation Panel**

The VCCEP Peer Consultation Panel for n-Alkanes consists of eleven members: seven of the nine VCCEP Core Panel Members for Year 2 and four additional *ad hoc* members specifically selected for this meeting. The Panel includes scientific experts in toxicity testing, risk assessment, exposure assessment, and children's health. Collectively, this panel has many publications and presentations on topics related to children's health risk.

A core group of panel members participates in all panel meetings to ensure consistency among the reviews. *TERA* received 50 nominations for core panel members in early 2002 from VCCEP stakeholders and other interested parties. After a thorough review of these nominees, as well as others independently identified, *TERA* selected a group of nine scientists in June 2002. The original core panelists were invited to return for Year 2 (2004). One core panel member choose not to return for the second year, therefore, the Year 2 core panel consists of the original eight panel members and one new member.

Additional *ad hoc* experts are invited by *TERA* to participate in panel meetings on a case-by-case basis to provide additional expertise relevant to a specific chemical or issue. Nominations for *ad hoc* panelists were solicited from interested parties or independently selected by *TERA*. *Ad hoc* panelists have the same status and responsibilities as the core group panelists.

Each panel member has disclosed information regarding potential conflicts of interest and biases related to the VCCEP program, the sponsor, and n-Alkanes. *TERA* evaluated these disclosures when selecting panel members. Short biographical sketches and disclosure statements for panel members are provided in this package.

### **Conduct of the Peer Consultation**

*TERA* developed a "charge" document that identifies the scientific issues to be discussed by the panel. The panel received a copy of the submission, the charge, and key references

approximately a month prior to the meeting, to ensure adequate time to carefully review the document and be prepared for the discussions.

The meeting will be organized to make the best use of the time available to hear the opinions of the experts on the charge questions and the data needs. The meeting will begin with panel introductions and discussion of conflict of interest and bias issues. The discussion will then address the four assessment sections of the sponsor's submission (hazard, exposure, risk characterization, and data needs). To start each discussion section, the authors of the assessment document will make a short presentation. These presentations will highlight the salient points and issues, and give the panel the opportunity to ask clarifying questions of the authors.

### **Public Observation and Comments**

Members of the public are invited to attend the VCCEP peer consultation meetings and observe the Panel discussions. To ensure that adequate space is available, we ask people to register in advance for the meeting. The public was also given the opportunity to prepare brief technical comments on the assessment document and submit these in writing prior to the meeting. Several public comments were received on n-Alkanes. Observers will be permitted to make brief technical comments at the meeting as time permits. Panel members and sponsors may ask clarifying questions of those making comments.

### **Meeting Report**

*TERA* will prepare a meeting report summarizing the sponsor presentations, the opinions and recommendations expressed by the panel, and any oral comments from the public. Written public comments will also be included. The meeting report will not be a transcript. The report will be reviewed by the panel for accuracy. Sponsors and observers presenting oral comments will be offered the opportunity to review the summaries of their presentations. The finalized report will then be made available to the public at <http://www.tera.org/peer/VCCEP/n-alkanes/n-alkanesWelcome.html>.

## **Panel Charge for N-Alkanes**

**(Decane, Undecane, and Dodecane)**

### Introduction

The primary objective of this Peer Consultation Panel is to discuss whether the potential hazards, exposures, and risks for children have been adequately characterized for decane, undecane, and dodecane, based on the information contained in assessment documents submitted by the sponsors and on other available information. If the potential hazards, exposures, and risks cannot be adequately characterized, then data needs should be identified. The panel's job is not to critique the assessment document *per se*; rather, the panelists use the document and its references as a source of information. The panel is not required to reach consensus positions on any issues or conclusions. Panelists who believe a chemical has not been adequately characterized will be asked to identify what additional information is needed and why it is necessary. All the panelists will be encouraged to discuss and debate each other's suggestions and comments, providing scientific rationales for their points of view. *TERA* will compile the panel discussions in a meeting report that will be sent to the sponsor and made available to the public.

*TERA* has prepared this charge to help the panel discuss the sponsor's submission and address whether a chemical has been adequately characterized. The topics are consistent with the directions for VCCEP submissions given in the December 26, 2000, Federal Register: <http://www.epa.gov/oppt/chemrtk/ts00274d.htm>.

Panelists should keep in mind the following directives from the Federal Register regarding any recommendations for additional testing: (1) If specific toxicity studies are indicated, they should be chosen from the next tier of studies within the overall framework. They should allow flexibility to pursue either additional toxicity testing and/or exposure evaluation, allowing sponsors to select the option which will most quickly, directly, and cost-effectively reduce uncertainty and allow the creation of a risk assessment; (2) EPA is committed to avoiding duplicative testing, and to reducing, refining, and replacing animal testing when valid alternatives exist; (3) if relevant alternative test methods become validated, EPA will consider their immediate implementation in the program; (4) EPA encourages sponsors to combine tests where possible to conserve resources and reduce the number of animals required for testing; and (5) the Tier 2 and Tier 3 testing will be limited to chemicals for which there is a clear need.

### ***Hazard Assessment***

1. Discuss whether the information available on mode of action, toxicity studies, and ADME (absorption, distribution, metabolism, and elimination) is adequate to identify and assess potential hazards a) to the prospective parents, b) to the embryo and fetus, and c) to the infant and child.
2. Discuss whether the quantitative hazard and dose-response information (e.g., RfD, RfC) is appropriately chosen or selected.

### ***Exposure Assessment***

3. Discuss whether the fates of these chemicals are adequately understood.
4. Based on the information at hand, discuss whether the available data are adequate to characterize exposure, taking into consideration the conditions of exposure (sources, routes, frequency, duration, intensity, etc.).
5. Discuss whether all times relevant to childhood exposure [(a) parental exposure prior to conception, (b) prenatal development, (c) and postnatal development to the age of sexual maturation] have been adequately considered.
6. Discuss whether the estimates of exposure have been calculated appropriately and correctly.

### ***Risk Characterization***

7. Discuss whether the Risk Characterization appropriately integrates the exposure and hazard information for this chemical and adequately characterizes the risk a) to the prospective parents, b) to the embryo and fetus, and c) to the infant and child.

### ***Data Needs***

8. Identify any additional hazard information that is needed and discuss why it is necessary. The focus should be on those studies listed in the next VCCEP tier.
9. Identify any additional exposure data and analyses that are needed and discuss why this information is necessary.

## **Conflict of Interest and Panel Biographical Sketches**

An essential part of Peer Consultation Panel selection is the identification and disclosure of conflicts of interest and biases. Prior to selecting the core and *ad hoc* panelists, each panel member is asked to complete a questionnaire to determine whether their activities, financial holdings, or affiliations could pose a real or perceived conflict of interest or bias. (See <http://www.tera.org/peer/COI.html> for *TERA*'s policy and questionnaire for the Peer Consultation Program related to VCCEP). Questionnaires are reviewed by *TERA* staff and discussed further with panel candidates as needed.

For the Peer Consultation Program related to VCCEP, a conflict of interest (COI) for a candidate would include:

- Working for an organization sponsoring the chemical to be reviewed at the panel meeting,
- Having direct personal financial investments in the sponsoring organization or in the chemical itself, or
- Authoring the sponsoring organization's assessment document submitted to the VCCEP panel.

Bias for a peer consultation panel candidate would be a predisposition towards the subject matter to be discussed at the panel meeting that could influence the candidate's viewpoint. Examples of potential bias would be situations in which a candidate:

- Has previously taken a public position on subjects to be discussed by the panel, or
- Is affiliated with an industry, governmental, public interest, or other group with a partiality regarding subjects to be discussed by the panel.

Most scientists with technical expertise in areas relevant to these peer consultation panels will have existing opinions about the subject matter. Therefore, they may be considered to have some degree of bias.

The purpose of these peer consultation panels is to gather expert scientific opinion from a range of experts, including those who may be affiliated with organizations or companies with an interest in the outcome. All panelists were selected by *TERA* based upon their expertise and qualifications. They are employed by many types of organizations. *TERA* strives to create a balance of expertise and affiliations for each peer consultation meeting; however, individual panel members represent their own expertise and views, not those of their employer, of any group who may have nominated them, or any group with whom they may be associated. This peer consultation panel is a distinguished group with many years experience in a wide range of disciplines.

Toxicology Excellence for Risk Assessment (*TERA*) is conducting this VCCEP peer consultation under its Peer Consultation Program. This program is principally funded by a Cooperative Agreement with the U.S. EPA, the purpose of which is to design, develop, and manage a Peer Consultation process that will serve as a public scientific forum. *TERA*'s role in managing the peer consultation is undertaken primarily at the request of and for the benefit of non-federal stakeholders, particularly the sponsors of VCCEP chemicals.

*TERA* has performed work for organizations associated with VCCEP, both in the past and at the present time. These include the U.S. EPA, the American Chemistry Council, and some companies that are sponsors of VCCEP chemicals. In the past, *TERA* has conducted assessments and analysis for a number of chemicals included in the VCCEP pilot program (i.e., acetone, decabromodiphenyl ether, methyl ethyl ketone, and toluene) and is currently doing work on trichloroethylene. This work has been done for a variety of public and private sponsors, but none of it is directly related to the VCCEP assessments.

A brief biographical sketch of each panel member is provided below, together with a disclosure statement describing any potential conflict of interest or bias issues. The disclosure statements do not address funding provided by organizations unrelated to VCCEP or these chemicals and sponsor. For the core panelists, the disclosure statements cover the chemicals and sponsors in the entire VCCEP pilot program. For the *ad hoc* panelists, the disclosures are specific to n-Alkanes and the n-Alkanes sponsor. Brief biographical sketches of the sponsors' presenters follow the panelist biographical sketches.

## ***Dr. John Balbus***

Dr. John Balbus is currently the Director of the Environmental Health Program for Environmental Defense, where he is working on projects related to antibiotic resistance, health impacts of urban sprawl and transportation policy, and chemical testing and right-to-know. Before his current position, he served as the founding Director of the Center for Risk Science and Public Health, as well as an Associate Professor at the George Washington University Medical Center. Dr. Balbus' research activities at the Center for Risk Science and Public Health included addressing susceptibility in risk assessment and risk management, children's susceptibility to waterborne contaminants, and health impacts of climate change. Dr. Balbus was a founding co-director of the Mid-Atlantic Center for Children's Health and the Environment, one of 11 Pediatric Environmental Health Specialty Units funded by the U.S. EPA and ATSDR.

Dr. Balbus received his M.D. from the University of Pennsylvania, an M.P.H. from the Johns Hopkins School of Hygiene and Public Health, and an A.B. in Biochemistry from Harvard University. He completed residencies in internal medicine at Pennsylvania Hospital and in occupational and environmental medicine at Johns Hopkins School of Hygiene and Public Health. Dr. Balbus has also held a variety of additional academic appointments that include: Assistant Professor of Medicine at George Washington University Medical Center, Clinical Fellow in Medicine at John Hopkins School of Medicine, Assistant Professor in Medicine at Uniformed Services University of the Health Sciences, and Clinical Instructor in Medicine at the University of Pennsylvania, School of Medicine.

Dr. Balbus is currently certified by the American Board of Internal Medicine, and the American Board of Preventive Medicine, specialty in Occupational Medicine.

In addition to Dr. Balbus' extensive professional and academic career, he has published numerous articles relating to a variety of topics in risk assessment, public health, and environmental health.

### **DISCLOSURE:**

Dr. Balbus is a VCCEP Core Panel member. He is employed by Environmental Defense. Environmental Defense has taken public positions on chemicals included in the VCCEP pilot program and on the VCCEP program itself.

## ***Mr. Thomas Brennan***

Mr. Thomas Brennan is currently a Team Leader/Environmental Protection Specialist with the Office of Pesticide Programs, Special Review & Reregistration Division, Reregistration Branch 1 of the U.S. EPA. He has extensive experience in developing and evaluating risk assessment methods and models. He managed the development of the Pesticide Inert Risk Assessment Tool (PIRAT), which estimates the exposures to inert ingredients of pesticide products used in residential settings. Mr. Brennan is also the Project Manager of the Office of Prevention, Pesticides, and Toxic Substances “International Toolbox” project. The International Toolbox is a CD-ROM- and Web-based directory allowing access to over 50 databases, models, software, and documents to better assess and manage risks to human health and the environment, as well as to prevent pollution. While working for US EPA’s Office of Pollution Prevention and Toxics (OPPT), he managed the development of the Exposure & Fate Assessment Screening Tool (E-FAST) that provides screening-level estimates of consumer, general population, and environmental exposures.

Mr. Brennan has been active in communicating EPA science, policy, and computer modeling issues to varied stakeholder groups. He has helped teach chemical and pesticide risk assessment modeling and policy issues at: Duke University, at Society for Toxicology continuing education seminars, as part of the OPPT P2Framework workshops, directly to representatives for industry and foreign governments, and elsewhere.

Mr. Brennan received his M.S. and B.S. in Botany from Ohio University, Environmental and Plant Biology Department. He joined the U.S. EPA in 1997 and has held several scientific and communications positions during his tenure. In his current position, Mr. Brennan leads multi-disciplinary teams that assess exposures and subsequent risks to human and ecological health from pesticide active and inert ingredients. These assessments include assessing human and ecological risks, considering any alternatives to the chemical, as well as economic impacts of possible regulatory activities. Before joining the Agency, he worked several years for government consulting firms in the Washington DC area. He is a member of the Society for Risk Analysis.

### **DISCLOSURE:**

Mr. Brennan is an *ad hoc* member of the VCCEP n-Alkanes Panel. He is employed by the U.S. EPA, working in the Office of Pesticide Programs, Special Review & Reregistration Division. EPA has taken public positions on the VCCEP pilot chemicals and on the tests included in the VCCEP Tiers.

## ***Dr. George Daston***

Dr. George Daston is a Research Fellow for the Procter & Gamble Company (P&G) where he has worked since 1985. He has worked the past 21 years in the field of developmental toxicology and risk assessment, particularly in the area of children's risk assessment. Dr. Daston is also an adjunct professor in the Department of Pediatrics and Developmental Biology Program at the University of Cincinnati and Children's Hospital Research Foundation, and lectures in courses on teratology, developmental biology, toxicology, and risk assessment.

Dr. Daston received his Ph.D. in Developmental Biology and Teratology and a B.S. in Biology from the University of Miami. Before joining the Procter & Gamble Company, Dr. Daston worked for the U.S. EPA's Health Effects Research Laboratory as a National Research Council Research Associate and as an assistant professor for the Department of Biological Sciences at the University of Wisconsin.

His research interests include teratogenic mechanisms, *in vitro* methodologies, and risk assessment. His most recent research includes toxicant-nutrient (especially zinc) and maternal-embryonal interactions in developmental toxicity, the role of pattern formation genes in abnormal development, genomic approaches to endocrine disrupter screening, and improvements in risk assessment methodology for noncancer endpoints.

Dr. Daston's activities in professional societies include serving as Chair of the Reproductive and Developmental Effects Subcommittee of the American Industrial Health Council, Chair of the Developmental and Reproductive Toxicology Technical Committee of ILSI-Health Effects Sciences Institute; President of the Society of Toxicology's Reproductive and Developmental Toxicology Specialty Section, President of the Teratology Society, member of the National Academy of Sciences Board on Environmental Studies and Toxicology, and member of EPA's Endocrine Disrupter Screening and Testing Advisory Committee (EDSTAC).

Dr. Daston has recently served on the organizing committees for an ILSI/EPA/AIHC workshops on benchmark dose methodology and human variability in toxic response; an EPA workshop on endocrine mediated toxicity; and as co-chair of an AIHC/EPA workshop on Leydig cell tumors, an ILSI/EPA workshop on interpreting reproductive toxicity endpoints, and a NIEHS workshop on the state of validation of the FETAX assay for teratogen screening.

Dr. Daston is an Associate Editor of *Toxicological Sciences*, Editor-in-Chief of *Birth Defects Research Part B: Developmental and Reproductive Toxicology*, on the Editorial Board of *Human and Ecological Risk Assessment* and *Reproductive Toxicology*, and an *ad hoc* reviewer for *Teratology*, *Journal of Nutrition* and other journals. He has published over 90 peer-reviewed articles, reviews and book chapters, and has edited three books.

### **DISCLOSURE:**

Dr. Daston is a VCCEP Core Panel member. He is employed by the Procter & Gamble Company (P&G). P&G uses thousands of chemicals, which it purchases individually, or in mixtures. It is possible that some VCCEP pilot chemicals are included in these purchases. P&G purchases chemicals from numerous suppliers, including companies that are sponsors of the VCCEP pilot chemicals.

## ***Dr. Michael L. Dourson***

Dr. Michael Dourson directs Toxicology Excellence for Risk Assessment (*TERA*), a nonprofit corporation dedicated to the best use of toxicity data for estimating risk assessment values. *TERA*'s projects include the development of complex risk assessments, such as soluble nickel salts; research into improvements of risk methods, such as differential sensitivity of children and adults to chemical toxicity, organizing peer review and consultation meetings for risk assessment topics and documents; and education and outreach on risk assessment values through lectures and data bases, including the International Toxicity Estimates for Risk (*ITER*).

Before founding *TERA* in 1996, Dr. Dourson held leadership roles in the U.S. Environmental Protection Agency for fifteen years; as chair of EPA's Reference Dose (RfD) Work Group, charter member of the EPA's Risk Assessment Forum and chief of the group that helped create the Integrated Risk Information System (IRIS) in 1986. Dr. Dourson received his Ph.D. in Toxicology from the University of Cincinnati and a B.A. in biology from Wittenberg University. Dr. Dourson's research interests include investigating methods to extrapolate toxicity data garnered on experimental animals or healthy adults to the appropriate sensitive human population. Topic such as adversity of effect, and characterization of risk are also of interest.

