2 Pollution Prevention, Risk Assessment and Sustainable Futures

2.1 Pollution Prevention and the Risk Assessment Process

2.1.1 What Is Pollution Prevention (P2)?

Pollution Prevention (P2) is the common sense understanding that it is easier and expensive to prevent problems than to correct them. Pollution prevention is reducing or eliminating waste at the source by promoting the use of non-toxic or less-toxic substances, modifying production processes, implementing conservation techniques, and re-using materials rather than discarding them. Congress, by enacting the Pollution Prevention Act of 1990 (42 U.S.C. 13101 and13102, s/s et seq.), created a bold national objective for environmental protection by outlining a hierarchy in dealing with pollution:

- Pollution should be prevented or reduced at the source whenever feasible;
- Pollution that cannot be prevented should be recycled in an environmentally safe manner whenever feasible;
- Pollution that cannot be prevented or recycled should be treated in an environmentally safe manner whenever feasible; and
- Disposal or other releases into the environment should be employed only as a last resort and should be conducted in an environmentally safe manner.

Pollution prevention means "source reduction," as defined under the Pollution Prevention Act. The Pollution Prevention Act defines "source reduction" to mean any practice which:

- Reduces the amount of any hazardous substance, pollutant, or contaminant entering any waste stream or otherwise released into the environment prior to recycling, treatment, or disposal; and
- Reduces the hazards to public health and the environment associated with the release of such substances, pollutants, or contaminants.

Source reduction can be achieved through equipment or technology modifications, processes or procedure modification, reformulation or redesign of products, substitution of materials, etc.

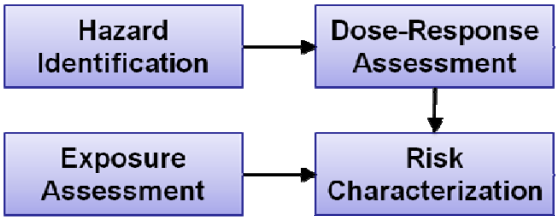
2.1.2 The Risk Assessment Process

In 1983, the National Academy of Sciences developed a paradigm describing risk assessment and risk management*:

- **Hazard (Toxicity) Identification** – Determining if a particular chemical is or is not causally links to particular health effects (for example, could it increase cancer cases, birth defects, or kill fish); **An important part of the Hazard Identification step is Dose-Response Assessment** – Determining the relation between the magnitude of exposure and the probability of occurrence of the toxicity / hazard effects of concern, also referred to as Hazard Characterization. This is the step at which effects levels like No Observable Adverse Effect Levels (NOAELs) and Lowest Observable Adverse Effect Levels (LOAELs) are determined;
- **Exposure Assessment** – Determining the extent (magnitude, frequency, and duration) of exposure before or after application of regulatory controls; and
- **Risk Characterization** – Determining the potential for, and magnitude of, risk to an exposed individual or population nature, including accompanying uncertainty.

The components of the risk assessment process are illustrated in the figure below.

The Risk Assessment Paradigm*



*NRC. 1983. Risk Assessment in the Federal Government: Managing the Process. National Research Council. National Academy Press, Washington, DC. ISBN: 0-309-03349-7. http://www.nap.edu/books/0309033497/html

2.2 The Pollution Prevention (P2) Framework

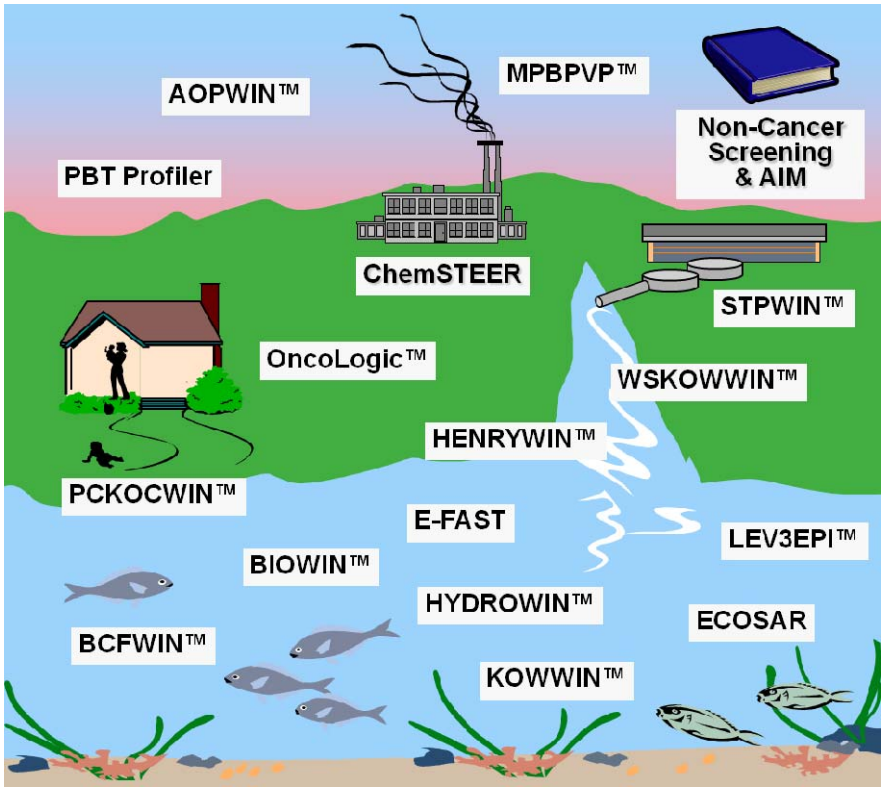
Methods included in the P2 Framework are intended to provide screening level information to help in assessing potential risk posed by a chemical or group of chemicals. Screening level information should never be used instead of experimental data from properly conduced laboratory studies, but can be used to prioritize chemicals and identify those needing additional review.

2.2.1 The P2 Framework Methods Provide Information in Four Areas

The P2 Framework methods provide information in the following four areas:

1. Physical/Chemical Properties
2. Chemical Fate in the Environment
3. Hazard to Humans and the Environment
4. Exposure and/or Risk

2.2.2 A "Road Map" to the P2 Framework Methods



The P2 Framework methods described in this document are listed below, and shown in the following illustration. The illustration can be used as an informal "road map" to approximate the endpoints the model addresses and help decide which models you might wish to use.

PHYSICAL/CHEMICAL PROPERTY MODELS (integrated into EPISuite™):

- MPBPWIN™ - Estimates Melting Point, Boiling Point, and Vapor Pressure of a chemical
- KOWWIN™ - Estimates KOW or octanol-water partition coefficient, which describes partitioning between octanol (which represents lipids, or body fat of biota) and water
- WSKOWWIN™ - Estimates KOW, octanol-water partition coefficient, and water solubility
- HENRYWIN™ - Calculates partitioning between air and water (Henry's Law constant)

ENVIRONMENTAL FATE MODELS (integrated into EPISuite™):

- AOPWIN™ - Estimates Atmospheric Oxidation Potential, or breakdown in air
- HYDROWIN™ - Estimates hydrolysis, or the breakdown of a chemical in water bodies
- BIOWIN™ - Estimates biodegradation of chemicals in the presence of oxygen
- PCKOCWIN™ - Estimates KOC, or adsorption of a chemical to the organic carbon portion of soil and sediment
- BCFWIN™ - Calculates the fish BioConcentration Factor
- STPWIN™ - Predicts the removal of a chemical in a Sewage Treatment Plant
- LEV3EPI™ - Level 3 fugacity model that predicts partitioning of chemicals between air, soil, sediment, and water

HAZARD MODELS:

- OncoLogic™ - Estimates the potential for a chemical to cause cancer in humans
- Non-Cancer Screening - A stepwise process, not computerized, to screen chemicals for non-cancer health effects
- Analog Identification Methodology (AIM): Identifies analogous chemicals with available measured data
- ECOSAR - Predicts a chemical's toxicity to aquatic biota

P, B, T POTENTIAL:

- PBT Profiler - Screens chemicals for potential to persist, bioaccumulate, and be toxic

EXPOSURE and/or RISK MODELS:

- E-FAST - Estimates chemical releases and dose rates to humans from these releases
- ChemSTEER - Estimates environmental releases and worker exposures resulting from chemical manufacture, processing, and/or use in industrial and commercial workplaces

2.3 How EPA Uses These Models and Methods

The predictive methods that OPPT scientists developed to screen new chemicals include computational toxicology and expert systems, among other approaches. Endpoints addressed include physical/chemical properties, environmental fate, cancer hazard, aquatic toxicity, exposure, and risk. In the years since TSCA was implemented OPPT has received a wealth of Confidential Business Information (CBI) data on tens of thousands of chemicals covering the vast range of chemistry. Whenever possible, CBI knowledge from PMN submissions is used to develop SARs. The SARs themselves are not CBI and can be released to the public. An example is the model ECOSAR which contains numerous SARs developed with CBI data. The calculations comprising the SARs are provided in the "help" screens within ECOSAR. This component of "transferring the technology" and using CBI data to develop publicly-available methods are two of the greatest values provided by Sustainable Futures.

While OPPT scientists do use these models to screen PMNs, they have access to additional information that cannot be made public. Examples include previous analogous cases and their own scientific judgment.

2.4 Sustainable Futures

2.4.1 What is Sustainable Futures?

P2 Framework Outreach

OPPT wanted to learn if its predictive screening level tools could be transferred to industry and if these methods could be used early in Research and Development (R&D) to provide risk-related information on PMN candidate chemicals and processes. While EPA sees approximately 2,000 PMNs per year, industry has made thousands of other decisions early in R&D, long before they submit the PMN. By the time the company decides on a specific chemical or process and submits the PMN to EPA, many of the P2 opportunities have been lost.

In 1995 OPPT began to work with the chemical industry to help transfer the chemical screening methods to developers of new chemicals and new chemical products. OPPT developed P2 Partnerships with many industry sectors to help them explore the application of the P2 Framework methods to their design and chemical management practices.

P2 Framework-based XL Projects

Eastman Kodak and PPG Industries both applied the P2 Framework methods to their chemicals of interest. Based on their experiences, both companies proposed P2 Framework-based XL Projects. Project XL http://www.epa.gov/projectxl/ (eXellence and Leadership) was a voluntary national program in

which EPA offered some flexibility in its regulations to encourage companies, communities and other project participants to develop and test cleaner, cheaper and smarter alternatives that could produce superior environmental results beyond those that would have been achieved under current regulations and policies. Both companies used the P2 Framework methods during the early stages of product development, allowing them to improve the environmental performance of products while reducing costs, saving time, enhancing competitive advantage and decreasing potential liability.

Under their XL Project, PPG verified the accuracy of the P2 Framework by comparing aquatic toxicity data on 38 polymers with estimates from the P2 Framework with agreement between the two being 87-90% (Citation: Chun, J.S., Nabholz, J.V., & Wilson, M.J. (2000). Comparison of aquatic toxicity experimental data with EPA/OPPT/SAR prediction on PPG polymers. Pittsburgh, PA, and Washington, DC: PPG Industries and EPA Office of Prevention, Pesticides and Toxic Substances.)

Kodak conducted an analysis of the economic and business benefits of application of the P2 Framework, and found that using the P2 Framework helped identify environmentally preferable products, lowered product development costs, reduced time to market and lowered fullscale manufacturing costs. The Kodak experience was published by the Tellus Institute (Citation: Votta, T.J., & White, A.L. (1999). Design for competitive advantage: The business benefits of the-EPA pollution-prevention assessment framework in new product development. Boston: The Tellus Institute.) Both of these reports are available on the Sustainable Futures web site at http://www.epa.gov/oppt/sf/pubs/index.htm#case.

Sustainable Futures Pilot Project

Sustainable Futures www.epa.gov/oppt/sf evolved directly out of the successful P2 Framework-based XL Projects. EPA selected both XL Projects to be "scaled-up" and offered nationwide. As a result, since 2002 when the Sustainable Futures Initiative was launched, any company can become eligible for expedited Pre-manufacture Notice (PMN) which was previously only available to participants in Project XL.