Dr. Dourson has served on numerous expert panels, such as EPA's peer review panels for IRIS assessments and its Risk Assessment Forum, *TERA*'s International Toxicity Estimates for Risk (*ITER*) independent peer reviews and consultations, FDA's Science Board Subcommittee on Toxicology, the NSF's Health Advisory Board, and SOT's harmonization of cancer and non-cancer risk assessment. Dr. Dourson has also organized over 16 symposia for 9 different organizations on a variety of topics, including: effective risk communication; chromium; information resources for toxicology and environmental health; risk assessment of essential trace elements; risk characterization; EPA's IRIS; role of toxicology in tomorrow's risk assessment practice; techniques for quantifying uncertainty in risk assessment; statistical and dose response models in risk assessment; workshop on benchmark dose methodology; basics of risk assessment; improvements in quantitative noncancer risk assessment; and neurotoxicity risk assessment.

Dr. Dourson is a Diplomate of the American Board of Toxicology and served on its Board as President, Vice President, and Treasurer. He is currently Secretary for the Society for Risk Analysis. He has also served as president of the Dose-Response Specialty Group of the Society for Risk Analysis, of the Society of Toxicology's Specialty Section on Risk Assessment and of the Ohio Chapter of the Society for Risk Analysis. He is currently on the editorial board of three journals. Dr Dourson has published more than 70 papers on risk assessment methods, has co-authored over 100 government risk assessment documents, and has made over 90 invited presentations.

### **DISCLOSURE:**

Dr. Dourson is a VCCEP Core Panel member. He is Director of the non-profit organization Toxicology Excellence for Risk Assessment (*TERA*). Previously, he was employed by the U.S. EPA. *TERA* has performed work for organizations associated with VCCEP. These include the U.S. EPA, the American Chemistry Council, and some companies that are sponsors of VCCEP chemicals. In the past, *TERA* has conducted assessments and analysis for a number of chemicals included in the VCCEP pilot program (i.e., acetone, decabromodiphenyl ether, methyl ethyl ketone, and toluene) and is currently doing work on trichloroethylene. This work has been done for a variety of public and private sponsors, but none of it is directly related to the VCCEP assessments.

## ***Dr. Jeffrey Fisher***

Dr. Jeffrey Fisher is Professor and Department Head in the Department of Environmental Health Sciences at the University of Georgia. He has 18 years of experience in physiological modeling and has trained 20 graduate students and postdoctoral fellows on the concepts and application of physiological models. His modeling and research activities with solvents have focused on the development and validation of mathematical models for cancer risk assessment, estimating lactational transfer of solvents, understanding *in utero* and neonatal dosimetry, and quantifying metabolism of solvent introduced as mixtures. His work includes research on trichloroethylene and its P450 mediated metabolites, trichloroacetic and dichloroacetic acid; perchloroethylene, methanol, and carbon tetrachloride. Recently, he has worked on pharmacokinetic and pharmacodynamic models for hypothyroidism in rats using perchlorate to induce hypothyroidism. He currently teaches a graduate class in PBPK modeling and trains graduate students in the application of PBPK models in toxicology and environmental health.

Dr. Fisher has a B.S. degree in biology from the University of Nebraska at Kearney, a M.S. degree in biology/ecology from Wright State University, and a Ph.D. in Zoology/Toxicology from Miami University. He spent most of his career at the Toxicology Laboratory, Wright Patterson AFB, where he was Principal Investigator and Senior Scientist in the Toxics Hazards Division and Technical Advisor for the Operational Toxicology Branch. He was a Visiting Scientist at the Chemical Industry Institute of Toxicology in 1996 and at the NIOSH Taft Laboratory in 1999. During this time, he also served as Adjunct Professor in the Department of Pharmacology and Toxicology at Wright State University. He accepted an academic position at the University of Georgia in July 2000.

Dr. Fisher has published over 50 papers on pharmacokinetics and PBPK modeling in laboratory animals and humans. He has served on several panels and advisory boards for the Department of Defense, the Agency for Toxic Substances and Disease Registry, the U.S. EPA, and for non-profit organizations. He also has been a U.S. delegate for the North Atlantic Treaty Organization.

Dr. Fisher also served on the International Life Sciences Institute Steering Committee, which evaluated chloroform and dichloroacetic acid using EPA-proposed Carcinogen Risk Guidelines. He is Past President of the Biological Modeling Specialty Section of the Society of Toxicology, reviewer for several toxicology journals, and was Co-Principal Investigator on a National Institutes of Health (NIH)-supported workshop on Mathematical Modeling at the University of Georgia in the fall of 2003.

### **DISCLOSURE:**

Dr. Fisher is a VCCEP *ad hoc* Panel member. He is a Professor and Department Head in the Department of Environmental Health Sciences at the University of Georgia.

## ***Dr. Pertti (Bert) Hakkinen***

Dr. Hakkinen is on the staff of the European Commission at the EC's Joint Research Centre (JRC) in Ispra, Italy. He is in the JRC's Physical and Chemical Exposure Unit of the Institute for Health and Consumer Protection where he helps develop and manage work packages for EIS-ChemRisks, the European Information System on risks from chemicals released from consumer products and articles (textiles, toys, etc.).

Dr. Hakkinen is a member of the Scientific Advisory Panel of the (U.S.) Mickey Leland National Urban Air Toxics Research Center and has served as the vice chair of this panel since March 2003. Prior to joining the European Commission's staff, Dr. Hakkinen was on the staff of Toxicology Excellence for Risk Assessment (*TERA*). Before joining *TERA*, he worked at the Procter & Gamble Company to provide global human exposure and risk assessment support for numerous types of consumer products and chemicals. While at Procter & Gamble, he chaired the Exposure Assessment Task Group of the Chemical Manufacturers Association (Washington, DC; now the American Chemistry Council) for several years, and was a chair of the American Chemistry Council's Human Exposure Assessment Technical Implementation Panel.

Dr. Hakkinen earned a B.A. in Biochemistry and Molecular Biology from the University of California, Santa Barbara, and received his Ph.D. in Comparative Pharmacology and Toxicology from the University of California, San Francisco. He served as a postdoctoral investigator in respiratory toxicology, and exposure and risk assessment at the Biology Division of the Oak Ridge National Laboratory. Dr. Hakkinen has been an invited expert or reviewer for U.S. EPA-, Health Canada-, and other associations to develop or revise human exposure assessment guidance, resource documents, and software. He has lectured on exposure and risk assessment, risk perception, and risk communication at the University of Cincinnati and elsewhere.

Dr. Hakkinen is a member of the Society of Toxicology (SOT), and a charter member of the Society for Risk Analysis (SRA) and the International Society of Exposure Analysis (ISEA). He proposed the idea for the "Residential Exposure Assessment. A Sourcebook," developed and published in 2001 via the expertise and involvement of members of SRA's Exposure Assessment Specialty Group, ISEA members, and many others. Dr. Hakkinen received SRA's Outstanding Service Award in 1996.

He was on the editorial board of *Toxicology* and was a co-editor and co-author of the latest edition of *Information Resources in Toxicology*. Further, he is a co-editor and co-author of the upcoming new edition of the *Encyclopedia of Toxicology*. Dr. Hakkinen has authored and co-authored numerous other publications, including ones on consumer product exposure and risk assessments, consumer risk perceptions, toxicological interactions, respiratory tract toxicology, and computer software and databases.

### **DISCLOSURE:**

Dr. Hakkinen is a VCCEP *ad hoc* Panel member. His employer, the European Commission, has interest in the potential exposures and hazards of n-alkanes and other VCCEP chemicals; however, the views that Dr. Hakkinen expresses as a VCCEP panelist are his own and do not necessarily represent official views of the European Commission. Before joining the European Commission in 2003, he was employed by *TERA* and, prior to that, by the Procter & Gamble Company. While at P&G, Dr. Hakkinen chaired the Exposure Assessment Task Group of the Chemical Manufacturers Association (now the American Chemistry Council). He also previously chaired the ACC's Human Exposure Assessment Technical Implementation Panel.

## ***Dr. Elaine Cohen Hubal***

Dr. Elaine Cohen Hubal is currently the Acting Associate Director for Human Exposure Modeling in the Human Exposure and Atmospheric Sciences Division of the U.S. EPA's National Exposure Research Laboratory (NERL). In this position, she has worked to develop and direct NERL's human exposure modeling research program. This research program is designed to develop modeling tools and conduct modeling analyses to characterize and estimate human exposure to environmental pollutants and to reduce uncertainty in risk assessments for the general population and for highly-exposed subpopulations. A significant focus of the lab's human exposure research program is on understanding and characterizing children's residential exposures to environmental contaminants. She previously worked as a chemical engineer for the Research Triangle Institute, and Camp Dresser and McKee. She also served as a Predoctoral Fellow at the Chemical Industry Institute of Toxicology.

Dr. Hubal received her Ph.D. and M.S. in Chemical Engineering from North Carolina State University and a S.B. in Chemical Engineering from Massachusetts Institute of Technology.

Dr. Hubal has served on a variety workgroups, panels, and committees. She currently serves as a member of EPA's Risk Assessment Forum Cumulative Risk Assessment Technical Panel, the Study Design Working Group for the National Children's Study, ILSI Health and Environmental Sciences Institute Biomonitoring Workshop Steering Team, and the Occupational and Environmental Exposures of Skin to Chemicals (OEESC) 2005 Program Committee.

Dr. Hubal's current research interests focus on characterizing exposure-to-dose relationships and enhancing quantitative risk assessment through application of computational tools and a systems approach. Her general research interest is on reducing uncertainty in risk assessment with a specific focus on children's exposure. She has designed and conducted studies to evaluate dermal exposure assessment approaches and collect exposure factor data in support of the Food Quality Protection Act. She has developed and worked with a variety of computational models to describe the simultaneous mass transport and reaction of inhaled gases in the airway lining. Dr. Hubal has also worked on the development of a modeling platform to predict contaminant fate and transport of environmental pollutants to perform exposure assessments in support of the Hazardous Waste Identification Rule, and conducted research in the area of industrial pollution prevention by developing a framework to evaluate the environmental impact of pollution prevention activities that directly relates the energy requirements to process air, water, and solid waste emissions.

Dr. Hubal has published in the areas of children's exposure and human health risk modeling.

### **DISCLOSURE:**

Dr. Hubal is a VCCEP Core Panel member. She is employed by the U.S. EPA, working at the National Exposure Research Laboratory. EPA has taken public positions on the VCCEP pilot chemicals and on the tests included in the VCCEP Tiers. Dr. Hubal is also a public member of the American Chemistry Council's Human Exposure Assessment Technical Implementation Panel.

## ***Dr. Sam Kacew***

Dr. Sam Kacew is a Professor in the Department of Cellular and Molecular Medicine, Faculty of Medicine, as well as a scientist of the Institute of Population Health at the University of Ottawa. His responsibilities include teaching medical students and graduate students the techniques required to write and publish peer-review papers. His current research involves the effects of chemical contaminants in breast milk on infants, the role of confounding factors in toxicity testing, as well as the basis for differences in responsiveness to chemicals between infants and adults.

Dr. Kacew received his Ph.D. in Pharmacology from the University of Ottawa. He served as a Postdoctoral Fellow for the Medical Research Council of Canada at the University of Montreal. Dr. Kacew was certified in 1994 as a Fellow of Academy of Toxicological Sciences. He has received numerous awards, including several achievement, recognition, public communications, and travel awards from the Society of Toxicology (SOT), the United States-China Foundation, and the National Science Council of the Republic of China.

Dr. Kacew has served on numerous expert panels and committees, including as a member of the National Advisory Committee on Environmental Contaminants and the Implications for Child Health, and as a member of the National Academy of Sciences (U.S.) Committee on Toxicology and Chair of the National Academy of Sciences Subcommittee on Iodotrifluoromethane. He has also served as a chairman for a variety of symposiums, panels, and committees including the SOT Annual Meeting's General Toxicology Session, the Federation of American Societies for Experimental Biology Annual Meeting, an Assessment Panel for the Canadian Council on Animal Care, a SOT Symposium on Use of Moderate Dietary Restriction in Safety Assessment, and a SOT Symposium on the Role of Diet and Obesity in Endocrine Disruption.

He has presented hundreds of invited lectures for a variety of federal and state government agencies, colleges and universities, private companies, and international organizations. He was an invited participant to the American Society for Pharmacology and Experimental Therapeutics Meeting, the Federation of American Societies for Experimental Biology Annual Meeting, the International Life Sciences Institute, the Chalk River Nuclear Labs, Turkey Society of Biochemistry, Society of Toxicology of Taiwan and the Korea Society of Toxicology.

Dr. Kacew is on a number of grant committees and has served as an external referee for grants and fellowships for a wide variety of organizations and government agencies. He is currently the Editor-in-Chief the *Journal of Toxicology and Environmental Health*, an Associate Editor for *Toxicology and Applied Pharmacology*, an assistant editor for TOMES (Micromedex, Inc.), Guest Editor for Toxicology and Applied Pharmacology special issue on Toxicological Reviews in Fetal Childhood Development as well as a member of the editorial board of a number of other journals. Dr. Kacew has over 140 publications in peer-reviewed journals and books in the area of toxicology, risk assessment, and children's health. He has also served as an editor for a number of books on toxicology and children.

### **DISCLOSURE:**

Dr. Kacew is a VCCEP Core Panel member. He is a Professor in the Department of Cellular & Molecular Medicine in the Faculty of Medicine at the University of Ottawa in Canada.

## ***Dr. Chad Sandusky***

Dr. Chad Sandusky is currently Director of Research and senior toxicology advisor to the Physicians Committee for Responsible Medicine (PCRM), a non-profit organization that promotes good nutrition, conducts clinical trials and promotes nonanimal experimental methods in medical and scientific research. For PCRM, Dr. Sandusky coordinates the review and preparation of comments on the EPA's High Production Volume Challenge Program (HPV) and Voluntary Children's Chemical Evaluation Program (VCCEP) chemical assessments. As such, he stresses the weight-of-evidence approach in these assessments and the development of exposure scenarios as key to the success of these programs. He is actively engaged in identifying methods which use alternatives to animal testing to meet the needs of the safety assessments, including tests undergoing validation at the European Center for Alternative Methods (ECVAM) and the Interagency Coordinating Committee on the Validation of Alternative Methods (ICCVAM).

Dr. Sandusky was the past Manager of Toxicology and Risk Assessment at ENVIRON and has extensive experience at both the EPA and ENVIRON in pesticide toxicology as well as exposure and risk assessments. For example, he evaluated the toxicology of pesticides and extrapolated these effects in risk assessments; directed the dietary exposure and risk assessments for agrochemicals and other potentially toxic residues in foods using the TAS Dietary exposure software; served as toxicology team leader and senior author of numerous EPA documents, including Registrations Standards and Position Documents; and since the passage of the FQPA in August 1996, coordinated the review and assessment of numerous agrochemicals to address the full range of new requirements, including: assessing aggregate exposure from multiple pathways (e.g., drinking water and residential use), cumulative exposure to chemicals with a common mode of action, accounting for potential sensitivity to infants and children, and assessing the potential for endocrine disruption.

Dr. Sandusky has extensive international experience including the coordination and submission of dossiers for the EU Reauthorization process under EU 91/414 and presentation of the results to member states. Dr. Sandusky also represented the Institute of Food Technology at the Codex Committee for Pesticide Residues (CCPR) in The Hague for several years. In addition, he also coordinated preparation and reviews of dossiers for chemicals approved as GRAS as well as directed the preparation and submission of Food Contact Notifications (FCNs) to the FDA. More recently, Dr. Sandusky represented the International Coalition of Animal Protection Organizations (ICAPO) at the OECD meetings in Paris on the Existing Chemicals Programme.

Dr. Sandusky received his Ph.D. in Pharmacology from the Emory University. He served as a Postdoctoral Fellow at the Georgetown University Schools of Medicine and Dentistry, Washington, D.C. He is currently a member of the Society of Toxicology, and was previously affiliated with such organizations as the International Society of Exposure Analysis and the Society of Environmental Toxicology and Chemistry.

### **DISCLOSURE:**

Dr. Sandusky is a VCCEP Core Panel member. He currently is employed by the Physicians Committee for Responsible Medicine (PCRM). The PCRM actively promotes non-animal experimental methods in toxicology studies. PCRM has taken public positions on the VCCEP pilot chemicals, the tiered test methods, and on the VCCEP program itself. Several years ago, Dr. Sandusky did consulting work for Shell and Chevron, related to their agricultural chemicals business.

## ***Dr. Kimberly Thompson***

Dr. Kimberly M. Thompson is Associate Professor of Risk Analysis and Decision Science in the Departments of Health Policy and Management and Society, Human Development and Health at the Harvard School of Public Health. She is the Director of the Kid Risk Project that seeks to improve the lives of children by using analytical methods to characterize children's risks and strategies to reduce those risks. Dr. Thompson directs a professional education course on Probabilistic Risk Analysis: Assessment, Management, and Communication, and she seeks to effectively integrate technological, social, political, legal, and economic issues into risk analyses that inform public policy and improve decision making. Her research interests focus on the issues related to developing and applying quantitative methods for risk assessment and risk management, and consideration of the public policy implications associated with including uncertainty and variability in risk characterization.