OPPT published a Federal Register notice announcing the voluntary Sustainable Futures Initiative on December 11, 2002. The FR notice is available at http://www.epa.gov/fedrgstr/EPA-TOX/2002/December/Day-11/t31243.pdf.

The intention of Sustainable Futures is to offer the chemical industry and other stakeholders an integrated path to safer chemical products and processes. Sustainable Futures includes: (1) comprehensive P2 Framework hands-on training, and (2) specialized technical assistance within each industry sector.

Incentives

The regulatory flexibility available to companies that graduate from Sustainable Futures allows them to submit prescreened new chemical notices that are considered a PreManufacture Notice AND a Test Manufacturing Exemption application. The new chemical that is the subject of these combined notices, once dropped from further review, can be manufactured in 45-days under the terms of the TME, rather than the 90-day time-period under the PMN. This is a powerful incentive for many companies. In addition to getting to market sooner, regulatory uncertainty is greatly reduced because the P2 Framework helps anticipate, and engineer away from, chemicals of concern. This is Pollution Prevention in its purest form.

Industry response to Sustainable Futures has been positive. Hundreds of individuals representing chemical companies and other stakeholders have taken Sustainable Futures hands-on training. EPA has

seen an increase in the percentage of PMNs submitted containing predictions from Sustainable Futures chemical risk screening methods.

Benefits

Sustainable Futures is helping EPA realize a goal of making their predictive models and methods publicly available and promoting transparency in screening processes. Another major benefit to EPA is capturing and transferring a wealth of chemical knowledge and state-of-the art predictive technology to the general public to promote pollution prevention and chemical safety.

Participants in Sustainable Futures have reported the following benefits

- Assist in chemical R&D and stakeholder business planning;
- Identify potential concerns allowing for development of safer chemicals;
- Help prioritize limited resources;
- Identify chemical substitution opportunities;
- Identify pathways for risk-based testing strategies;
- Increase Pollution Prevention (P2) opportunities;
- Increase opportunities for innovation;
- Focus initial hazard testing to area of greatest concern or uncertainty versus conducting base set testing for all chemicals, even those posing low hazard concerns;
- Limit testing for chemicals where exposure is expected to be minimal or limited; and
- Reduce generation of chemical waste.

Avoiding problem chemicals and the potential high costs associated with those chemicals, sometimes called chemicals "left on the cutting room floor," may well be the source of the greatest cost savings to companies participating in Sustainable Futures. The ultimate identification and commercialization of safer chemicals benefits the participant, as well as the general public and the environment.

The Risk Standard Is Not Lowered

OPPT continues to conduct an independent risk evaluation of each PMN submitted, and those that EPA finds to be low hazard/low risk can qualify for relief once the submitting company has graduated from Sustainable Futures. EPA makes this determination in the first 30 days of the 90-day review period. Chemicals that do not make the low hazard/low risk cut in the first 30 days won't qualify for relief. As a result, there will be no lowering of the risk standard.

2.4.2 How Companies Can Graduate from SF and Qualify for Regulatory Relief

EPA provides hands-on training in the proper use and application of OPPT's P2 Framework models and methods in the Sustainable Futures training workshops. Participants in the 2- or 3-day training sessions each receive a workbook and CD with copies of the methods, workshop materials, and background documents. Participants are walked through a complete risk assessment using sample chemicals, and shown how to record the model results in a worksheet (discussed below). Training opportunities are announced on the SF web site at http://www.epa.gov/oppt/sf/meetings/train.htm#how.

Here are the steps participants representing companies must go through to graduate from Sustainable Futures and qualify for regulatory relief of subsequent prescreened low hazard, low risk new chemical notices.

Four Steps to Graduation

Step 1: Take Training
Step 2: Use Screening Models
Step 3: Submit Sustainable Futures PMNs
Step 4: Notify EPA

Step 1: Take Sustainable Futures Training

Take training to become competent in the proper use of chemical risk screening models. Participants must take training to understand the Sustainable Futures Initiative and acquire an understanding of the scope, applicability, interpretation, and limitations of chemical hazard, exposure, and risk screening tools that can be used to conduct screening level assessments on chemicals based on an analysis of chemical structure or other considerations. Sustainable Futures Partners are offering fee-for-service training in proper use of the Sustainable Futures models. Get information on available training sessions or arrange to host a session.

Step 2: Use Screening Models to Develop PMNs

Use chemical- risk screening models, such as the Sustainable Futures / P2 Framework models to develop new chemical notices. Participants must apply hazard and exposure screening models, where appropriate, to gain hazard-, exposure-, and risk-related information on alternative chemicals or processes under consideration in the research and development and product development stages (i.e., before submission of a PMN). Use of chemical risk-screening models and methods other than the Sustainable Futures / P2 Framework models is also acceptable.

Step 3: Submit Sustainable Futures PMNs

Submit five Sustainable Futures PMNs that have the information requested (listed below) and that are not regulated by EPA. PMNs that are acceptable and not regulated will count towards graduation. An example of a Sustainable Futures PMN has been developed using the chemical isodecyl acrylate (CAS 1330-61-6) to show the kinds of information that should be included in the submission. The Sustainable Futures PMN is presented in chapter 14 of this document. This example is for illustration only and is intended to show the type of information that will indicate to EPA how the use of the screening models informed the submitter's judgment in development of the PMN.

Sustainable Futures submissions should include:

- Cover letter stating that the notice is being submitted under Sustainable Futures (see the cover letter example in the SF PMN in Appendix H);
- A low-hazard, low-risk chemical substance;
- Evidence showing the chemical was prescreened and evaluated using chemical risk screening models. Acceptable examples are:
  - model outputs;
  - SF Summary Assessment worksheet (see Appendix H); or
  - SF Chemical Hazard - Risk Screening Single Page Information Sheet (also included in Appendix H).
- Summaries of potential hazard, exposure, and risk associated with the PMN chemical; and
- Submitter's impressions of the usefulness of the information provided by the screening models in the development of the PMN chemical.