Over the last decade, for both private and public clients Dr. Thompson has consulted on computer applications, projects concerning environmental quality, fate and transport of toxic chemicals in the environment, analysis of remedial alternatives at landfills and abandoned sites, efforts to characterize uncertainty and variability in risks, and development of white papers for the EPA on topics related to children's risks. Dr. Thompson's most recent consulting includes work with the MIT Lincoln Laboratory as part of an integration team studying the development of a national health surveillance and biodefense system, and her recent book Overkill focuses on microbiological risks in what she calls this "Age of Risk Management."

Dr. Thompson received a Sc.D. in Environmental Health from Harvard University's School of Public Health. She received a M.S. and B.S. in Chemical Engineering from the Massachusetts Institute of Technology. Dr. Thompson has served on several National Academy of Sciences committees and subcommittees and a number of other expert review panels. She has been an invited presenter at a variety of workshops, conferences, and annual meetings, such as the Boston Mayor's Symposium on Youth Development, the Congressional Research Services Children's Environmental Risks: Federal Activities in Perspective Symposium on Risk Assessment and Risk Communication, and a NIH/NIEHS Workshop on the Role of Human Exposure Assessment in the Prevention of Environmental Disease. She also served as the chair of the Exposure Assessment Specialty Group and is currently a Councilor of the Society for Risk Analysis.

Dr. Thompson has written over 30 peer-reviewed journal publications in the areas of human health modeling, probabilistic risk assessment, children's health and risk communication. She has also reviewed manuscripts for over a dozen journals, including the Journal of Toxicology and Environmental Health, Risk Analysis, Health Policy, and the Journal of the American Medical Association.

### **DISCLOSURE:**

Dr. Thompson is a VCCEP Core Panel member. She is Associate Professor of Risk Analysis and Decision Science and Director of the Kids Risk Project at Harvard University in the School of Public Health. She received funding from EPA in 2000 to chair a workshop and prepare a publication discussing changes in children's exposure as a function of age. Dr. Thompson's research program benefits from unrestricted grants made to Harvard University by the American Chemistry Council and Synthetic Organic Chemicals Manufacturers Association. Both of these organizations are sponsors of VCCEP chemicals. ExxonMobil donated its Christmas 2003 advertising space to the Kids Risk Project and ran the piece that Dr. Thompson wrote, titled "Children Are Our Present."

## ***Dr. Pamela Williams***

Dr. Pamela Williams is a Principal Health Scientist at ChemRisk, where she manages a variety of large-scale projects and a team of six scientists in the Boulder, Colorado office. Her areas of expertise include risk assessment, retrospective exposure assessment, and decision analysis. She has used her expertise in these areas to characterize human exposures and health risks, prioritize health and safety risks, identify potential risk tradeoffs, and establish cost-effective risk management goals. She has been active in providing expert testimony (including before the U.S. Congress) and litigation support regarding chemicals found in air, soil, food, and drinking water. These chemicals include asbestos, benzene, ethanol, elemental mercury, hexavalent chromium, hydrogen sulfide, methanol, methyl tertiary butyl ether (MTBE), sulfur dioxide, tetrachloroethylene, trichloroethylene, and vinyl chloride.

Dr. Williams has a Sc.D. in Environmental Health and Health Policy & Management from Harvard University, a M.S. in Public Health from Harvard University, and a B.A. in Sociology/Applied Social Research from San Diego State University. Her pre-doctoral experience includes an internship at the Agency for Toxic Substances and Disease Registry (ATSDR) in Atlanta, as well as work for environmental health consulting firms in California and Massachusetts. She has also lectured on the topics of environmental health and risk assessment at the Harvard School of Public Health and conducted research on different food safety hazards and public perceptions of risk at the Harvard Center for Risk Analysis. Before joining ChemRisk in 2003, she was a Senior Scientist at Exponent, where her exposure and risk/benefit work earned her national recognition as an expert on MTBE.

Dr. Williams is the author of numerous publications and abstracts related to individual chemicals and to exposure and risk assessment methodologies. Some of her recent interests and publications include evaluating children's exposures and health risks and using comparative risk analyses to better communicate risk findings. She belongs to several professional societies, including the International Society of Exposure Analysis (ISEA) and the Society for Risk Analysis (SRA). She has been especially active in this latter society, where she has chaired a number of symposia and is the current Treasurer-Elect.

### **DISCLOSURE:**

Dr. Williams is a VCCEP *ad hoc* Panel member. The ACC and at least two consortium members have been clients of Dr. Williams's current employer, ChemRisk. Dr. Williams's current and former employers (ChemRisk and Exponent) have been involved in work related to some VCCEP chemicals, but they are not involved with work related to the VCCEP n-Alkanes peer consultation.

## **Sponsor Presenter Biographical Sketches**

### ***Dr. Ralph Gingell***

Senior Toxicology Advisor  
Shell Chemical LP

Dr. Gingell is a Senior Toxicology Advisor with Shell Chemical LP in Houston, where he has worked since joining Shell in 1980. In his current position he primarily supports Shell's Solvents, Aromatics and EO/Glycols businesses. Dr. Gingell received his Ph.D. in Biochemistry from London University in 1971, and became a Diplomat of the American Board of Toxicology in 1985. Prior to joining Shell, he was a research professor at the University of Nebraska Medical Center studying the metabolic activation of chemical carcinogens. Dr. Gingell has more than 50 peer-reviewed publications, has authored two chapters in Patty's Industrial Hygiene and Toxicology, and represents Shell on several trade association panels.

### ***Mr. Andrew Jaques***

CHEMSTAR Director  
American Chemistry Council

Andrew Jaques is a Director in the CHEMSTAR group of the American Chemistry Council (ACC); he joined ACC in 1998. He manages several panels and consortia at ACC on hydrocarbon solvents, aliphatic and aromatic hydrocarbons. Prior to joining ACC, Mr. Jaques worked for the American Petroleum Institute (API) as a Regulatory Analyst in its Health and Environmental Affairs Department. He was responsible for managing health, hazard communication and industrial hygiene regulatory and research programs. Prior to this, Mr. Jaques worked as a Safety and Fire Protection Associate with API, overseeing the development of safety and fire protection standards. He received a B.A. in Physics and Economics from Drew University in Madison, NJ. He also has completed all course work towards a M.P.H. in Environmental and Occupational Health from George Washington University in Washington, DC.

### ***Dr. Ross Macdonald***

Consultant to n-Alkanes Consortium

Dr. Macdonald is a consultant with over 20 years experience in inhalation toxicology, exposure assessment, risk assessment and dose response assessment. He holds a Ph.D in Chemistry from the University of Bristol (U.K.). Dr. Macdonald was a Higher Scientific Officer for the British Health and Safety Executive researching the behavior of particulates before moving to Shell where he conducted inhalation studies on the company's products. More recently, as a Staff Toxicologist and Risk Assessor he has participated in numerous RCRA and CERCLA investigations and corrective actions. He has also been involved in dose-response assessment, and development of Shell internal exposure standards. Dr. Macdonald was a focal point for assessment of waste sites, refinery emissions, and public and occupational risk from exposure to Shell products.

***Dr. Dave Penney***

Senior Toxicologist  
Sasol North America Inc.

Dr. Dave Penney is Senior Toxicologist at Sasol North America Inc. where he has worked since originally joining the Research and Development Department of the company (then as Vista Chemical Company) in 1989. In 1995, he transferred to the Product Safety and Occupational Health Department in Houston where he has various responsibilities for Sasol North America's Product Safety Evaluation and Regulatory programs. Dr. Penney received his Ph.D. in Toxicology from The University of Kansas in 1982. He is a member of the ACC Hydrocarbons Panel and Toxicology Research Task Group, and represents Sasol North America in various domestic and international High Production Volume program consortia.

# **Appendix C**

## **Public Comments**

**Voluntary Children's Chemical Evaluation  
Program (VCCEP)  
Peer Consultation on  
n-Alkanes  
(Decane, Dodecane, and Undecane)**

**Public Comments**

**September 14, 2004**

**Kingsgate Conference Center, Salon A  
University of Cincinnati  
Cincinnati, Ohio**

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**Ms. Lynn A. Delpire**  
**Chemist**  
**U.S. Environmental Protection Agency**

### **Physical, Chemical, and Environmental Fate Properties**

The VCCEP submission for n-decane, n-undecane, and n-dodecane would benefit from more discussion supporting the statements about environmental persistence and partitioning. The submission states that the chemicals will not persist in the environment because they will volatilize and photo-oxidize. The submission should discuss the Level I fugacity modeling and how it does or does not support this claim.

The submission states that the chemicals biodegrade, but does not give a reference. Biodegradation is a characteristic that can significantly affect environmental fate and exposure, and it is important to include references.

The submission mixed up two of the estimated half lives for atmospheric oxidation; the correct half lives are: n-decane, 11.5 hours; n-undecane, 10.2 hours; n-dodecane, 9.2 hours.

The submission should give references for the vapor pressure values. Vapor pressure is an important physical chemical property for these chemicals, and it is used as an input to fugacity modeling.

The submission should include the inputs used for the Level I fugacity model so that reviewers can confirm the results.

In the High Production Volume program, the Office of Pollution Prevention and Toxics accepts the results of a Level I fugacity model, but makes it clear that results of a Level III fugacity model are preferred. The submission should include the results of Level III fugacity modeling.

Level III fugacity results for these chemicals show that the model does not predict that all of the chemicals will partition out of water at steady state. In fact, the Level III results suggest that water, soil, and sediment are the major compartments for these chemicals when equal, continuous emissions to air, water, and soil occur. This is quite different from the Level I results cited in the submission.

Level I fugacity modeling considers only equilibrium partitioning, ignoring all types of degradation. Level III fugacity modeling is more complicated than Level I fugacity modeling, and includes degradation, advection (physical movement of a substance), atmospheric deposition, etc. A Level III fugacity model is not an equilibrium model. A Level III fugacity model does assume that steady state is attained.

The submission cites a 1999 version of EPIWIN for the atmospheric half lives. The sponsor could and should have used EPI Suite v3.11 to estimate a variety of physical chemical properties

and predict environmental fate. For example, the submission cites the water solubility as "negligible" according to the CRC Handbook. EPI Suite v3.11 gives several values for water solubility, including experimental (measured) and estimated values. The submission cites a 1998 version of the Mackay Level I fugacity model for fugacity/partitioning in the environment. EPI Suite v3.11 makes Level III fugacity calculations. EPI Suite v3.11 is readily available at

<http://www.epa.gov/opptintr/exposure/docs/episuitedi.htm>

and here are results of running EPI Suite v3.11 for all three chemicals: see attached files: EPI\_decane.txt; EPI\_undecane.txt; EPI\_dodecane.txt

## Exposure Assessment

An important aspect of this study is the unusual production pattern of n-alkanes; their production as pure chemicals is far exceeded by their production as constituents of fuels such as kerosene, diesel, and home heating oil. Because the Consortium members include only manufacturers of the pure substances, the majority of production of these chemicals is not covered by the VCCEP submission. This calls into question the usefulness of the report as an indicator of overall exposure to the target chemicals.

The submission presents screening level data in which certain exposure routes, such as oral ingestion, dermal contact, and exposure via breast milk, were considered. The bounding limits of exposure under these scenarios were found to be very low, and these scenarios were not considered further in the assessment. Some occupational and nonoccupational exposures were ignored because other scenarios had a higher exposure concentration; it does not appear that any other factors, such as differences in exposure frequency, exposure duration, or work/use environment, were considered. This may have resulted in the omission of a significant exposure pathway.

The occupational scenarios focus on only two occupational activities, both of which involve the use of products containing the target chemicals. There is no consideration of occupational exposure during manufacturing and processing of the chemicals. This may also have resulted in the omission of a significant exposure pathway.

The submission could be improved by a more thorough discussion of why the five scenarios evaluated represent the only significant exposure pathways. In addition, the submission does not include information about occupational exposure or general population exposure resulting from manufacturing and processing; this could be significant. More important, the submission as a whole is of limited usefulness as an assessment of n-alkane exposure because, as the submission states, the assessed uses only account for a small amount of the n-alkanes that are manufactured; most of the n-alkanes are produced in the petroleum refining industry, which is outside the scope of the submission. This results in two potential problems. First, the assessment does not account for all exposure scenarios. Second, some of the studies cited in the submission include measurements of VOCs in ambient air; these measurements do not distinguish between n-alkanes

derived from activities within the scope of the submission and n-alkanes derived from other sources, such as automobile exhaust. These limitations must be considered in evaluating the conclusions of the submission.

The information presented in Section 6 and Appendix G on the EPA Research House Study does not support some of the numbers used in MOE calculations. In Table 8.7, Margin of Exposure (EPA Research House), the Representative Exposure Concentrations for 1 day, 2 days, and 4 days are not adequately supported by the information in Section 6 and Appendix G; they appear to be too low. The Representative Exposure Concentrations for 15 days and 23 days appear to be adequately supported by the data on page G-6. The submission should provide a better explanation of how the Representative Exposure Concentrations were chosen for 1 day, 2 days, and 4 days.

## Ms. Delpire's Attachment 1 – Decane EPI Suite Results

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C10 H22

MOL WT : 142.29

----- EPI SUMMARY (v3.11) -----

Physical Property Inputs:

Water Solubility (mg/L): -----

Vapor Pressure (mm Hg) : -----

Henry LC (atm-m<sup>3</sup>/mole) : -----

Log Kow (octanol-water): -----

Boiling Point (deg C) : -----

Melting Point (deg C) : -----

KOWWIN Program (v1.67) Results:

=====

Log Kow(version 1.67 estimate): 5.25

Experimental Database Structure Match:

Name : Decane

CAS Num : 000124-18-5

Exp Log P: 5.01

Exp Ref : Coates,M et al. (1985)

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C10 H22

MOL WT : 142.29

TYPE	NUM	LOGKOW	FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3	[aliphatic carbon]	0.5473	1.0946
Frag	8	-CH2-	[aliphatic carbon]	0.4911	3.9288
Const		Equation Constant			0.2290

Log Kow = 5.2524

MPBPWIN (v1.41) Program Results:

=====

Experimental Database Structure Match:

Name : N-DECANE

CAS Num : 000124-18-5

Exp MP (deg C): -29.7

Exp BP (deg C): 174.1

Exp VP (mm Hg): 1.43E+00

Exp VP (deg C): 25

Exp VP ref : DAUBERT,TE & DANNER,RP (1989)

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C10 H22

MOL WT : 142.29

----- SUMMARY MPBPWIN v1.41 -----

Boiling Point: 164.60 deg C (Adapted Stein and Brown Method)

Melting Point: -70.70 deg C (Adapted Joback Method)

Melting Point: -17.55 deg C (Gold and Ogle Method)

Mean Melt Pt : -44.13 deg C (Joback; Gold,Ogle Methods)

Selected MP: -44.13 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):  
 (Using BP: 174.10 deg C (exp database))  
 (MP not used for liquids)  
 VP: 1.89 mm Hg (Antoine Method)  
 VP: 1.58 mm Hg (Modified Grain Method)  
 VP: 1.79 mm Hg (Mackay Method)  
 Selected VP: 1.73 mm Hg (Mean of Antoine & Grain methods)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	2	-CH3	21.98	43.96
Group	8	-CH2-	24.22	193.76
*		Equation Constant		198.18

---

RESULT-uncorr	BOILING POINT in deg Kelvin	435.90
RESULT- corr	BOILING POINT in deg Kelvin	437.76
	BOILING POINT in deg C	164.60

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	2	-CH3	-5.10	-10.20
Group	8	-CH2-	11.27	90.16
*		Equation Constant		122.50

---

RESULT	MELTING POINT in deg Kelvin	202.46
	MELTING POINT in deg C	-70.70

Water Sol from Kow (WSKOW v1.41) Results:

Water Sol: 1.252 mg/L

Experimental Water Solubility Database Match:

Name : N-DECANE  
 CAS Num : 000124-18-5  
 Exp WSol : 0.052 mg/L (25 deg C)  
 Exp Ref : YALKOWSKY,SH & DANNENFELS, RM (1992)

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C10 H22

MOL WT : 142.29

----- WSKOW v1.41 Results -----

Log Kow (estimated) : 5.25

Log Kow (experimental): 5.01

Cas No: 000124-18-5

Name : Decane

Refer : Coates, M et al. (1985)

Log Kow used by Water solubility estimates: 5.01

Equation Used to Make Water Sol estimate:

Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction  
 (used when Melting Point NOT available)

Correction(s):	Value
----------------	-------

Hydrocarbon	-0.537
-------------	--------

Log Water Solubility (in moles/L) : -5.055

Water Solubility at 25 deg C (mg/L): 1.252

WATERNT Program (v1.01) Results:

=====

Water Sol (v1.01 est): 0.091706 mg/L

Experimental Water Solubility Database Match:

Name : N-DECANE  
CAS Num : 000124-18-5  
Exp WSol : 0.052 mg/L (25 deg C)  
Exp Ref : YALKOWSKY,SH & DANNENFELSER,RM (1992)

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C10 H22

MOL WT : 142.29

TYPE	NUM	WATER SOLUBILITY	FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3	[aliphatic carbon]	-0.3213	-0.6425
Frag	8	-CH2-	[aliphatic carbon]	-0.5370	-4.2962
Factor	1	Hydrocarbon	[unsubst. alkane] correction	-1.5013	-1.5013
Const		Equation Constant			0.2492

Log Water Sol (moles/L) at 25 dec C = -6.1908

Water Solubility (mg/L) at 25 dec C = 0.091706

ECOSAR Program (v0.99g) Results:

=====

SMILES : CCCCCCCCCC

CHEM :

CAS Num:

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C10 H22

MOL WT : 142.29

Log Kow: 5.25 (KowWin estimate)

Melt Pt:

Wat Sol: 0.3063 mg/L (calculated)

ECOSAR v0.99g Class(es) Found

-----

Neutral Organics

ECOSAR Class	Organism	Predicted Duration	End Pt	mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.282
Neutral Organics	: Fish	96-hr	LC50	0.093
Neutral Organics	: Fish	14-day	LC50	0.282
Neutral Organics	: Daphnid	48-hr	LC50	0.125
Neutral Organics	: Green Algae	96-hr	EC50	0.094
Neutral Organics	: Fish	30-day	ChV	0.020
Neutral Organics	: Daphnid	16-day	EC50	0.026
Neutral Organics	: Green Algae	96-hr	ChV	0.061
Neutral Organics	: Fish (SW)	96-hr	LC50	0.102
Neutral Organics	: Mysid Shrimp	96-hr	LC50	0.003

mg/kg (ppm)  
dry wt soil

Neutral Organics : Earthworm 14-day LC50 87.330 \*

Note: \* = asterick designates: Chemical may not be soluble enough to measure this predicted effect.

Fish and daphnid acute toxicity log Kow cutoff: 5.0

Green algal EC50 toxicity log Kow cutoff: 6.4

Chronic toxicity log Kow cutoff: 8.0

MW cutoff: 1000

HENRY (v3.10) Program Results:

Bond Est : 5.30E+000 atm-m3/mole

Group Est: 6.74E+000 atm-m3/mole

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C10 H22

MOL WT : 142.29

----- HENRYWIN v3.10 Results -----

Experimental Database Structure Match:

Name : N-DECANE

CAS Num : 000124-18-5

Exp HLC : 5.15E+00 atm-m3/mole

Temper : 25 deg C

Exp VP : 1.43E+00 mm Hg

Exp WSol : 5.20E-02 mg/L

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	22 Hydrogen to Carbon (aliphatic) Bonds		-2.6329
FRAGMENT	9 C-C		1.0467
FACTOR	* Linear or branched alkane		-.7500

RESULT | BOND ESTIMATION METHOD for LWAPC VALUE | TOTAL | -2.336

HENRYs LAW CONSTANT at 25 deg C = 5.30E+000 atm-m3/mole  
= 2.17E+002 unitless

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	2 CH3 (X)		-1.24
	8 CH2 (C)(C)		-1.20

RESULT | GROUP ESTIMATION METHOD for LOG GAMMA VALUE | TOTAL | -2.44

HENRYs LAW CONSTANT at 25 deg C = 6.74E+000 atm-m3/mole  
= 2.75E+002 unitless

Henrys LC [VP/WSol estimate using EPI values]:

HLC: 2.587E-001 atm-m3/mole

VP: 1.73 mm Hg

WS: 1.25 mg/L

BIOWIN (v4.01) Program Results:

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C10 H22  
MOL WT : 142.29

----- BIOWIN v4.01 Results -----

Linear Model Prediction : Biodegrades Fast  
Non-Linear Model Prediction: Biodegrades Fast  
Ultimate Biodegradation Timeframe: Days-Weeks  
Primary Biodegradation Timeframe: Days  
MITI Linear Model Prediction : Biodegrades Fast  
MITI Non-Linear Model Prediction: Biodegrades Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Linear C4 terminal chain [CCC-CH3]	0.1084	0.2169
MolWt	*	Molecular Weight Parameter		-0.0677
Const	*	Equation Constant		0.7475
RESULT   LINEAR BIODEGRADATION PROBABILITY				0.8967

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Linear C4 terminal chain [CCC-CH3]	1.8437	3.6874
MolWt	*	Molecular Weight Parameter		-2.0205
RESULT   NON-LINEAR BIODEGRADATION PROBABILITY				0.9908

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Linear C4 terminal chain [CCC-CH3]	0.2983	0.5967
MolWt	*	Molecular Weight Parameter		-0.3144
Const	*	Equation Constant		3.1992
RESULT   SURVEY MODEL - ULTIMATE BIODEGRADATION				3.4814

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Linear C4 terminal chain [CCC-CH3]	0.2691	0.5381
MolWt	*	Molecular Weight Parameter		-0.2053
Const	*	Equation Constant		3.8477
RESULT   SURVEY MODEL - PRIMARY BIODEGRADATION				4.1806

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks  
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Methyl [-CH3]	0.0004	0.0008
Frag	8	-CH2- [linear]	0.0494	0.3953
MolWt	*	Molecular Weight Parameter		-0.4233

Const| \* | Equation Constant | | 0.7121  
 =====  
 RESULT | MITI LINEAR BIODEGRADATION PROBABILITY | | 0.6850  
 =====

-----+-----+-----+-----+-----  
 TYPE | NUM | BIOWIN FRAGMENT DESCRIPTION | COEFF | VALUE  
 -----+-----+-----+-----+-----  
 Frag | 2 | Methyl [-CH3] | 0.0194 | 0.0389  
 Frag | 8 | -CH2- [linear] | 0.4295 | 3.4360  
 MolWt| \* | Molecular Weight Parameter | | -4.1076  
 =====  
 RESULT | MITI NON-LINEAR BIODEGRADATION PROBABILITY | | 0.8691  
 =====

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable  
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.91) Results:

=====  
 SMILES : CCCCCCCCCC  
 CHEM :  
 MOL FOR: C10 H22  
 MOL WT : 142.29  
 ----- SUMMARY (AOP v1.91): HYDROXYL RADICALS -----  
 Hydrogen Abstraction = 11.1105 E-12 cm3/molecule-sec  
 Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec  
 Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec  
 Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec  
 Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec  
 Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 11.1105 E-12 cm3/molecule-sec  
 HALF-LIFE = 0.963 Days (12-hr day; 1.5E6 OH/cm3)  
 HALF-LIFE = 11.552 Hrs

----- SUMMARY (AOP v1.91): OZONE REACTION -----  
 \*\*\*\*\* NO OZONE REACTION ESTIMATION \*\*\*\*\*  
 (ONLY Olefins and Acetylenes are Estimated)

Experimental Database Structure Match:  
 Chem Name : n-Decane  
 CAS Number: 000124-18-5  
 Exper OH rate constant : 11.6 E-12 cm3/molecule-sec  
 Exper OH Reference: ATKINSON,R (1989)  
 Exper Ozone rate constant: --- cm3/molecule-sec  
 Exper NO3 rate constant : 2.59 E-16 cm3/molecule-sec

PCKOC Program (v1.66) Results:

=====  
 Koc (estimated): 1.72e+003  
 SMILES : CCCCCCCCCC  
 CHEM :  
 MOL FOR: C10 H22  
 MOL WT : 142.29  
 ----- PCKOCWIN v1.66 Results -----  
 First Order Molecular Connectivity Index ..... : 4.914  
 Non-Corrected Log Koc ..... : 3.2365  
 Fragment Correction(s) --> NONE : ---  
 Corrected Log Koc ..... : 3.2365

Estimated Koc: 1724

HYDROWIN Program (v1.67) Results:

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C10 H22

MOL WT : 142.29

----- HYDROWIN v1.67 Results -----

Currently, this program can NOT estimate a hydrolysis rate constant for the type of chemical structure entered!!

ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens) and Specific Alkyl Halides can be estimated!! For more information, (Click OVERVIEW in Help or see the User's Guide)

\*\*\*\*\* CALCULATION NOT PERFORMED \*\*\*\*\*

BCF Program (v2.15) Results:

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C10 H22

MOL WT : 142.29

----- Bcfwin v2.15 -----

Log Kow (estimated) : 5.25

Log Kow (experimental): 5.01

Log Kow used by BCF estimates: 5.01

Equation Used to Make BCF estimate:

$$\text{Log BCF} = 0.77 \log \text{Kow} - 0.70 + \text{Correction}$$

Correction(s):	Value
Alkyl chains (8+ -CH2- groups)	-1.000

Estimated Log BCF = 2.158 (BCF = 143.8)

Volatization From Water

Chemical Name:

Molecular Weight : 142.29 g/mole

Water Solubility : ----

Vapor Pressure : ----

Henry's Law Constant: 5.15 atm-m<sup>3</sup>/mole (Henry experimental database)

	RIVER	LAKE
	-----	-----
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	1.217	113.3
HALF-LIFE (days) :	0.05072	4.721

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

PROPERTIES OF:

-----  
Molecular weight (g/mol) 142.29

Aqueous solubility (mg/l) 0  
 Vapour pressure (Pa) 0  
 (atm) 0  
 (mm Hg) 0  
 Henry 's law constant (Atm-m3/mol) 5.15  
 Air-water partition coefficient 210.62  
 Octanol-water partition coefficient (Kow) 102329  
 Log Kow 5.01  
 Biomass to water partition coefficient 20466.7  
 Temperature [deg C] 25  
 Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):  
 -Primary tank 0.00 9761.53 10000.00  
 -Aeration tank 0.00 9761.53 10000.00  
 -Settling tank 0.00 9761.53 10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	7.0E-002	100.00
Primary sludge	4.81E+000	3.4E-002	48.07
Waste sludge	4.64E-003	3.3E-005	0.05
Primary volatilization	2.61E-002	1.8E-004	0.26
Settling volatilization	9.91E-005	7.0E-007	0.00
Aeration off gas	5.14E+000	3.6E-002	51.44
Primary biodegradation	1.44E-002	1.0E-004	0.14
Settling biodegradation	6.01E-006	4.2E-008	0.00
Aeration biodegradation	7.92E-005	5.6E-007	0.00
Final water effluent	3.50E-003	2.5E-005	0.03
Total removal	1.00E+001	7.0E-002	99.97
Total biodegradation	1.45E-002	1.0E-004	0.14

(\*\* Total removal recommended maximum is 99 percent)

Level III Fugacity Model (Full-Output):

Chem Name :  
 Molecular Wt: 142.29  
 Henry's LC : 5.15 atm-m3/mole (Henry database)  
 Vapor Press : 1.73 mm Hg (Mpbpwin program)  
 Log Kow : 5.01 (Kowwin program)  
 Soil Koc : 4.2e+004 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	18.4	22.1	1000
Water	49.7	208	1000
Soil	14.9	208	1000
Sediment	17	832	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	9.12e-011	1.66e+003	531	55.4	17.7
Water	2.43e-005	478	144	15.9	4.79
Soil	8.22e-008	143	0	4.76	0
Sediment	4.41e-006	40.9	0.982	1.36	0.0327

Persistence Time: 96.2 hr  
 Reaction Time: 124 hr

Advection Time: 427 hr  
Percent Reacted: 77.5  
Percent Advected: 22.5

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 22.13  
Water: 208.1  
Soil: 208.1  
Sediment: 832.3  
Biowin estimate: 3.481 (days-weeks )

Advection Times (hr):

Air: 100  
Water: 1000  
Sediment: 5e+004

---

## Ms. Delpire's Attachment 2 – Dodecane EPI Suite Results

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C12 H26

MOL WT : 170.34

----- EPI SUMMARY (v3.11) -----

### Physical Property Inputs:

Water Solubility (mg/L): -----

Vapor Pressure (mm Hg) : -----

Henry LC (atm-m3/mole) : -----

Log Kow (octanol-water): -----

Boiling Point (deg C) : -----

Melting Point (deg C) : -----

### KOWWIN Program (v1.67) Results:

=====

Log Kow(version 1.67 estimate): 6.23

### Experimental Database Structure Match:

Name : Dodecane

CAS Num : 000112-40-3

Exp Log P: 6.10

Exp Ref : Coates,M et al. (1985)

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C12 H26

MOL WT : 170.34

-----+-----+-----+-----+-----

TYPE	NUM	LOGKOW	FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3	[aliphatic carbon]	0.5473	1.0946
Frag	10	-CH2-	[aliphatic carbon]	0.4911	4.9110
Const		Equation Constant			0.2290

-----+-----+-----+-----+-----

Log Kow = 6.2346

### MPBPWIN (v1.41) Program Results:

=====

### Experimental Database Structure Match:

Name : DODECANE

CAS Num : 000112-40-3

Exp MP (deg C): -9.6

Exp BP (deg C): 216.3

Exp VP (mm Hg): 1.35E-01

Exp VP (deg C): 25

Exp VP ref : DAUBERT,TE & DANNER,RP (1993)

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C12 H26

MOL WT : 170.34

----- SUMMARY MPBPWIN v1.41 -----

Boiling Point: 205.71 deg C (Adapted Stein and Brown Method)

Melting Point: -48.16 deg C (Adapted Joback Method)

Melting Point: 6.45 deg C (Gold and Ogle Method)

Mean Melt Pt : -20.85 deg C (Joback; Gold,Ogle Methods)

Selected MP: -20.85 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):  
 (Using BP: 216.30 deg C (exp database))  
 (MP not used for liquids)  
 VP: 0.253 mm Hg (Antoine Method)  
 VP: 0.22 mm Hg (Modified Grain Method)  
 VP: 0.245 mm Hg (Mackay Method)  
 Selected VP: 0.236 mm Hg (Mean of Antoine & Grain methods)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	2	-CH3	21.98	43.96
Group	10	-CH2-	24.22	242.20
*		Equation Constant		198.18

---

RESULT-uncorr| BOILING POINT in deg Kelvin | 484.34  
 RESULT- corr | BOILING POINT in deg Kelvin | 478.87  
                   | BOILING POINT in deg C     | 205.71

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	2	-CH3	-5.10	-10.20
Group	10	-CH2-	11.27	112.70
*		Equation Constant		122.50

---

RESULT | MELTING POINT in deg Kelvin | 225.00  
           | MELTING POINT in deg C     | -48.16

Water Sol from Kow (WSKOW v1.41) Results:

Water Sol: 0.1099 mg/L

Experimental Water Solubility Database Match:

Name : DODECANE  
 CAS Num : 000112-40-3  
 Exp WSol : 0.0037 mg/L (25 deg C)  
 Exp Ref : KERTES,AS (1989)

SMILES : CCCCCCCCCCCC  
 CHEM :  
 MOL FOR: C12 H26  
 MOL WT : 170.34

----- WSKOW v1.41 Results -----

Log Kow (estimated) : 6.23  
 Log Kow (experimental): 6.10  
 Cas No: 000112-40-3  
 Name : Dodecane  
 Refer : Coates,M et al. (1985)  
 Log Kow used by Water solubility estimates: 6.10

Equation Used to Make Water Sol estimate:

Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction  
 (used when Melting Point NOT available)

Correction(s):	Value
Hydrocarbon	-0.537

Log Water Solubility (in moles/L) : -6.190

Water Solubility at 25 deg C (mg/L): 0.1099

WATERNT Program (v1.01) Results:

=====

Water Sol (v1.01 est): 0.0092579 mg/L

Experimental Water Solubility Database Match:

Name : DODECANE  
CAS Num : 000112-40-3  
Exp WSol : 0.0037 mg/L (25 deg C)  
Exp Ref : KERTES,AS (1989)

SMILES : CCCCCCCCCCCC

CHEM :

MOL FOR: C12 H26

MOL WT : 170.34

TYPE	NUM	WATER SOLUBILITY	FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3	[aliphatic carbon]	-0.3213	-0.6425
Frag	10	-CH2-	[aliphatic carbon]	-0.5370	-5.3702
Factor	1	Hydrocarbon	[unsubst. alkane] correction	-1.5013	-1.5013
Const		Equation Constant			0.2492

Log Water Sol (moles/L) at 25 dec C = -7.2648

Water Solubility (mg/L) at 25 dec C =0.0092579

ECOSAR Program (v0.99g) Results:

=====

SMILES : CCCCCCCCCCCC

CHEM :

CAS Num:

ChemID1:

ChemID2:

ChemID3:

MOL FOR: C12 H26

MOL WT : 170.34

Log Kow: 6.23 (KowWin estimate)

Melt Pt:

Wat Sol: 0.0367 mg/L (calculated)

ECOSAR v0.99g Class(es) Found

-----

Neutral Organics

ECOSAR Class	Organism	Predicted Duration	End Pt	mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.047 *
Neutral Organics	: Fish	96-hr	LC50	0.013
Neutral Organics	: Fish	14-day	LC50	0.047 *
Neutral Organics	: Daphnid	48-hr	LC50	0.019
Neutral Organics	: Green Algae	96-hr	EC50	0.015
Neutral Organics	: Fish	30-day	ChV	0.003
Neutral Organics	: Daphnid	16-day	EC50	0.006
Neutral Organics	: Green Algae	96-hr	ChV	0.018
Neutral Organics	: Fish (SW)	96-hr	LC50	0.024
Neutral Organics	: Mysid Shrimp	96-hr	LC50	0.000188

mg/kg (ppm)  
dry wt soil

Neutral Organics : Earthworm 14-day LC50 52.177 \*

Note: \* = asterick designates: Chemical may not be soluble enough to measure this predicted effect.