The Sustainable Futures Summary Assessment Worksheet that is used during Sustainable Futures hands-on training is offered as a suggestion on what to include in a SF PMN – it is not required. Types of data and screening assessments included in notices submitted under Sustainable Futures will vary.

Step 4: Notify EPA of Eligibility

Once your company representative has completed the training, learned how to use the models and methods to develop at least five unregulated PMNs your company is ready to graduate. Write to EPA to let us know your company is ready to graduate and become eligible for Expedited Review of subsequent prescreened low hazard, low risk PMNs.

As explained in the Federal Register Notice announcing the Sustainable Futures Initiative participants should write to the director of OPPT's Chemical Control Division (address below) and provide the following non-CBI documentation:

- The date(s) your company scientists completed Sustainable Futures training;
- List of the Sustainable Futures PMNs your company submitted and the outcome of EPA's review, i.e., that the chemicals were not regulated;
- Summary listing of the hazard and exposure screening tools used to evaluate each PMN substance; and
- Overall assessment of the value of the use of hazard and exposure screening tools to evaluate the PMN substances submitted.

Mail the information listed above to:

Director, Chemical Control Division (7405M)
U.S. Environmental Protection Agency
1200 Pennsylvania Ave, NW
Washington, DC 20460

Please also email a PDF of the original graduation request to:

Bill Waugh, 202-564-7657, waugh.bill@epa.gov
Kelly Mayo, 202-564-7662, mayo.kelly@epa.gov or
Maggie Johnson, 202-564-8924 johnson.maggie@epa.gov

EPA staff will then review and verify the information your company submitted. The decision to allow your company to graduate from Sustainable Futures will be presented to the OPPT Division Directors for their approval and you will be notified that your company has graduated and can join the list of companies that are SF Graduates, including:

- PPG Industries
- Eastman Kodak, Inc.
- Cytec Industries, Inc.
- Clariant Corporation
- International Flavors and Fragrances, Inc.
- NALCO, an Ecolab Company
- Chevron Phillips Chemical Company
- Cabot Corporation

Sustainable Futures Graduates Can Take Advantage of Expedited Review

Companies that have met the requirements and graduated from Sustainable Futures can take advantage of the expedited review of their subsequent PreManufacture Notices (PMNs). As described in the Federal Register Notice announcing Sustainable Futures the expedited review is achieved by EPA allowing the submission to be considered *both* as a PMN and a Test Marketing Exemption (TME) Application. The

advantage of the simultaneous submission is that the case will be considered a TME and the submitter will be able to manufacture at day 45 instead of having to wait until the PMN 90 day review period ends. This in effect cuts the review time in half.

Create and Submit the PMN and the TME Using the ePMN Software

Under the electronic PMN system the Sustainable Futures Graduate will need to create and submit two separate notices, the PMN and the TME, as the combined Sustainable Futures submission. Using the electronic PMN submission system, the submitter should "create" the TME by doing the following:

1. copy the PMN file;
2. renaming the file;
3. open the new file in the e-PMN software;
4. make the changes needed to meet the requirements of a TME (note in the cover letter that your company is a graduate of Sustainable Futures and that your submission meets the requirements of a TME); PMN page 1 mark it as a TME, PMN page 7 change the production volume as needed, etc); and
5. finalize the submission and submit the TME.

Must Meet Requirements of a TME

The TME component of the combined submission must be a legitimate TME http://www.epa.gov/oppt/newchems/pubs/tmeranddbulletin.pdf. When the TME is submitted, the company must specify (1) the amount of material to be produced and distributed, (2) the number of potential customers to whom it is distributed, and (3) the time period of the test marketing must be specified to EPA in advance of distribution. EPA does not require a production volume or use limit regarding the TME, but the company will be held to the production volume they stated in the TME. Therefore, if you need to manufacture 1,000 pounds during the TME period for a specialty use, state this in the TME. Likewise, if you need to manufacture 1,000,000 pounds for a variety of specific consumer product uses, state that in the TME.

The status of PMNs is available on the New Chemicals Web site at http://www.epa.gov/oppt/newchems/tools/status1.htm.

We have developed draft language demonstrating the submission is a legitimate TME and you are free to model your cover letter after this note. You may modify the language in any way you think is appropriate. The language, included below, is posted on the SF Frequent Questions page at http://www.epa.gov/oppt/sf/pubs/faqs.htm.

Draft Language Demonstrating a Submission is a Legitimate TME

[The company] has developed this new chemical substance using the pollution prevention hierarchy as articulated in the Pollution Prevention Act of 1990 and EPA's Pollution Prevention Strategy (56 Federal Register 7849, February 26, 1991). In this Strategy, the Agency ranks source reduction as the first preference in methods of controlling chemical risks.

[The company] has addressed source reduction through the application of SAR and risk screening methodologies that comprise EPA's Pollution Prevention (P2) Framework. The P2 Framework is designed to evaluate potential chemical risk or hazards based on an analysis of chemical structure and other factors. This represents a unique approach to product development in the industrial chemical sector and constitutes a significant departure from standard practice in new product development.

Standard practice typically does not include P2, SAR, and other risk screening approaches in early product development. This approach to product development may result in the selection of a material to be commercialized that is different from a material which might have been selected based on more traditional approaches to product development (i.e., cost, efficacy, yield, performance, etc.).

The new chemical will be used as a component in a product. [The company] plans to test market the new chemical that was developed with this unique P2-based product development paradigm to ensure acceptability of the product in the marketplace. During the test marketing period, [the company] plans to do the following activities as part of an effort to evaluate the acceptability of the product based on the new chemical:

(COMPANIES WOULD LIST ACTIVITIES, HERE ARE SOME EXAMPLES)

- For a period of six months, [the company] will judge the marketability of a currently sold product which now uses a new isolated intermediate (the TME substance) in the manufacturing process for that existing product. The TME substance will be distributed and consumed by two Divisions within our company, but the final product's market will be unchanged.
- For a period of 45 days to one year, we will judge market acceptance of a "new and improved" general consumer coating that includes the TME material as a new component. Production is estimated at 150,000 kg and the TME substance will be distributed in this coating in commerce to a very large general consumer customer base.
- For a period of _____, we will judge market acceptance of a TME material used as a dye coupler in general photographic applications.
- The TME substance will be distributed in film to thousands of consumer photographic supply outlets . . . to judge the market acceptance of a TME material used in manufacturing adhesives for automotive glass.

As a result, we believe that this test marketing of the product developed using the P2 Framework satisfies the requirement to distinguish this test marketing activity from full-scale commercial production and research and development, as required under 40 CFR 720.38(b)(5).

2.5 Sustainable Futures Frequent Questions

Sustainable Futures participants often asked similar questions, and we have combined these into Frequent Questions and posted them on the SF web site at http://www.epa.gov/oppt/sf/pubs/faqs.htm). Most questions have dealt with training, participating in SF, graduation, how to submit combined SF PMNs. We are including the SF Frequent Questions in this Chapter for your information.

2.5.1 Training & Graduation

What qualifies as "taking training" for the purposes of graduation?
While EPA recognizes that there are many qualified groups that can offer training in these methods, we consider "taking training" as having attended one of the Sustainable Futures hands-on workshops given by, or cosponsored by the EPA Office of Pollution Prevention and Toxics. An important component of the Sustainable Futures training is gaining an understanding of the concepts, goals, and benefits of the Sustainable Futures Initiative, including the benefits of prescreening chemicals at the R&D stage.

Does an individual or company "graduate?"
The FR notice indicates that the Sustainable Futures Program is designed so “companies subject to… reporting requirements…. demonstrate experience and competence with the P2 Framework or other scientifically acceptable approaches to chemical risk screening…. Companies interested in participating in this pilot project must demonstrate an understanding of the scope, applicability, interpretation, and limitations of pollution prevention and chemical hazard and exposure screening tools...”. These excerpts emphasize that Sustainable Futures program graduation status is granted to the company, and not simply associated with intellectual property or select staff. In turn, if a trained individual moves to another company, "graduate" status remains with the company and does not travel with the person to his or her next company.

Can contractors or consultants obtain Sustainable Futures graduate status?
The FR notices emphasizes that Sustainable Futures program graduation status and associated regulatory incentives are given to companies who are subject to TSCA section 5 reporting requirements. Therefore, contractors and consultants who do not manufacture substances or are required to report under TSCA Section 5 are not able to “graduate” under the program. However, consultants and contractors can still derive a business benefit by attending training and understanding the graduation process since this information can be used to inform customers of the potential regulatory outcomes of their submissions and can be used to identify associated hazards and risks of particular chemistries along the development pathway.

If my company contractor takes training does that count as my company taking training?
No, a representative employed directly by the company, not a contractor, must take training before the company will be considered as having taken training. EPA wants a company employee to attend so that the company will understand the scope, applicability, and limitations of the Sustainable Futures risk screening methods and understand the programmatic and administrative issues associated with Sustainable Futures. It is then assumed that the employee of the company will then circulate the information and insights gained during the training class with his/her colleagues within the company.

If my company has a consultant do the prescreening on chemicals my company submits as PMNs, can those submissions count toward our total needed for graduation?
Yes, those submissions developed by a consultant or contractor can count towards graduation as long as the submissions meet other criteria for graduation. Remember that in order for a company to qualify for graduation a company employee must attend the training.

Do prescreened submissions count towards the five required PMN submissions if they were sent in before we took training?
Yes, prescreened submissions sent in prior to taking training will count towards graduation as long as the submission has been adequately screened, demonstrates an appropriate level of knowledge of the tools and assessment approaches, and is deemed “successful” by EPA.

Does a PMN that was dropped with a non-5(e) SNUR count towards graduation from Sustainable Futures?
EPA may consider a submission regulated with a non section 5(e) SNUR as “successful” and count that submission towards graduation on a case-by-case basis pending the review of cases after EPA receives the company’s graduation request. For notifications concerning substances regulated by a TSCA non-section 5(e) SNUR, the review must indicate EPA did not find that the submitter’s use may present an unreasonable risk to human health or the environment. It is important to note that EPA’s non-section 5(e) SNUR actions apply to potential new uses that are different from those uses identified in the original PMN

submission. A non-section 5(e) SNUR indicates that an additional evaluation would be required of any new uses of the chemical to determine whether exposures to, or releases of, that substance from the new use may result in an unreasonable risk to health or the environment.

Will Low Volume Exemptions (LVEs) count towards graduation from Sustainable Futures?
Yes, Low Volume Exemptions (LVEs) will count towards the total PMN submissions needed as long as they are prescreened and not regulated, and for a low volume exemption "not regulated" means it is granted by EPA.

When a company graduates will they get something in writing from EPA?
Yes, once a company graduates they will receive correspondence from EPA indicating that, by virtue of their participation in Sustainable Futures, and their use of risk screening tools, they can now submit a simultaneous TMEA and PMN. When the company submits a combined PMN/TMEA they should add to the submission cover letter that they have graduated from Sustainable Futures and are allowed to submit a combined PMN/TMEA.

2.5.2 SF Submissions

Why is EPA asking for my company's impressions of the usefulness of the methods?
As explained in the Federal Register Notice announcing the Sustainable Futures Initiative, EPA is considering creating a new Pollution Prevention (P2)-based exemption to TSCA that would make the regulatory relief currently available only to graduates of the Sustainable Futures Initiative available also to any company that prescreens a low hazard, low risk new chemical notice. In order to do this EPA needs to provide evidence that risk screening at R&D results in health and environmental benefits.

What should I include in the summary of the usefulness of the methods?
The summary does not need to be detailed. The summary can be a table or brief text that could be included in the cover letter, in the pollution prevention information on page 11 of the PMN form, or included as an attachment to the submission.