Fish and daphnid acute toxicity log Kow cutoff: 5.0

Green algal EC50 toxicity log Kow cutoff: 6.4

Chronic toxicity log Kow cutoff: 8.0

MW cutoff: 1000

HENRY (v3.10) Program Results:

Bond Est : 9.35E+000 atm-m3/mole

Group Est: 1.34E+001 atm-m3/mole

SMILES : CCCCCCCCCCCC

CHEM :

MOL FOR: C12 H26

MOL WT : 170.34

----- HENRYWIN v3.10 Results -----

Experimental Database Structure Match:

Name : DODECANE

CAS Num : 000112-40-3

Exp HLC : 8.24E+00 atm-m3/mole

Temper : 25 deg C

Exp VP : 1.36E-01 mm Hg

Exp WSol : 3.70E-03 mg/L

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	26 Hydrogen to Carbon (aliphatic) Bonds		-3.1116
FRAGMENT	11 C-C		1.2793
FACTOR	* Linear or branched alkane		-0.7500

RESULT | BOND ESTIMATION METHOD for LWAPC VALUE | TOTAL | -2.582

HENRYs LAW CONSTANT at 25 deg C = 9.35E+000 atm-m3/mole  
= 3.82E+002 unitless

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	2 CH3 (X)		-1.24
	10 CH2 (C)(C)		-1.50

RESULT | GROUP ESTIMATION METHOD for LOG GAMMA VALUE | TOTAL | -2.74

HENRYs LAW CONSTANT at 25 deg C = 1.34E+001 atm-m3/mole  
= 5.50E+002 unitless

Henrys LC [VP/WSol estimate using EPI values]:

HLC: 4.813E-001 atm-m3/mole

VP: 0.236 mm Hg

WS: 0.11 mg/L

BIOWIN (v4.01) Program Results:

SMILES : CCCCCCCCCCCC

CHEM :

MOL FOR: C12 H26  
MOL WT : 170.34

----- BIOWIN v4.01 Results -----

Linear Model Prediction : Biodegrades Fast  
Non-Linear Model Prediction: Biodegrades Fast  
Ultimate Biodegradation Timeframe: Days-Weeks  
Primary Biodegradation Timeframe: Days  
MITI Linear Model Prediction : Biodegrades Fast  
MITI Non-Linear Model Prediction: Biodegrades Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Linear C4 terminal chain [CCC-CH3]	0.1084	0.2169
MolWt	*	Molecular Weight Parameter		-0.0811
Const	*	Equation Constant		0.7475
RESULT   LINEAR BIODEGRADATION PROBABILITY				0.8833

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Linear C4 terminal chain [CCC-CH3]	1.8437	3.6874
MolWt	*	Molecular Weight Parameter		-2.4188
RESULT   NON-LINEAR BIODEGRADATION PROBABILITY				0.9863

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Linear C4 terminal chain [CCC-CH3]	0.2983	0.5967
MolWt	*	Molecular Weight Parameter		-0.3764
Const	*	Equation Constant		3.1992
RESULT   SURVEY MODEL - ULTIMATE BIODEGRADATION				3.4194

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Linear C4 terminal chain [CCC-CH3]	0.2691	0.5381
MolWt	*	Molecular Weight Parameter		-0.2458
Const	*	Equation Constant		3.8477
RESULT   SURVEY MODEL - PRIMARY BIODEGRADATION				4.1401

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks  
(Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	Methyl [-CH3]	0.0004	0.0008
Frag	10	-CH2- [linear]	0.0494	0.4942
MolWt	*	Molecular Weight Parameter		-0.5068

Const| \* | Equation Constant | | 0.7121  
 =====  
 RESULT | MITI LINEAR BIODEGRADATION PROBABILITY | | 0.7004  
 =====

-----+-----  
 TYPE | NUM | BIOWIN FRAGMENT DESCRIPTION | COEFF | VALUE  
 -----+-----  
 Frag | 2 | Methyl [-CH3] | 0.0194 | 0.0389  
 Frag | 10 | -CH2- [linear] | 0.4295 | 4.2949  
 MolWt| \* | Molecular Weight Parameter | | -4.9175  
 =====  
 RESULT | MITI NON-LINEAR BIODEGRADATION PROBABILITY | | 0.8746  
 =====

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable  
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.91) Results:

=====

SMILES : CCCCCCCCCCCC  
 CHEM :  
 MOL FOR: C12 H26  
 MOL WT : 170.34

----- SUMMARY (AOP v1.91): HYDROXYL RADICALS -----

Hydrogen Abstraction = 13.9366 E-12 cm3/molecule-sec  
 Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec  
 Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec  
 Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec  
 Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec  
 Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 13.9366 E-12 cm3/molecule-sec  
 HALF-LIFE = 0.767 Days (12-hr day; 1.5E6 OH/cm3)  
 HALF-LIFE = 9.210 Hrs

----- SUMMARY (AOP v1.91): OZONE REACTION -----

\*\*\*\*\* NO OZONE REACTION ESTIMATION \*\*\*\*\*  
 (ONLY Olefins and Acetylenes are Estimated)

Experimental Database Structure Match:

Chem Name : n-Dodecane  
 CAS Number: 000112-40-3  
 Exper OH rate constant : 14.2 E-12 cm3/molecule-sec  
 Exper OH Reference: ATKINSON,R (1994)  
 Exper Ozone rate constant: --- cm3/molecule-sec  
 Exper NO3 rate constant : --- cm3/molecule-sec

PCKOC Program (v1.66) Results:

=====

Koc (estimated): 5.86e+003

SMILES : CCCCCCCCCCCC  
 CHEM :  
 MOL FOR: C12 H26  
 MOL WT : 170.34

----- PCKOCWIN v1.66 Results -----

First Order Molecular Connectivity Index ..... : 5.914  
 Non-Corrected Log Koc ..... : 3.7682  
 Fragment Correction(s) --> NONE : ---  
 Corrected Log Koc ..... : 3.7682

Estimated Koc: 5864

HYDROWIN Program (v1.67) Results:

=====

SMILES : CCCCCCCCCCCC  
CHEM :  
MOL FOR: C12 H26  
MOL WT : 170.34

----- HYDROWIN v1.67 Results -----

Currently, this program can NOT estimate a hydrolysis rate constant for the type of chemical structure entered!!

ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens) and Specific Alkyl Halides can be estimated!! For more information, (Click OVERVIEW in Help or see the User's Guide)

\*\*\*\*\* CALCULATION NOT PERFORMED \*\*\*\*\*

BCF Program (v2.15) Results:

=====

SMILES : CCCCCCCCCCCC  
CHEM :  
MOL FOR: C12 H26  
MOL WT : 170.34

----- Bcfwin v2.15 -----

Log Kow (estimated) : 6.23  
Log Kow (experimental): 6.10  
Log Kow used by BCF estimates: 6.10

Equation Used to Make BCF estimate:

$$\text{Log BCF} = 0.77 \log \text{Kow} - 0.70 + \text{Correction}$$

Correction(s):            Value  
Alkyl chains (8+ -CH2- groups) -1.500

Estimated Log BCF = 2.497 (BCF = 314.1)

Volatization From Water

=====

Chemical Name:  
Molecular Weight : 170.34 g/mole  
Water Solubility : ----  
Vapor Pressure : ----  
Henry's Law Constant: 8.24 atm-m<sup>3</sup>/mole (Henry experimental database)

	RIVER	LAKE
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05
HALF-LIFE (hours) :	1.332	124
HALF-LIFE (days ) :	0.0555	5.165

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

=====

PROPERTIES OF:

-----

Molecular weight (g/mol)                    170.34  
Aqueous solubility (mg/l)                    0

Vapour pressure (Pa) 0  
(atm) 0  
(mm Hg) 0  
Henry 's law constant (Atm-m3/mol) 8.24  
Air-water partition coefficient 336.992  
Octanol-water partition coefficient (Kow) 1.25893E+006  
Log Kow 6.1  
Biomass to water partition coefficient 251786  
Temperature [deg C] 25  
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):  
-Primary tank 0.00 9980.18 10000.00  
-Aeration tank 0.00 9980.18 10000.00  
-Settling tank 0.00 9980.18 10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	5.9E-002	100.00
Primary sludge	5.87E+000	3.4E-002	58.72
Waste sludge	2.80E-002	1.6E-004	0.28
Primary volatilization	2.59E-003	1.5E-005	0.03
Settling volatilization	4.91E-005	2.9E-007	0.00
Aeration off gas	4.07E+000	2.4E-002	40.73
Primary biodegradation	1.72E-002	1.0E-004	0.17
Settling biodegradation	3.58E-005	2.1E-007	0.00
Aeration biodegradation	4.72E-004	2.8E-006	0.00
Final water effluent	6.33E-003	3.7E-005	0.06
Total removal	9.99E+000	5.9E-002	99.94
Total biodegradation	1.77E-002	1.0E-004	0.18

(\*\* Total removal recommended maximum is 99 percent)

Level III Fugacity Model (Full-Output):

=====  
Chem Name :  
Molecular Wt: 170.34  
Henry's LC : 8.24 atm-m3/mole (Henry database)  
Vapor Press : 0.236 mm Hg (Mpbpwin program)  
Log Kow : 6.1 (Kowwin program)  
Soil Koc : 5.16e+005 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	5.24	18.1	1000
Water	20.1	208	1000
Soil	25.9	208	1000
Sediment	48.7	832	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	4.81e-011	1.29e+003	336	42.9	11.2
Water	1.7e-005	430	129	14.3	4.3
Soil	3.58e-008	553	0	18.4	0
Sediment	3.04e-006	260	6.24	8.65	0.208

Persistence Time: 213 hr  
Reaction Time: 253 hr  
Advection Time: 1.36e+003 hr

Percent Reacted: 84.3  
Percent Advected: 15.7

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):

Air: 18.08  
Water: 208.1  
Soil: 208.1  
Sediment: 832.3  
Biowin estimate: 3.419 (days-weeks )

Advection Times (hr):

Air: 100  
Water: 1000  
Sediment: 5e+004

---

## Ms. Delpire's Attachment 3 – Undecane EPI Suite Results

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C11 H24

MOL WT : 156.31

----- EPI SUMMARY (v3.11) -----

### Physical Property Inputs:

Water Solubility (mg/L): -----

Vapor Pressure (mm Hg) : -----

Henry LC (atm-m<sup>3</sup>/mole) : -----

Log Kow (octanol-water): -----

Boiling Point (deg C) : -----

Melting Point (deg C) : -----

### KOWWIN Program (v1.67) Results:

=====

Log Kow(version 1.67 estimate): 5.74

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C11 H24

MOL WT : 156.31

TYPE	NUM	LOGKOW	FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3	[aliphatic carbon]	0.5473	1.0946
Frag	9	-CH2-	[aliphatic carbon]	0.4911	4.4199
Const			Equation Constant		0.2290

-----  
Log Kow = 5.7435

### MPBPWIN (v1.41) Program Results:

=====

#### Experimental Database Structure Match:

Name : N-UNDECANE

CAS Num : 001120-21-4

Exp MP (deg C): -25.6

Exp BP (deg C): 195.9

Exp VP (mm Hg): 4.12E-01

Exp VP (deg C): 25

Exp VP ref : DAUBERT,TE & DANNER,RP (1989)

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C11 H24

MOL WT : 156.31

----- SUMMARY MPBPWIN v1.41 -----

Boiling Point: 185.61 deg C (Adapted Stein and Brown Method)

Melting Point: -59.43 deg C (Adapted Joback Method)

Melting Point: -5.29 deg C (Gold and Ogle Method)

Mean Melt Pt : -32.36 deg C (Joback; Gold,Ogle Methods)

Selected MP: -32.36 deg C (Mean Value)

#### Vapor Pressure Estimations (25 deg C):

(Using BP: 195.90 deg C (exp database))

(MP not used for liquids)

VP: 0.681 mm Hg (Antoine Method)

VP: 0.576 mm Hg (Modified Grain Method)

VP: 0.65 mm Hg (Mackay Method)

Selected VP: 0.629 mm Hg (Mean of Antoine & Grain methods)

TYPE	NUM	BOIL DESCRIPTION	COEFF	VALUE
Group	2	-CH3	21.98	43.96
Group	9	-CH2-	24.22	217.98
*		Equation Constant		198.18

---

RESULT-uncorr| BOILING POINT in deg Kelvin | 460.12  
RESULT- corr | BOILING POINT in deg Kelvin | 458.77  
| BOILING POINT in deg C | 185.61

TYPE	NUM	MELT DESCRIPTION	COEFF	VALUE
Group	2	-CH3	-5.10	-10.20
Group	9	-CH2-	11.27	101.43
*		Equation Constant		122.50

---

RESULT | MELTING POINT in deg Kelvin | 213.73  
| MELTING POINT in deg C | -59.43

Water Sol from Kow (WSKOW v1.41) Results:

Water Sol: 0.2571 mg/L

Experimental Water Solubility Database Match:

Name : N-UNDECANE  
CAS Num : 001120-21-4  
Exp WSol : 0.0044 mg/L (25 deg C)  
Exp Ref : YALKOWSKY,SH & DANNENFELSER,RM (1992)

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C11 H24

MOL WT : 156.31

----- WSKOW v1.41 Results -----

Log Kow (estimated) : 5.74

Log Kow (experimental): not available from database

Log Kow used by Water solubility estimates: 5.74

Equation Used to Make Water Sol estimate:

$\text{Log S (mol/L)} = 0.796 - 0.854 \log \text{Kow} - 0.00728 \text{ MW} + \text{Correction}$   
(used when Melting Point NOT available)

Correction(s): Value

-----  
Hydrocarbon -0.537

Log Water Solubility (in moles/L) : -5.784

Water Solubility at 25 deg C (mg/L): 0.2571

WATERNT Program (v1.01) Results:

Water Sol (v1.01 est): 0.029256 mg/L

Experimental Water Solubility Database Match:

Name : N-UNDECANE  
CAS Num : 001120-21-4

Exp WSol : 0.0044 mg/L (25 deg C)  
 Exp Ref : YALKOWSKY,SH & DANNENFELSER,RM (1992)

SMILES : CCCCCCCCCC  
 CHEM :  
 MOL FOR: C11 H24  
 MOL WT : 156.31

TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	2	-CH3 [aliphatic carbon]	-0.3213	-0.6425
Frag	9	-CH2- [aliphatic carbon]	-0.5370	-4.8332
Factor	1	Hydrocarbon [unsubst. alkane] correction	-1.5013	-1.5013
Const		Equation Constant		0.2492

Log Water Sol (moles/L) at 25 dec C = -6.7278  
 Water Solubility (mg/L) at 25 dec C = 0.029256

ECOSAR Program (v0.99g) Results:

=====

SMILES : CCCCCCCCCC  
 CHEM :  
 CAS Num:  
 ChemID1:  
 ChemID2:  
 ChemID3:  
 MOL FOR: C11 H24  
 MOL WT : 156.31  
 Log Kow: 5.74 (KowWin estimate)  
 Melt Pt:  
 Wat Sol: 0.1065 mg/L (calculated)

ECOSAR v0.99g Class(es) Found

-----  
 Neutral Organics

ECOSAR Class	Organism	Predicted		
		Duration	End Pt	mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	0.116 *
Neutral Organics	: Fish	96-hr	LC50	0.035
Neutral Organics	: Fish	14-day	LC50	0.116 *
Neutral Organics	: Daphnid	48-hr	LC50	0.049
Neutral Organics	: Green Algae	96-hr	EC50	0.038
Neutral Organics	: Fish	30-day	ChV	0.008
Neutral Organics	: Daphnid	16-day	EC50	0.013
Neutral Organics	: Green Algae	96-hr	ChV	0.033
Neutral Organics	: Fish (SW)	96-hr	LC50	0.049
Neutral Organics	: Mysid Shrimp	96-hr	LC50	0.000706
			mg/kg (ppm) dry wt soil	
Neutral Organics	: Earthworm	14-day	LC50	67.776 *

Note: \* = asterick designates: Chemical may not be soluble enough to measure this predicted effect.  
 Fish and daphnid acute toxicity log Kow cutoff: 5.0  
 Green algal EC50 toxicity log Kow cutoff: 6.4  
 Chronic toxicity log Kow cutoff: 8.0

MW cutoff: 1000

HENRY (v3.10) Program Results:

=====  
Bond Est : 7.04E+000 atm-m3/mole  
Group Est: 9.52E+000 atm-m3/mole

SMILES : CCCCCCCCCC  
CHEM :  
MOL FOR: C11 H24  
MOL WT : 156.31

----- HENRYWIN v3.10 Results -----

Experimental Database Structure Match:

Name : N-UNDECANE  
CAS Num : 001120-21-4  
Exp HLC : 1.93E+00 atm-m3/mole  
Temper : 25 deg C  
Exp VP : 4.12E-01 mm Hg  
Exp WSol : 4.40E-03 mg/L

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN	24 Hydrogen to Carbon (aliphatic) Bonds		-2.8722
FRAGMENT	10 C-C		1.1630
FACTOR	* Linear or branched alkane		-0.7500
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	-2.459

HENRYs LAW CONSTANT at 25 deg C = 7.04E+000 atm-m3/mole  
= 2.88E+002 unitless

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	2 CH3 (X)		-1.24
	9 CH2 (C)(C)		-1.35
RESULT	GROUP ESTIMATION METHOD for LOG GAMMA VALUE	TOTAL	-2.59

HENRYs LAW CONSTANT at 25 deg C = 9.52E+000 atm-m3/mole  
= 3.89E+002 unitless

Henrys LC [VP/WSol estimate using EPI values]:

HLC: 5.032E-001 atm-m3/mole  
VP: 0.629 mm Hg  
WS: 0.257 mg/L

BIOWIN (v4.01) Program Results:

=====  
SMILES : CCCCCCCCCC  
CHEM :  
MOL FOR: C11 H24  
MOL WT : 156.31

----- BIOWIN v4.01 Results -----

Linear Model Prediction : Biodegrades Fast  
Non-Linear Model Prediction: Biodegrades Fast  
Ultimate Biodegradation Timeframe: Days-Weeks  
Primary Biodegradation Timeframe: Days