Do I need to run exposure models on a low hazard chemical?
During the period when a submitter is demonstrating their knowledge of the P2 Framework methods while working on their 5-10 successful submissions, the submitter needs to evaluate the full suite of risk assessment sections including exposure to gain experience in using the tools and characterizing the endpoints. Creating this exposure section may or may not require actually running the modeling tools. After a submitter has achieved graduation status and is completing the prescreening for the purposes of the dual TMEA/PMN submissions they may choose not to run the exposure tools on low hazard substances. However, the EPA would encourage submitters to take the time to understand their engineering processes and environmental releases even for chemicals they deem as low hazard, in the event the EPA characterizes the submitted chemical with a higher hazard concern and requires follow-up on your operations.

Will EPA review my prescreening assessment?
EPA considers all information submitted with every PMN; however, we do not have the resources to review in detail each Sustainable Futures prescreening assessment done by the submitting company. EPA will always conduct an independent review of each PMN. If you have specific questions on your assessment, please contact OPPT with your questions and we will do our best to provide you feedback.

Can I get a copy of EPA's review of my PMN?
EPA often uses previously submitted PMNs as analogs in the assessment of a new PMN, and as a result the EPA report is CBI. You may contact your program manager for the case to inquire about receiving a sanitized copy.

If a company is sold, acquired or merged, what happens to the company's graduation status?
The Sustainable Future program graduation status is attached to specific companies and not simply associated with intellectual property or select staff as a result of asset acquisition. Experience, understanding and competence obtained by graduate companies can not necessarily be transferred through asset acquisition of another company. Therefore, if intellectual property assets of a company (Company A) have been acquired by another company (Company B) rather than taking place via merger of two companies and, Company A, a Sustainable Futures Program graduate no longer controls the assets associated with the Sustainable Futures Program, then, Company B may not maintain an existing graduation status under the Sustainable Futures Program by relying on acquisition of assets from Company A. Instead, Company B must satisfy the requirements for Sustainable Futures graduation and work through the process to obtain their own graduate status. The EPA will not be involved in evaluating whether the above discussion directly relates to any particular situation, instead the EPA will leave that determination up to a company's legal counsel and will expect that appropriate steps are taken based on the above discussion.

2.5.3 Submissions From Companies That Have Graduated

Once a company does graduate, how will EPA reduce the PMN review period from 90 days to 45 days?
EPA is not reducing the review period for a PMN from 90 to 45 days. There will be two concurrent review periods - a 90-day Premanufacture Notice (PMN) review period and a 45-day Test Marketing Exemption Application (TMEA) review period. Once a company graduates, they will be permitted to send in a PMN and a TMEA for the same substance at the same time, i.e., a simultaneous or combined submission of the PMN and TMEA. PMNs and TMEAs have different review periods - 90 days for a PMN and 45 days for a TMEA. When a Graduate submits a combined PMN/TMEA, and if the TMEA is granted, the company is free to begin test marketing manufacture at day 45 under the provisions of the TMEA. Manufacture under a TMEA does not mean the substance would go on the TSCA inventory. When the PMN reaches day 90 and if EPA has not regulated the PMN, the company is free to begin commercial manufacture under the terms of the PMN. If the company made several batches of the substance under test marketing manufacture (between day 45 and day 90), they would be permitted to sell or use the material from those batches until the amount made under test marketing manufacture is gone. Commercial manufacture that may begin after the PMN review period closes on day 90 must take place before a company can submit a notice of commencement (NOC). A company may not use leftover material made under the TMEA in submitting an NOC. With the submission of the NOC, the substance that is the subject of the PMN then would be added to the TSCA inventory. The substance won't be added to the Inventory until EPA receives the NOC.

The TMEA component of the combined submission must be a legitimate TME. When the TMEA is submitted, the company must specify (1) the amount of material to be produced and distributed, (2) the number of potential customers to whom it is distributed, and (3) the time period of the test marketing must be specified to EPA in advance of distribution (see http://www.epa.gov/oppt/newchems/pubs/tmeranddbulletin.pdf). EPA does not require a production volume or use limit regarding the TMEA, but the company will be held to the production volume they stated in the TMEA. Therefore, if you need to manufacture 1,000 pounds during the TMEA period for a

specialty use, state this in the TMEA. Likewise, if you need to manufacture 1,000,000 pounds for a variety of specific consumer product uses, state that in the TMEA.

We have developed draft language demonstrating the submission is a legitimate TMEA and you are free to model your cover letter after this note. You may modify the language in any way you think is appropriate. A number of companies have used this, or similar, language and the Agency determined that this language demonstrates the application is in fact a legitimate TMEA. The central argument made in the draft language is that because the new substance was developed using risk screening tools at R&D, the substance is unique because risk reduction and/or pollution prevention were considered at R&D, resulting in a potentially unique product that warrants test marketing. The draft language refers to the "P2 Framework" which is the computerized chemical screening models. Sustainable Futures is the programmatic structure EPA uses to deliver the P2 Framework risk screening tools to industry together with training and regulatory relief for qualifying low hazard/low risk PMN submissions.

Submit the customary PMN and add to the cover letter a statement that says you have graduated from Sustainable Futures and that this is a simultaneous PMN/TMEA submission under Sustainable Futures. Your submission will then receive both a PMN and TMEA number.

Do I still need to continue to prescreen my chemicals after I graduate in the program?
Yes, your graduation status reflects the companies commitment to prescreening activities which help inform the decision making process. Therefore, the subsequent TMEA/PMN submissions should still contain a prescreening review. After a submitter has achieved graduation status and is submitting the dual TMEA/PMN submissions, they may choose not to run the exposure tools on low hazard substances. However, the EPA would encourage submitters to take the time to understand their engineering processes and environmental releases even for chemicals they deem as low hazard, in the event the EPA characterizes the submitted chemical with a higher hazard concern and requires follow-up on your operations.