MITI Linear Model Prediction : Biodegrades Fast  
 MITI Non-Linear Model Prediction: Biodegrades Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Linear C4 terminal chain [CCC-CH3]	0.1084	0.2169	
MolWt	*	Molecular Weight Parameter		-0.0744	
Const	*	Equation Constant		0.7475	
RESULT				LINEAR BIODEGRADATION PROBABILITY	0.8900

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Linear C4 terminal chain [CCC-CH3]	1.8437	3.6874	
MolWt	*	Molecular Weight Parameter		-2.2197	
RESULT				NON-LINEAR BIODEGRADATION PROBABILITY	0.9888

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast  
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Linear C4 terminal chain [CCC-CH3]	0.2983	0.5967	
MolWt	*	Molecular Weight Parameter		-0.3454	
Const	*	Equation Constant		3.1992	
RESULT				SURVEY MODEL - ULTIMATE BIODEGRADATION	3.4504

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Linear C4 terminal chain [CCC-CH3]	0.2691	0.5381	
MolWt	*	Molecular Weight Parameter		-0.2255	
Const	*	Equation Constant		3.8477	
RESULT				SURVEY MODEL - PRIMARY BIODEGRADATION	4.1604

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks  
 (Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag	2	Methyl [-CH3]	0.0004	0.0008	
Frag	9	-CH2- [linear]	0.0494	0.4447	
MolWt	*	Molecular Weight Parameter		-0.4650	
Const	*	Equation Constant		0.7121	
RESULT				MITI LINEAR BIODEGRADATION PROBABILITY	0.6927

TYPE	NUM	BIOWIN FRAGMENT DESCRIPTION	COEFF	VALUE
------	-----	-----------------------------	-------	-------

```

Frag | 2 | Methyl [-CH3] | 0.0194 | 0.0389
Frag | 9 | -CH2- [linear] | 0.4295 | 3.8654
MolWt | * | Molecular Weight Parameter | | -4.5126
=====
RESULT | MITI NON-LINEAR BIODEGRADATION PROBABILITY | | 0.8718
=====

```

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable  
A Probability Less Than 0.5 indicates --> NOT Readily Degradable

AOP Program (v1.91) Results:

```

=====
SMILES : CCCCCCCCCC
CHEM :
MOL FOR: C11 H24
MOL WT : 156.31
----- SUMMARY (AOP v1.91): HYDROXYL RADICALS -----
Hydrogen Abstraction = 12.5235 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Aromatic Rings = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec

OVERALL OH Rate Constant = 12.5235 E-12 cm3/molecule-sec
HALF-LIFE = 0.854 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE = 10.249 Hrs
----- SUMMARY (AOP v1.91): OZONE REACTION -----

***** NO OZONE REACTION ESTIMATION *****
(ONLY Olefins and Acetylenes are Estimated)

```

Experimental Database Structure Match:

```

Chem Name : n-Undecane
CAS Number: 001120-21-4
Exper OH rate constant : 13.2 E-12 cm3/molecule-sec
Exper OH Reference: KWOK,ESC & ATKINSON,R (1994)
Exper Ozone rate constant: --- cm3/molecule-sec
Exper NO3 rate constant : --- cm3/molecule-sec

```

PCKOC Program (v1.66) Results:

```

=====
Koc (estimated): 3.18e+003

SMILES : CCCCCCCCCC
CHEM :
MOL FOR: C11 H24
MOL WT : 156.31
----- PCKOCWIN v1.66 Results -----

First Order Molecular Connectivity Index ..... : 5.414
Non-Corrected Log Koc ..... : 3.5023
Fragment Correction(s) --> NONE : ---
Corrected Log Koc ..... : 3.5023

Estimated Koc: 3179

```

HYDROWIN Program (v1.67) Results:

```

=====
SMILES : CCCCCCCCCC
CHEM :
MOL FOR: C11 H24

```

MOL WT : 156.31

----- HYDROWIN v1.67 Results -----

Currently, this program can NOT estimate a hydrolysis rate constant for the type of chemical structure entered!!

ONLY Esters, Carbamates, Epoxides, Halomethanes (containing 1-3 halogens) and Specific Alkyl Halides can be estimated!! For more information, (Click OVERVIEW in Help or see the User's Guide)

\*\*\*\*\* CALCULATION NOT PERFORMED \*\*\*\*\*

BCF Program (v2.15) Results:

=====

SMILES : CCCCCCCCCC

CHEM :

MOL FOR: C11 H24

MOL WT : 156.31

----- Bcfwin v2.15 -----

Log Kow (estimated) : 5.74

Log Kow (experimental): not available from database

Log Kow used by BCF estimates: 5.74

Equation Used to Make BCF estimate:

Log BCF = 0.77 log Kow - 0.70 + Correction

Correction(s): Value  
Alkyl chains (8+ -CH2- groups) -1.000

Estimated Log BCF = 2.722 (BCF = 527.8)

Volatization From Water

=====

Chemical Name:

Molecular Weight : 156.31 g/mole

Water Solubility : ----

Vapor Pressure : ----

Henry's Law Constant: 1.93 atm-m<sup>3</sup>/mole (Henry experimental database)

	RIVER	LAKE
	-----	-----
Water Depth (meters):	1	1
Wind Velocity (m/sec):	5	0.5
Current Velocity (m/sec):	1	0.05

HALF-LIFE (hours) : 1.276 118.8

HALF-LIFE (days) : 0.05317 4.948

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

=====

PROPERTIES OF:

-----

Molecular weight (g/mol)	156.31
Aqueous solubility (mg/l)	0
Vapour pressure (Pa)	0
(atm)	0
(mm Hg)	0
Henry's law constant (Atm-m <sup>3</sup> /mol)	1.93
Air-water partition coefficient	78.9313
Octanol-water partition coefficient (Kow)	549541
Log Kow	5.74
Biomass to water partition coefficient	109909

Temperature [deg C] 25  
 Biodeg rate constants (h<sup>-1</sup>), half life in biomass (h) and in 2000 mg/L MLSS (h):  
 -Primary tank 0.00 9954.71 10000.00  
 -Aeration tank 0.00 9954.71 10000.00  
 -Settling tank 0.00 9954.71 10000.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	6.4E-002	100.00
Primary sludge	5.73E+000	3.7E-002	57.27
Waste sludge	5.36E-002	3.4E-004	0.54
Primary volatilization	5.79E-003	3.7E-005	0.06
Settling volatilization	2.15E-004	1.4E-006	0.00
Aeration off gas	4.18E+000	2.7E-002	41.80
Primary biodegradation	1.68E-002	1.1E-004	0.17
Settling biodegradation	6.87E-005	4.4E-007	0.00
Aeration biodegradation	9.04E-004	5.8E-006	0.01
Final water effluent	1.54E-002	9.8E-005	0.15
Total removal	9.98E+000	6.4E-002	99.85
Total biodegradation	1.78E-002	1.1E-004	0.18

(\*\* Total removal recommended maximum is 99 percent)

Level III Fugacity Model (Full-Output):

=====  
 Chem Name :  
 Molecular Wt: 156.31  
 Henry's LC : 1.93 atm-m<sup>3</sup>/mole (Henry database)  
 Vapor Press : 0.629 mm Hg (Mpbpwin program)  
 Log Kow : 5.74 (Kowwin program)  
 Soil Koc : 2.25e+005 (calc by model)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	5.95	19.4	1000
Water	23.7	208	1000
Soil	36.6	208	1000
Sediment	33.7	832	0

	Fugacity (atm)	Reaction (kg/hr)	Advection (kg/hr)	Reaction (percent)	Advection (percent)
Air	5.31e-011	1.21e+003	340	40.4	11.3
Water	6.13e-006	452	136	15.1	4.52
Soil	2.65e-008	697	0	23.2	0
Sediment	1.1e-006	161	3.86	5.35	0.129

Persistence Time: 191 hr  
 Reaction Time: 227 hr  
 Advection Time: 1.19e+003 hr  
 Percent Reacted: 84  
 Percent Advected: 16

Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):  
 Air: 19.45  
 Water: 208.1  
 Soil: 208.1  
 Sediment: 832.3

Biowin estimate: 3.450 (days-weeks )

Advection Times (hr):

Air: 100

Water: 1000

Sediment: 5e+004

---

**Mr. Scott Prothero**  
**Senior Chemical Engineer**  
**US Environmental Protection Agency**

My branch, the Chemical Engineering Branch (CEB) of US EPA, has reviewed the American Chemistry Council n-Alkane VCCEP Consortium's VCCEP submission for the n-Alkane category, including decane, undecane, and dodecane (CAS Nos. 124-18-5, 1120-21-4, 112-40-3) submitted by the n-Alkane VCCEP Consortium and dated June 17, 2004. We offer for consideration by the peer consultation panel the following comments, which focus primarily on the charge questions 4, 5, and 6 under Exposure Assessment. Our review focused on elements of this submission pertaining to occupational exposures and environmental releases, and whether these elements provide sufficient data to complete an exposure assessment. This review focuses on the appropriate use of data (we did not verify the calculations used for the exposure assessments in the submission), additional data needs, and the methodologies to conduct the assessments.

The submission presents the exposure data collected for the assessment, and indicates which studies were used for this analysis. The sources for all data are documented, and a list of references is provided. The methodology for use of the data in the exposure sections is described, including exposure calculations, where appropriate. For those exposure routes evaluated, the submission is considered to be transparent, in that it is possible to reproduce results and evaluate the conclusions.

A criteria for determining whether occupational exposure should be addressed in the assessment is whether the reproductive and / or developmental hazard potential for the chemical is low. On page 56, the submission makes the following statement: "The weight of evidence indicates that n-decane, n-undecane and n-dodecane have a low potential to cause reproductive or developmental toxicity." If the submission is correct on this issue, the occupational exposure issues noted below may not need further consideration based on this criteria.

There are several occupational exposure issues that were not given adequate coverage in the submission. Although the submission seems to indicate that the Air Force base workers with exposures covered in section 6.4.6 (Air Force / Airline Industry / Re-Fueling) are the highest exposed population, the submission should explicitly state that this population is the highest exposed population found in the literature search for this submission. In section 6.4, the submission should include further discussion about other exposed populations that are not covered by the literature search (occupational exposures during petroleum refining, n-alkanes processing, and formulation; and during paint, adhesive, carpet, wallpaper, and furniture manufacturing (industrial uses for products that contain n-alkanes, as described in the submission)). The Consortium authors should state whether monitoring data exists for workers in their own facilities and present any exiting data to demonstrate that their workers have lower exposures than the Air Force base workers' exposures. Screening level exposure assessments should assure that no higher exposed populations can reasonably be expected to exist before concluding that no further exposure data are needed, and this submission does not adequately present this assurance. Both the exposure assessment and the risk assessment sections should address this issue of completeness by transparently addressing this

issue.

In addition, the submission does not present any estimates of environmental releases from industrial processes (e.g., manufacturing, processing or industrial use of these chemicals). If the non-occupational exposure data set in the submission is considered by the panel to be complete, then such releases need not be addressed further. However, if the non-occupational exposure data set in the submission is considered by the panel to be incomplete, then such releases may need further consideration and coverage as the releases may relate to and impact non-occupational exposures.

The submission states in Section 5.4 that "this assessment is not intended to address petroleum substances which may contain one or more of these n-alkanes," although it recognizes that petroleum substances represent the predominant use of these n-alkanes. The submission does not completely omit petroleum substances; however, it does not address all of the industrial uses of these chemicals. In section 9.2 of the submission, this data gap should be stated and its significance should be given proper discussion.

**Dr. Louis Scarano<sup>2,3</sup>**  
**Toxicologist**  
**US Environmental Protection Agency**

### **Overall**

Given the risk assessment as presented in the submission, I agree with the conclusions and do not believe that additional Tier 2 (or higher) hazard or exposure information is necessary. I further would like to recognize the complexity of trying to evaluate these three individual chemicals. They are most often found as components of complex mixtures and so are rarely observed as discrete entities.

### **General Technical Comments**

1. The category concept. I am a proponent of the category concept and its use in hazard assessment. In this case, it seems that there is sufficient information on the three subject chemicals for virtually all Tier 1 hazard endpoints and the limited “read-across” presented is reasonable. However, I do think it is important to define boundaries in a category. By definition, this would mean that all chemicals discussed that fall within the boundaries are considered category members. Boundaries are not explicitly stated in the submission. Throughout the submission, the structural analogs (i.e., nonane) are not considered category members – but I believe they should be.
2. Alpha-2u-globulin effect. The summary of repeat dose toxicity data in the main report (pp. 51-55 and Table 7.3) suggest that the alpha-2u-globulin effects observed in male rats is limited to alkane mixtures, all of which appear to have branched and cyclic components as well as linear alkanes. The robust summary for the Yoshimura study with undecane (beginning on p. B-22) indicates an “alpha-2u-globulin” finding. This appears inconsistent. (Although the Health Benchmark summary section on page 55 does mention that this was specifically measured in the Yoshimura study). My question is: what was exactly measured/identified in the Yoshimura study and how does it compare with the mixture studies and the decane data? In other words, were there male rat kidney pathological effects, hyaline droplet formation, etc. in the Yoshimura study? My point is that while I am convinced decane, undecane, and dodecane belong together as a category for hazard assessment purposes, I am not sure that the male rat nephropathy is an effect seen following exposure to these chemicals alone (i.e., pure linear alkanes between C10-12).
3. Viscosity (SUS) Measurements. It appears that the potential for aspiration hazard applies to decane, undecane, and dodecane. It would be useful to report the SUS values for these chemicals so they can be compared to the value of 100 that is generally used to label/identify potential aspiration hazards.

---

<sup>2</sup> Toxicologist, Office of Pesticide Programs, U.S. Environmental Protection Agency, Washington, DC.

<sup>3</sup> Views expressed are those of the author and do not represent EPA policy.

4. Dermal Hazard Potential. Although I agree with the overall conclusions about the lack of dermal effects due to irritancy and general lack of systemic effects, it is noteworthy that dodecane appears to be a skin tumor promoter.

**NOTE:** Dr. Scarano also made several editorial suggestions directly to the authors of the report.

## **Appendix D**

### **Sponsors' Presentation Slides**



# **n-Decane, n-Undecane, and n-Dodecane Tier 1 VCCEP Assessment**

n-Alkanes VCCEP Consortium:  
Chevron Phillips Chemical  
Sasol North America  
Shell Chemical

September 14, 2004

n-Alkanes VCCEP Consortium

## **Outline for Presentations**



- 1) Introductions/Background:  
Andrew Jaques, ACC Consortium Manager  
Exposure Assessment:  
Ross Macdonald, Consortium Consultant
- 2) Hazard Assessment:  
Ralph Gingell, Shell Chemicals LP
- 3) Risk Assessment:  
Ross Macdonald, Consortium Consultant  
Data Needs Assessment/Conclusion:  
Dave Penney, Sasol North America

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## Background



- Basis for VCCEP selection primarily due to indoor air and human breath data.
- n-Decane, n-undecane, and n-dodecane are linear aliphatic hydrocarbons. The three chemicals are being treated as a category because they are similar in chemistry and toxicity.
- Most exposures are to complex petroleum substances which contain these three chemicals, making a chain-of-commerce assessment impractical.

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## Production and Use



- Almost all of the decane, undecane, and dodecane reported on the TSCA Inventory are components of n-alkane process streams.
- These streams are generally consumed as chemical intermediates in the production of linear alkyl benzenes, which are themselves intermediates in the production of linear alkyl benzene sulfonate surfactants.
- Production of these alkane streams is <0.1% of the petroleum stream production containing these alkanes.

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## Petroleum Sources



- Decane, undecane, and dodecane are present in several petroleum products including kerosene, jet fuel, home heating oil, diesel fuel, and hydrocarbon solvents.
- These products are the primary sources of exposure to decane, undecane, and dodecane; as such, they were considered in the exposure assessment.
- Some hydrocarbon solvent toxicology data is provided in the hazard assessment as these data are used in the OECD SIDS category that includes decane, undecane, and dodecane.

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## n-Alkane VCCEP Exposure Assessment

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## Approach for n-Alkanes Exposure Assessment



### Approach:

- Focus on products/scenarios likely to result in highest exposure to children and prospective parents.
- Air monitoring studies in ambient, domestic, and workplace air.
- Monitoring data on human milk in urban areas.
- Modeling of dermal and drinking water pathways.

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## Sources of n-Alkanes Exposure



### Sources:

- Fuel: e.g. diesel fuel, jet fuel, home heating oil
- Paints (Alkyd) i.e. “oil-based paints”
- Solvents used in office products and construction materials (e.g. photocopier toner, glues)
- Laboratory reagent

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## Exposure Assessment Terms



### Definitions:

Representative Exposure Level:

- Arithmetic Average of measurements

Upper Bound Exposure Level:

- 95th percentile of distribution of measurements

Screening Estimate:

- A hypothetical exposure level considered to be unrealistically conservative (used for the purpose of screening out unlikely scenarios)

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## Exposure Routes Considered



- **Inhalation: (dozens of studies)**

- Ambient Air Measurements
- Indoor Domestic and Occupational Air Measurements

- **Oral (no data):**

- Screening : drinking water saturated with n-alkanes

- **Human Milk**

- Screening: based on analytical data

- **Dermal: (no data)**

- Screening: Occupational Exposure to Jet Fuel

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## Exposure Scenarios



- Chronic exposure of infants, children, and prospective parents to indoor air
- Short-term exposure of infants, children, and prospective parents in a newly painted home.
- Occupational exposure of prospective parents working with fuels and paints.

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## Highest Exposed Populations



Highest non-occupational exposure is in the home:

- Levels in homes are typically >2x higher than outside.
- Typical levels in autos are similar to home.
- Highest home exposure is during and after painting.

Highest occupational exposure is to workers involved in refueling airplanes and, to a lesser extent, painters.

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## Exposure Concentrations Highest Exposed Populations



Type of Measurement	Representative (Average) Concentration (ug/m3)	Upper Bound Concentration (ug/m3)
Indoor Air Home	42	129
Indoor Air Home During Painting	122	910
Occupational: Highest Exposed Fuel Workers	5,061	16,800

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## n-Alkanes VCCEP Hazard Assessment



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## Hazard Assessment: Introduction



- Similar toxic properties support consideration of the three n-alkanes as a category.
- Sufficient tier 1 studies.
- Few higher tier studies, on individual n-alkanes as they are not major articles of commerce.
- Additional data on n-nonane and selected hydrocarbon solvents containing these alkanes are included.
- Data on hydrocarbon fuels are generally not considered:
  - wider carbon range; contain aromatics and additives that may contribute to toxicity not typical of alkanes

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## Human Health Experience



- Acute effects include:
  - skin defatting from repeated dermal exposure
  - lung damage from aspiration
  - sensory irritation to eyes
- CNS depression by inhalation is generally not considered a hazard because C10-12 n-alkanes are not sufficiently volatile.
- No specific systemic effects identified for these n-alkanes, but anecdotal effects have been attributed to complex hydrocarbons:
  - eg. Liver/kidney damage, painter's syndrome
- Neither Sick Building Syndrome nor childhood asthma have been attributed to n-alkanes.

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## All Tier 1 Endpoints are met - 1



- Acute oral LD50 [rat]:
  - >2 - >5 g/kg – non-toxic [6 values]
- Acute dermal LD50 [rabbit]:
  - >2 - >5 g/kg – non-toxic [4 values]
- Acute inhalation LC50 [rat]:
  - no deaths at the maximum practical vapor concentration [3 values; 1000 – 8000 mg/m<sup>3</sup>]
- Oral limit dose of 5000 mg/kg is approximately equivalent to 35,000 mg/m<sup>3</sup> /6 hr [or 6000ppm]
- **Acute Toxicity Health Benchmark 5000 mg/m<sup>3</sup>**

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## All Tier 1 Endpoints are met - 2



- Several screening studies by gavage, dermal, or by inhalation route at 2000 – 5000 mg/m<sup>3</sup>, on several individual or mixed products
- Systemic toxic effects identified:
  - GI irritation; skin irritation; male rat nephropathy; adaptive liver hypertrophy, decreased wt gain.
- No reproductive effects at 1000 [C10] or 300 [C11] mg/kg oral doses in OECD 422 rat screening studies [300 mg/kg = 2000 mg/m<sup>3</sup> ]
- **Subchronic Health Benchmark: 1000 mg/m<sup>3</sup>**

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## Some Tier 2 Endpoints are addressed



- Genotoxicity: Negative *in vitro* and *in vivo* [mouse micronucleus] assays
- Developmental Toxicity: Negative in rat inhalation segment 2 study at 5000 mg/m<sup>3</sup> [maximum vapor concentration; mixed C9-C13 product].
- Metabolism: C10 is exhaled, metabolized and excreted; half-lives are approx 8 hr in blood and 30 hrs in fat, at high concentrations in rats.
- Reproductive/Developmental Toxicity Health Benchmark: 2000 (C11, inhalation equivalent) - 5000 mg/m<sup>3</sup> (mixed product; highest practical vapor conc.)

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## Some tier 3 endpoints are addressed



- Neurotoxicity: No apparent neurotoxic effects in subchronic studies
- n-Decane caused decreased fore-limb grip strength in rats on 3rd day of 8 hr inhalation repeated exposure at 5000 mg/m<sup>3</sup>, but not at 1500 mg/m<sup>3</sup>.
  - Recovery occurred within 24 hr after end of exposure: considered to be a pharmacological effect.
  - Consistent with 1000 mg/m<sup>3</sup> subchronic health benchmark.
- Carcinogenicity: No tumors in mouse skin initiation - promotion studies
- Can promote mouse skin carcinogenicity of polycyclic aromatics; due to chronic irritation?
  - Stoddard solvent caused small increase in benign adrenal tumors in male rats.

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## Hazard Conclusions



- No single target organ for systemic toxicity – decreased weight gain most sensitive effect.
- Reproduction/developmental toxicity not more sensitive than systemic toxicity.
- No data to address potential immunotoxicity or developmental neurotoxicity.
- Acute and subchronic toxicity health benchmarks are used with various exposure scenarios in risk assessment.
- Low exposures and high MOEs do not indicate need for additional hazard studies.

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## n-Alkanes VCCEP Risk Assessment



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## Risk Assessment Approach



$$\text{Risk} = \text{Exposure} \times \text{Hazard}$$

Assessed by Comparing Exposure with  
Health Benchmarks

- Margin of Exposure (MOE) = Animal Benchmark/Exposure
- Margin of Safety (MOS) = Human Benchmark/Exposure

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## Scenarios for n-Alkanes Risk Assessment



### Receptors/Pathways:

- Children at home/ chronic inhalation exposure
- Children at home/ short term inhalation exposures during renovation/painting
- Infants' oral exposure through human milk
- Prospective parents' occupational inhalation exposure
- Children/Parents: Screening of dermal and drinking water pathways

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## Health Benchmarks



Animal Health Benchmarks [Derived by the Consortium]	
Sub-chronic Inhalation	1,000 mg/m <sup>3</sup>
Acute Inhalation	5,000 mg/m <sup>3</sup>
Sub-chronic Oral	300 mg/kg/day
Human Health Benchmarks [Derived by Third Parties]	
Chronic RfC <sup>1</sup>	1 mg/m <sup>3</sup>
Chronic RfD <sup>1</sup>	0.1 mg/kg/day
Chronic Inhalation REL <sup>2</sup>	1.2 mg/m <sup>3</sup>
Occupational Exposure Limit <sup>3</sup> (OEL)	1,200 mg/m <sup>3</sup> (8-hr TWA)

<sup>1</sup> Total Petroleum Hydrocarbon Criteria Working Group

<sup>2</sup> Interim chronic recommended exposure limit (REL) for C10-C11 isoparaffinic hydrocarbon solvents, California OEHHA.

<sup>3</sup> Proposed (CEFIC)

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## Margins of Exposure and Safety : Children and Prospective Parents



Type of Measurement	Representative MOE	Upper Bound MOE	Representative MOS	Upper Bound MOS
Indoor Air Home (Chronic)	6,000	1,900	24	8
Indoor Air Home During Painting (Short term)	2,000	275	8	1.1

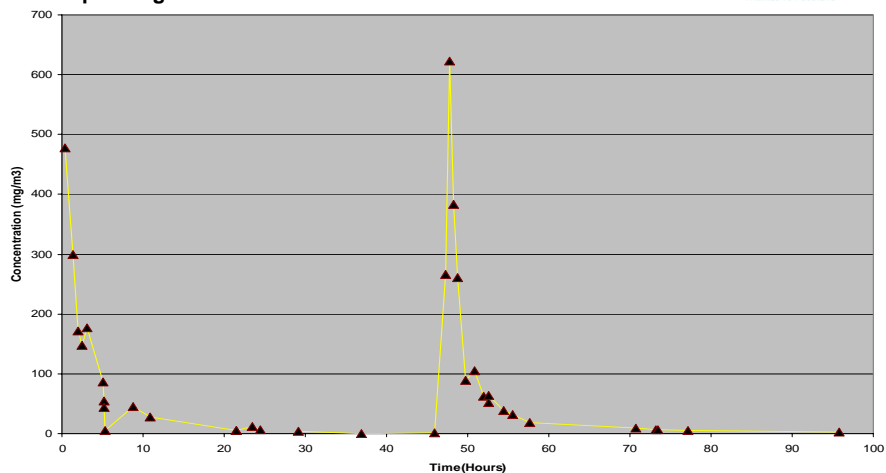
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## Acute Exposure: EPA Research House Data: (Sealed House)



Concentration of total C10-C12 n-alkanes after priming and painting bedroom



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## Acute Exposure During Painting EPA Research House Data<sup>\*\*\*</sup>: Screening Exercise



Time After Painting (hours)	Exposure Conc <sup>*</sup> (mg/m <sup>3</sup> )	Acute MOE <sup>*</sup> (child or worker)	MOS <sup>**</sup> (Worker)
<b>Highest 8 Hour Average Exposure</b>	<b>150</b>	<b>33</b>	<b>8</b>
<b>1</b>	<b>620</b>	<b>8</b>	<b>2</b>
<b>8</b>	<b>30</b>	<b>150</b>	<b>30</b>
<b>24</b>	<b>8</b>	<b>625</b>	<b>50</b>
<b>48</b>	<b>2</b>	<b>2,500</b>	<b>600</b>

\* MOE Based on Acute Health Benchmark of 5,000 mg/m<sup>3</sup>

\*\* MOS based on Occupational Exposure Limit (OEL) of 1,200 mg/m<sup>3</sup>

\*\*\* Sealed house; 0.45 air changes/hour

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## Screening Exercise : Milk, Water, Dermal Exposure



Receptor/Pathway	Representative MOE	Upper Bound MOE
Infant/Milk	64,000	45,000
Child/Drinking Water	>40,000	40,000
Worker/Dermal	270,000	13,000

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## Margins of Exposure and Safety: Aircraft Refueling Workers



Criterion	Representative Exposure	Upper Bound Exposure
MOE*	200	65
MOS**	237	71

\*MOE based on Sub-chronic Health Benchmark

\*\* MOS based on proposed Occupational Exposure Limit (OEL)

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## Aggregation of Exposures



- **Infants and Children:**  
Highest exposure is in the home and it was assumed 100% of time was spent at home so aggregation not necessary.
- **Prospective parents:**  
A refueler returning home from work to a freshly painted house would receive a 10 to 20% additional dose for a few days at most.
- **Nursing infants of occupationally exposed mothers:** No data to calculate dose in milk

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## Aggregation of Infant Exposure



Receptor/Pathway	Representative MOE	Upper Bound MOE
Infant Chronic in Home Inhalation	6,000	1,900
Infant/Drinking Water	> 40,000	40,000
Infant/Dermal	270,000	13,000
Infant/Mother's Milk	64,000	45,000
<b>Total MOE</b>	<b><u>≥4,700</u></b>	<b><u>1,500</u></b>

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## Aggregation of Infant Exposure



Receptor/Pathway	Representative MOE	Upper Bound MOE
Infant During Renovation*	2,000	275**
Infant/Drinking Water	> 40,000	40,000
Infant/Dermal	270,000	13,000
Infant/Mother's Milk	64,000	45,000
<b>Total MOE</b>	<b><u>&gt;1,800</u></b>	<b><u>266</u></b>

\* Sub-chronic/Acute Exposure

\*\* MOS =1

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## Risk Conclusions



### Chronic Exposure:

- MOE for children > 1,000
- MOS for children > 1

### Renovation (Painting):

- MOE >275 temporarily but, MOS >1

### Acute exposure [8 hr average]:

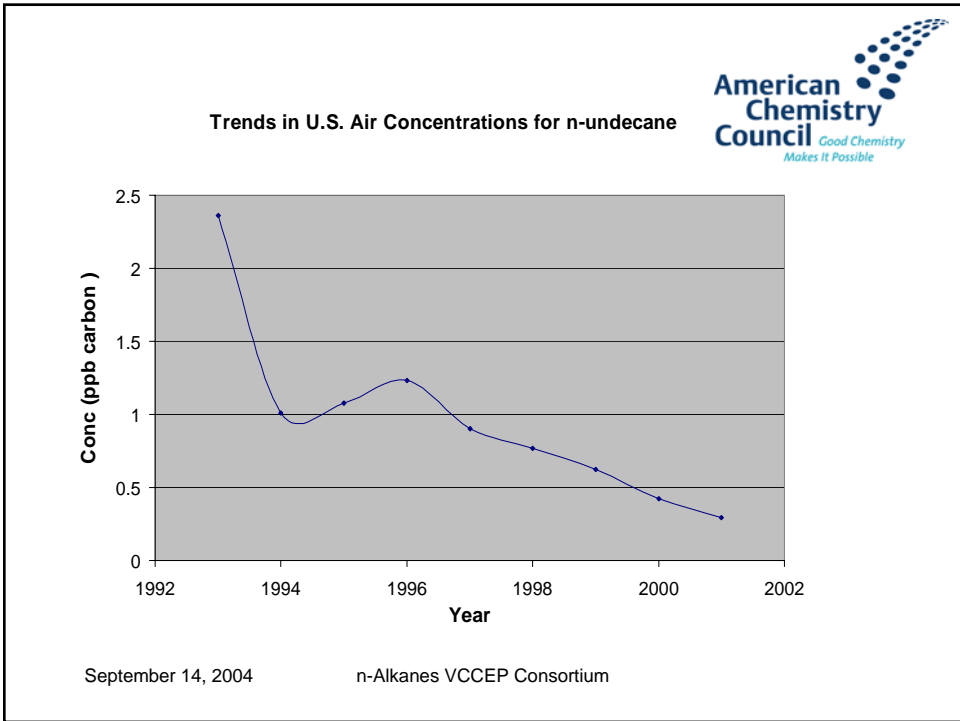
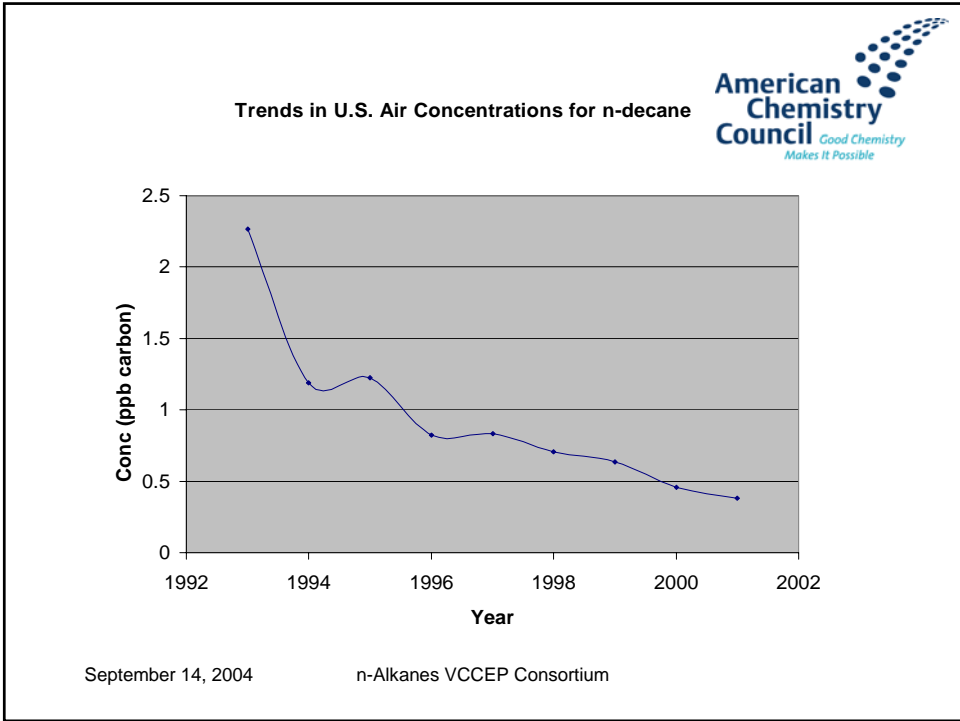
MOE for children > 150 (Sealed house painted)

### Occupational Exposure:

- MOE > 65
- MOS > 71

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# n-Alkane VCCEP Data Needs Assessment, Uncertainties and Conclusions

September 14, 2004

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## Hazard Data

- There are sufficient Tier 1 hazard data for the category.
- There is some information on Tier 2 and Tier 3 endpoints, including metabolism, in vivo genotoxicity, neurotoxicity and carcinogenicity.
- No data located on potential immunotoxicity or developmental neurotoxicity. However, there is no evidence or triggers that these are potential health hazards of n-alkanes.

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## Hazard Conclusions



- Low exposures and high MOEs do not indicate additional hazard studies are warranted
- No suggestion that children are more sensitive to any effects than adults
- There are already programs in place to examine the health hazards of complex hydrocarbon mixtures which are the major exposure sources for these alkanes:
  - jet and diesel fuel under the U.S. HPV Challenge program
  - jet fuels by the U.S. Air Force
  - hydrocarbon solvents in the OECD SIDS program

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## Exposure Conclusions-1



- Inhalation is the predominant route of exposure to these alkanes
- Ample peer-reviewed measurements of air concentrations in homes, schools, workplaces, automobiles, and outdoors exist for decane, undecane, and dodecane
- Low health risks exist for these materials based on large margins of exposure
- The vast majority of exposure to these materials occurs in combination with other components of hydrocarbon solvents and fuels, not as the individual alkanes
- No further exposure studies are warranted for these n-alkanes

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## Exposure Conclusions-2



- Uncertainty: Reported exposure levels may have included iso-alkanes and cyclic isomers in addition to the normal alkanes, and overestimated actual exposure levels
- No reliable data on human milk levels for occupationally exposed mothers. Non-occupational levels are very low, below detection limits, with MOEs (>100,000) suggesting that this would not likely be a significant exposure source even for children of occupationally exposed mothers.