Do we need to send in two copies of each submission?
Yes, under the electronic PMN system you will need to create and submit two separate notices as the combined Sustainable Futures submission. The electronic PMN system requires each submission to be a unique submission. This means that for Sustainable Futures submissions, the submitter will need to send to EPA two different notices - the PMN and the TMEA. Each submission will have a Submission Report Number (SRN) which EPA uses for tracking. Using the electronic PMN submission system, the submitter can "create" the TMEA by doing the following: (1) copy the PMN file; (2) renaming the file; (3) open the new file in the e-PMN software; (4) make the changes needed to meet the requirements of a TMEA (note in the cover letter that you are a graduate of Sustainable Futures and that your submission meets the requirements of a TMEA; PMN page 1 mark it as a TMEA submission, PMN page 7 change the production volume as needed, etc); (5) finalize the submission and submit the TMEA.

Can my company also get regulatory relief for Low Volume Exemptions (LVEs)?
The regulatory relief in the form of expedited (45-day) review applies to PMNs, which undergo a 90-day review, and not to LVEs, which undergo a 30-day review. No one is allowed to submit a LVE (Low Volume Exemption) and a PMN at the same time and only Sustainable Futures Graduates may submit a simultaneous Test Marketing Exemption Application (TMEA) and a PMN for the same chemical at the same time, but not a combined LVE/PMN.

After a Graduate submits a combined PMN/TMEA and day 45 of the TMEA has been reached with no EPA objection/regulation will the company be notified that they will be able to commence commercial manufacture of their PMN substance?
If and when the TMEA portion of the combined PMN/TMEA is granted and the PMN is dropped during the first 30 days of review, you will be notified by EPA's Sustainable Futures staff and/or staff in the OPPT Chemical Control Division. The email or phone call from the SF staff will most likely be from Kelly Mayo. You will be contacted by EPA staff in the OPPT Chemical Control Division if either the TMEA is not granted or the PMN is not dropped during the first 30 days of review. When you submit your combined PMN/TMEA, please email Kelly Mayo (mayo.kelly@epa.gov) to let the SF staff know it is coming and tell them who should be contacted if and when the TMEA is granted and the PMN is dropped during review.

When the TMEA portion (of a PMN/TMEA submission) is approved the SF Graduate will be able to commence manufacture for test marketing purposes as stipulated by the TMEA, but will not be able to commence manufacture for commercial purposes until day 90, as long as the Agency takes no action on the PMN portion of a combined PMN/TMEA. The PMN component of the simultaneous submission will still receive the normal 90-day PMN review period just like all other PMNs. If EPA grants the TMEA, but does not drop the PMN during the first 30 days of review, the submitter will be notified that they must choose, by letter within 15 days of being notified of the Agency's decision, to continue only one of the two notification procedures (i.e., withdraw the TMEA and continue with the PMN, or continue with the TMEA and withdraw the PMN).

2.5.4 PBT Profiler

Does EPA keep a record of the chemicals I evaluate using the PBT Profiler?
No user identification, chemical information, screening results, or any other electronic information entered into or generated by the PBT Profiler are intentionally tracked, stored, or collected. Information on user anonymity and security is provided on the PBT Profiler Web site.

Can I get a copy of the PBT Profiler as a stand-alone method like EPI Suite?
The PBT Profiler will not be available as a stand-alone method. The supporting modules and databases behind the PBT Profiler are routinely updated by Syracuse Research Corporation. If the model were a stand-alone there could eventually be multiple versions of the method in use, and this can create confusion. EPA prefers that the same version of the PBT Profiler be available to all users.

Will the PBT Profiler have a batch mode capability?
For an online method like the PBT Profiler to have a batch mode capacity would require that files be written to the server on which the method resides. Due to users' security concerns it was decided that the PBT Profiler would not have a batch mode capacity.

2.6 Sustainable Futures Training Materials

The P2 Framework models and methods which are contained in Sustainable Futures were developed to screen new chemicals submitted under TSCA. This manual walks the reader through a **Case Study** screening a sample chemical (isodecyl acrylate CAS RN 1330-61-6) using all the models in a step-wise process that follows the same sequence used when conducting a risk assessment (physical/chemical properties, fate properties, hazard or toxicity, exposure, and a final calculation of risk). Readers are instructed on how to interpret the results using **Interpretative Assistance Documents**, and how to enter the results into a **Sustainable Futures Summary Assessment Worksheet**.

The completed Sustainable Futures Summary Assessment Worksheet for the sample chemical isodecyl acrylate (CAS 1330-61-6) is included in this chapter and a blank worksheet is included in Appendix H. Chapter 14 of this document focuses on putting all of the model assessments together into a **Sustainable Futures PMN** to illustrate the kinds of information that Sustainable Futures participants can include in their PMNs while they are working towards graduating from Sustainable Futures and becoming eligible for regulatory relief (described in section 2.E.2 of this document). As of April 6, 2011 all new TSCA section 5 PMNs must be submitted electronically and must use e-PMN software which can be downloaded at http://www.epa.gov/opptintr/newchems/epmn/epmn-index.htm.

The Interpretative Assistance Documents and Sustainable Futures Summary Assessment Worksheet were developed specifically for the Sustainable Futures Initiative and are used in hands-on training. The Sustainable Futures Summary Assessment Worksheets for the example chemicals used during training are bound into a manual and designed so that, when opened the page on the left provides instructions on what information to include on the following page, which is on the right. All of the training materials, including the Interpretative Assistance Documents can be downloaded from the Sustainable Futures web site at http://www.epa.gov/oppt/sf/meetings/train.htm#materials.

Use of these suggested formats is not mandatory but is provided for illustration only.

2.6.1 Sustainable Futures Case Study Screening Isodecyl Acrylate

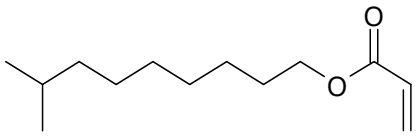
The following hypothetical information was developed for this case study and is not intended to represent an actual chemical or situation. Following the background information for the Case Study the Sustainable Futures Summary Assessment Worksheet is included with all the information filled in properly. A blank worksheet is included in Appendix H of this document.

NOTE: The background information for the Case Study is presented here however the information will be discussed in the chapters which present each model or method.

Introduction

The PMN substance, isodecyl acrylate (CAS No. 1330-61-6), also known by its trade name as MyCure 3310™, is a liquid that will be imported into the U.S. by the Green Chemical Company. Pure isodecyl acrylate will be used as a reactive diluent and processed to a 30% formulation for use in radiation curable coatings and adhesives, and related materials.