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**Appendix E**  
**Sponsors' Errata Sheet**

American Chemistry Council  
n-Alkane VCCEP Consortium

Errata and Clarifications to n-Alkane Category:  
Decane, Undecane, Dodecane  
(CAS Nos. 124-18-5, 1120-21-4, 112-40-3)  
Voluntary Children's Chemical Evaluation Program (VCCEP)  
Tier 1 Pilot Submission  
Docket Number OPPTS – 00274D

September 9, 2004

The following are corrections or clarifications to the text of the June 17, 2004, Tier 1 VCCEP submission for decane, undecane, and dodecane.

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Page 8: last sentence:

replace:

**"Reproductive/developmental NOAELs of 5g/m<sup>3</sup>, 300 mg/kg/day and 1,000 mg/kg/day (equivalent to approximately 2 g/m<sup>3</sup> and 7 g/m<sup>3</sup>, respectively) were identified. Since all of these values were larger than the subchronic NOAEL, no further risk assessment was conducted for reproductive or developmental effects."**

with:

"The developmental NOAEL is 5000 mg/m<sup>3</sup> and oral reproductive NOAELs are 1000 mg/kg/day for decane and 300 mg/kg/day for undecane; inhalation equivalents of about 7000 mg/m<sup>3</sup> and 2000 mg/m<sup>3</sup>, respectively. Thus, the overall NOAEL for reproductive/developmental effects is in the inhalation equivalent range of 2000 - 7000 mg/m<sup>3</sup>. As these NOAELs are in the same range of the systemic NOAEL of 1000 mg/m<sup>3</sup>, reproductive/developmental effects were not found to be more sensitive than systemic toxicity."

---

**page 9: 1<sup>st</sup> paragraph; clarification**

Replace

"Primary exposure of infants and children was in the home. In every domestic scenario relevant to infants, children and parents, including home renovation activities, Margins of Exposure (MOE) based on the subchronic NOAEL were comfortably in excess of 1,000 for both representative and upper bound exposures. Worst case short term exposure based on modeling a home painting scenario was comfortably in excess of 100 for a short term (days), increasing rapidly to greater than 1,000 despite very

conservative exposure assumptions. This suggests a low risk of harm to infants, children or parents."

with:

"Primary exposure of infants and children was in the home. In the chronic domestic scenario relevant to infants, children and parents, Margins of Exposure (MOE) based on the subchronic NOAEL were comfortably in excess of 1,000 for both representative and upper bound exposures. For short-term renovation activities (painting), MOEs based on the same subchronic NOAEL ranged from 2,000 for representative exposures to 275 for upper bound exposure. Considering such exposures would be of short duration, an MOE greater than 100 based on a subchronic NOAEL was considered protective. This is supported by the fact that the Margin of Safety (MOS) based on the chronic RfC was greater than 1.

Even worst case short term exposure concentrations based on EPA measurements in a home painting scenario with the infant in the room being painted, and with no ventilation other than 0.45 air changes per hour, was comfortably below the acute health criteria, and the subchronic based MOE exceeded 100 within 2 days, increasing rapidly to in excess of 1,000 despite the lack of additional ventilation. This suggests a low risk of harm to infants, children or parents."

---

**page 15, Section 3.2, 3<sup>rd</sup> paragraph;**

replace: "C<sub>10</sub>-C<sub>12</sub> aliphatic fraction"

with: "C<sub>9</sub>-C<sub>16</sub> aliphatic fraction"

**Clarification regarding Total Petroleum Hydrocarbon Criteria Working Group (TPHCWG) C<sub>9</sub>-C<sub>16</sub> aliphatic fraction RfC**

The calculation of the RfC for C<sub>9</sub>-C<sub>16</sub> aliphatic fraction is provided in the TPHCWG 1997 document on pages 21- 24. In deriving the RfC, the TPHCWG considered three subchronic rat studies and two developmental studies on complex aliphatic hydrocarbon products in this range (summarized in Table 5 of the TPHCWG document on page 22). The subchronic data considered for the RfC included: 1) a 12-week inhalation study (6 hr/day, 5 days/wk) of a C<sub>10</sub>-C<sub>11</sub> isoparaffin product with a NOAEL of 5226 mg/m<sup>3</sup> (Mullin, 1990), 2) a 12-week inhalation study (6 hrs/day 5 days/wk) of a C<sub>7</sub>-C<sub>11</sub> aliphatic product (n-alkanes, isoparaffins, and cycloparaffins) with a NOAEL of 5485 mg/m<sup>3</sup> (Phillips and Egan, 1984), and, 3) a 90-day continuous inhalation study of JP-8 with a NOAEL of 1000 mg/m<sup>3</sup> (Mattie, 1991). The developmental data were not used in deriving the RfC, but the NOAELs are 5226 mg/m<sup>3</sup> for the C<sub>10</sub>-C<sub>11</sub> isoparaffin product (Mullin, 1990) and 5485 mg/m<sup>3</sup> for the C<sub>7</sub>-C<sub>11</sub> aliphatic product (unpublished). The TPHCWG derived RfCs for each of these studies separately by converting to a continuous exposure, except for the Mattie 1991 study which was a continuous exposure study, and then dividing the

adjusted NOAELs by a total uncertainty factor of 1000. This total uncertainty factor was based on a subchronic to chronic uncertainty factor of 10, an uncertainty factor of 10 for interspecies extrapolation (animal to human), and an human intraspecies uncertainty factor of 10. For each study considered, the resulting RfC was approximately 1 mg/m<sup>3</sup>, forming the basis for the TPHCWG's recommended RfC of 1.0 mg/m<sup>3</sup>.

The TPHCWG RfC was used in the Risk Assessment (Section 8) derivations of chronic and short-term Margins of Safety (MOS), providing secondary support for the calculation of Margins of Exposure based the health benchmarks developed by the Consortium for C<sub>10</sub>-C<sub>12</sub> n-alkanes.

The data from the Phillips and Egan 1984 subchronic study and the unpublished developmental toxicity study of the C<sub>7</sub>-C<sub>11</sub> aliphatic product were considered in the VCCEP submission (Section 7). The data from the Mullin 1990 studies were not considered as they are specific to isoparaffins (no n-alkane content) and data from the Mattie study as not considered as no toxicology data on fuels were considered due to their wider range and aromatic content.

The published studies cited in the TPHCWG document were:

Phillips RD, Egan GF Subchronic inhalation exposure of dearomatized white spirit and C10-C11 isoparaffinic hydrocarbon in Sprague-Dawley rats. *Fundam Appl Toxicol.* 1984 Oct;4(5):808-18.

Mullin LS, Ader AW, Daughtrey WC, Frost DZ, Greenwood MR. Toxicology update isoparaffinic hydrocarbons: a summary of physical properties, toxicity studies and human exposure data. *J Appl Toxicol.* 1990 Apr;10(2):135-42.

Mattie DR, Alden CL, Newell TK, Gaworski CL, Flemming CD. A 90-day continuous vapor inhalation toxicity study of JP-8 jet fuel followed by 20 or 21 months of recovery in Fischer 344 rats and C57BL/6 mice. *Toxicol Pathol.* 1991;19(2):77-87.

-----  
**page 34:** last paragraph,

"These compare with a subchronic NOAEL of 1,000 mg/kg/day (see 7.3. Repeat Dose Toxicity: Health Benchmark) indicating Margin of Exposure in excess of 150,000."

Replace with:

"These compare with a reproductive/developmental NOAEL of 300 mg/kg/day (see section 7.4) indicating Margin of Exposure in excess of 45,000"  
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**page 35**

Table 6.3 "1. Representative Intake":  
Replace the line

"MOE*	Margin of Exposure	213,000"
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with:

"MOE*	Margin of Exposure	64,000"
-------	--------------------	---------

Table 6.3 "Upper Bound Intake":

Replace the line

"MOE*	Margin of Exposure	150,000"
-------	--------------------	----------

with:

"MOE*	Margin of Exposure	45,000"
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Replace the line:

"\*MOE based on subchronic NOAEL of 1,000 mg/kg/d (section 7.10.2)"

with:

"\*MOE based on reproductive/developmental NOAEL of 300 mg/kg/d (section 7.4)"

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## page 41

Replace the paragraph:

"Assuming even an unrealistic 25% n-dodecane content in the fuel, the dose per accidental exposure amounts to only  $8.2 \times 10^{-3}$  mg/kg and a chronic exposure of  $1.1 \times 10^{-3}$  mg/kg/day assuming 50 days per year of such incidents. These are essentially negligible doses compared with repeat dose subchronic oral NOAELs of 1,000 mg/kg/day and only 1% of the chronic RfD of 0.1 mg/kg/day. Margins of Exposure were in excess of 88,000 on a chronic basis for a fuel containing up to 25% of decane, undecane, and dodecane."

with:

"Assuming even an unrealistic 25% n-dodecane content in the fuel, the dose per accidental exposure amounts to only  $8.2 \times 10^{-3}$  mg/kg and a chronic exposure of  $1.1 \times 10^{-3}$  mg/kg/day assuming 50 days per year of such incidents. These are essentially negligible doses compared with repeat dose reproductive/developmental oral NOAELs

of 300 mg/kg/day and only 1% of the chronic RfD of 0.1 mg/kg/day. Margins of Exposure were in excess of 270,000 on a chronic basis for a fuel containing up to 25% of decane, undecane, and dodecane."

Replace the paragraph:

"Applying an even more conservative scenario by assuming 1 hour exposure per day to both hands on a daily basis (250 days per year), chronic margins of exposure still exceeded 4,000 as shown in Table 6.4 below."

with

"Applying an even more conservative scenario by assuming 1 hour exposure per day to both hands on a daily basis (250 days per year), chronic margins of exposure still exceeded 13,000 as shown in Table 6.4 below."

In Table 6.4:

1. Exposure Duration 15 minutes/day; 50 days/year

replace the lines:

"Sub-chronic NOAEL	100		mg/kg/d
MOE Per Event	3040	60800	12160
MOE Chronic	22192	443839	88768"

with:

"Sub-chronic NOAEL	300		mg/kg/d
MOE Per Event	9120	182399	36480
MOE Chronic	66576	1331516	266303"

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**page 42**

In Table 6.4:

2. Exposure Duration 60 minutes/day; 250 days/year

replace the lines:

"Sub-chronic NOAEL	100			mg/kg/d
MOE Per Event	760	15200	3040	
MOE Chronic	1110	22192	4438"	

with:

"Sub-chronic NOAEL	300			mg/kg/d
MOE Per Event	2280	45600	9120	
MOE Chronic	3329	66576	13315"	

Replace the third paragraph:

"The daily dose of such a contaminated water supply would result in dose of  $6.8 \times 10^{-3}$  mg/kg/day of n-decane and  $4.8 \times 10^{-4}$  mg/kg/day n-dodecane. Such intakes, unrealistic as they are, provide Margin of Exposure of about 150,000 based on the subchronic NOAEL of 1,000 mg/kg/day."

with:

"The daily dose of such a contaminated water supply would result in dose of  $6.8 \times 10^{-3}$  mg/kg/day of n-decane,  $5.7 \times 10^{-4}$  mg/kg/day n-undecane, and  $4.8 \times 10^{-4}$  mg/kg/day for n-dodecane. Such intakes, unrealistic as they are, provide Margin of Exposure of over 40,000 based on the reproductive/developmental NOAEL of 300 mg/kg/day."

---

**page 48**

replace: "MacFarland and Holdsworth 1987"

with: "Snyder, 1987"

Note: this is not a change in reference. MacFarland and Holdsworth were contributing authors to Ethel Browning's Toxicology and Metabolism of Industrial Solvents, Second Edition but the citation in the reference section is to Snyder, the editor.

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**page 49**

under Dermal:

Second sentence:

replace: "EMBSI 1983a,b"

with: "EMBSI 1983d,e"

Third sentence:

replace: "EMBSI 1983a"

with: "EMBSI 1983d"

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**page 55**

replace: "Carpenter, 1975"

with: "Carpenter, 1978"

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**page 58**

under Mutagenicity:

add: "c" after EMBSI, 1991

under Cytogenicity:

add "d" after EMBSI 1991

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**page 60**

replace: "Lammers et al, 2000"

with: "TNO, 2000"

Note: this is not a change in reference, Lammers was one of the authors of the TNO study but the citation in the reference section is to TNO.

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**page 75, 2<sup>nd</sup> full paragraph**

remove: "(See Appendix I)"

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**page 88-96, Reference Section**

The following references should be added to the reference section:

Barnes DG, Dourson M. Reference dose (RfD): description and use in health risk assessments. *Regul Toxicol Pharmacol*. 1988 Dec;8(4):471-86.

Bingham E, Falk HL. Environmental carcinogens. The modifying effect of cocarcinogens on the threshold response. *Arch Environ Health*. 1969 Dec;19(6):779-83.

Collins JF, Salmon AG, Budroe JD, Marty MA and Alexeeff. Available toxicity data on alternative dry cleaning chemicals. Abstract #1789 presented at the 2004 SOT meeting.

\*ExxonMobil Biomedical Sciences, Inc. 1978. A Segment II Teratology Study in Rats Following Inhalation Exposure. Study No. 77-1567. (Unpublished report – robust summary provided in Appendix B.)

ExxonMobil Biomedical Sciences, Inc. 1983a. Acute Oral Toxicity Study in the Rat. Study No. 320501. (Unpublished report – robust summary provided in Appendix B.)

ExxonMobil Biomedical Sciences, Inc. 1983b. Acute Oral Toxicity Study in the Rat. Study No. 320701. (Unpublished report – robust summary provided in Appendix B.)

ExxonMobil Biomedical Sciences, Inc. 1983c. Acute Oral Toxicity Study in the Rat. Study No. 320601A. (Unpublished report – robust summary provided in Appendix B.)

ExxonMobil Biomedical Sciences, Inc. 1983d. Acute Dermal Toxicity Study in the Rabbit. Study No. 320506. (Unpublished report – robust summary provided in Appendix B.)

ExxonMobil Biomedical Sciences. 1983e. Acute Dermal Toxicity Study in the Rabbit. Study No. 320706. (Unpublished report – robust summary provided in Appendix B.)

ExxonMobil Biomedical Sciences, Inc. 1991c. Microbial Mutagenesis in Salmonella Mammalian Microsome Incorporation Assay, Study No. 187425. (Unpublished report – robust summary provided in Appendix B.)

ExxonMobil Biomedical Sciences, Inc. 1991d. In vivo Mammalian Bone Marrow Micronucleus Assay. Study No. 187430. (Unpublished report – robust summary provided in Appendix B.)

ExxonMobil Biomedical Sciences, Inc. 1994. Acute Dermal Toxicity Study in the Rabbit. Study No. 140506C. (Unpublished report – robust summary provided in Appendix B.)

Krause, C Chutsch, M, et al, 1991; Umwelt-Survey band IIIc:Wohn-Innerraum: Raumluft (Living spaces:indoor air). WaBoLu-Hefte 4/1991. Institute for Water, Soil and Air Hygiene of the Federal Health Office, Berlin.

LeBret, E Van de Wiel, HJ et al, 1986. Volatile organic compounds in Dutch homes. Environ. Int. 12:2323-332

Petroquimia Espanola S.A. (PETRESA). 1984. Acute Oral Toxicity to Rats of PETREPAR® n-C14. (Unpublished report – robust summary provided in Appendix B.)

Sasol Italy. 1994. Study of the Capacity of the Test Article LINPAR® 10 to Induce Chromosome Aberrations in V79 Chinese Hamster Lung cells.

USEPA, 1986; Exposure Factors Handbook: Volume I - General Factors - EPA/600/P-95/002Ba, Volume II - Food Ingestion Factors - EPA/600-P-95/002Bb, Volume III - Activity Factors - EPA/600/P-95-002Bc

USEPA, 2002; Child-specific Exposure Factors Handbook EPA-600-P-00-002B Interim Report

Wallace, LA, Pellizzari, ED, Hartwell, TD, Sparacino, C, Whitmore, R, Sheldon, L, Zelo, H, Perritt, R (1987). The TEAM study: Personal exposures to toxic substances in air, drinking water and breath of 400 residents of New Jersey, North Carolina, and North Dakota. Environmental Research 43:290-307.

W.H.O., 1989: Indoor Air Quality: Organic Pollutants, Copenhagen, WHO Regional Office for Europe. (EURO Reports and Studies III)

Yoshimura et al., 1996. Ministry of Health and Welfare, Japan, 1996. Single Dose Oral Toxicity Test of Undecane in Rats. Toxicity City Testing Reports of Environmental Chemicals, Vol. 4, 578-614. (Robust summary provided in Appendix B.)

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## **Page 90, Reference Section**

Insert “a” after 1991 in first ExxonMobil Biomedical Sciences, Inc. reference.

Insert “b” after 1991 in second ExxonMobil Biomedical Sciences, Inc. reference.

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**page F-5**

Table F-1

1. Representative Intake:

replace the line :

"MOE\*                      Margin of Exposure                      213,000"

with:

"MOE\*                      Margin of Exposure                      64,000"

2. Upper Bound Intake:

replace the line :

"MOE\*                      Margin of Exposure                      150,000"

with:

"MOE\*                      Margin of Exposure                      45,000"

replace the line:

"\*MOE based on subchronic NOAEL of 1,000 mg/kg/d"

with:

"\*MOE based on reproductive/Developmental NOAEL of 300 mg/kg/d"