Isodecyl acrylate CAS RN 1330-61-6



Physical / Chemical Properties of Isodecyl Acrylate

- Molecular weight = 212.34 g/mole
- Melting point = –100 °C (measured)
- Boiling point = 158 °C at 50 mm Hg (measured)

Information about Import and Processing of Isodecyl Acrylate

Pure isodecyl acrylate will be imported in transport containers at 11,200 kg/year, and delivered directly to the facility where it will be processed. For each batch (10 batches/year), isodecyl acrylate will be transferred directly into a single reactor and processed to a 30% formulation. Worker exposure will be prevented during transfer of pure isodecyl acrylate into the reactor via automated transfer equipment. Furthermore, a fugitive emissions capture device will be utilized to prevent release of isodecyl acrylate into the environment during transfer into the reactor. After formulation of each batch, the processed

material will be transferred into the 55 gallon drums in which it will be transported to buyers. A single worker will be exposed dermally and by inhalation during drumming. The reactor is cleaned once per year; occupational exposure will not occur during cleaning of the reactor. Releases to the environment will occur during drumming (fugitive releases to air) and cleaning of the reactor (fugitive releases to air and releases to surface water).

Processing, exposure, and release scenarios for isodecyl acrylate are provided below and discussed in the ChemSTEER chapter of this document. ChemSTEER is used to estimate those values which will become inputs for other P2 Framework models and methods.

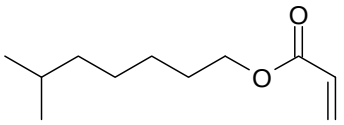

Worksheet for Isodecyl Acrylate Sustainable Futures Case Study
OPERATION(S):
Workplace / workplaces with same/similar operations such that estimates of releases and exposures can be assumed to be the same.
Examples of Media of Release
Water
Air
Landfill
Incineration
Potential Exposure Routes
Inhalation
Dermal
Drinking water
Manufacturing
(PMN chemical is created or formed)
Production Volume?
# of sites?
raw materials
Batch size?
Batches/Year?
Wt fraction?
# of workers?
Site(s) typically controlled by the submitter
minimum number (1 - 3), lower # of workers
larger, single point releases
Example Release(s)
* Equipment cleaning
* Sampling
Exposure Activities(s)
* Drumming
* Sampling
SUBSEQUENT OPERATION:
transport of product / chemical:
% and type of container:
Processing
(PMN chemical neither created nor destroyed)
Import PMN (11,200 kg/yr)
# of sites?: 1
Batches per year or operating days?: 10
Batch size?: 1120 kg
Hours per batch?: 24
Wt fraction of chemical in product?: 30%
# of workers?: 1
Release(s)
*Loading into 55 gal drums (fugitive air emissions), 10x/yr
*Cleaning reactor (surface water, fugitive air emissions), 1x/yr
Exposure Activities(s)
*Loading into 55 gal drums (dermal, inhalation), 10x/yr
SUBSEQUENT OPERATION:
transport of product / chemical:
% and type of container:
Use
(PMN is transformed or destroyed)
raw materials
Use Rate?
# of sites?
Operating days/year?
# of workers?
Sites typically controlled by others
Can have 1000's use sites, large # of workers
Smaller releases over a number of sites
Example Release(s)
*Equipment cleaning
*Container residue
*End-use releases
Exposure Activities(s)
*Unloading transport containers
*End-use activities
*Coating applications
*Unit operations and processing
*Miscellaneous activities

Ecotoxicity and Human Health Effects Data

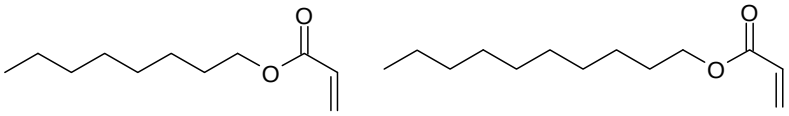
A search for publicly available aquatic toxicity and human health effects (cancer and non-cancer) did not locate data on isodecyl acrylate. Data were identified for several structural analogs. The analogs and data are summarized below but will be discussed in subsequent chapters. The background information on the Case Study is presented here however the information will be discussed in the chapters which present each model or method.

Analogs

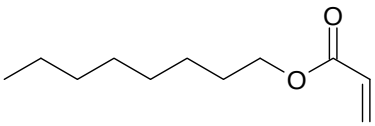
Isooctyl acrylate CAS RN 29590-42-9



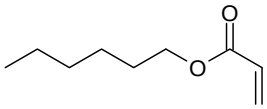
Mixture of Octyl and Decyl acrylate NO CAS



Octyl acrylate CAS RN 2499-59-4



Hexyl acrylate CAS RN 2499-95-8



Ecotoxicity

- No experimental data were identified for the PMN substance or structural analogues

Cancer Health Effects

- No experimental data were identified for the PMN substance.
- Isooctyl acrylate had negative results for carcinogenicity in a lifetime dermal carcinogenicity bioassay of the analogous substance isooctyl acrylate (CAS No. 29590-42-9) in male mice (Gordon et al., 1991).

Non-Cancer Human Health Effects

No experimental data were identified on the PMN substance; however, data were available for four structural analogues. These data are summarized below.

Isooctyl acrylate (CAS No. 29590-42-9)

- Acute rat LD50, oral gavage >5000 mg/kg (IUCLID data sheet)
- Irritating to the skin of rabbits (Gordon et al., 1981)
- Dermal sensitization in laboratory animals (TSCA Section 8(e) submission, 8(e)-3774)
- Negative in mutagenicity assay (CCRIS, 2004)
- Skeletal variations in offspring of pregnant rats treated during gestation via oral gavage; LOAEL = 1000 mg/kg-day (TSCA Section 8(e) submission, 8(e)-1524)
- Negative for developmental effects in the offspring of pregnant rats treated dermally during gestation (IUCLID data sheet)

Octyl acrylate (CAS No. 2499-59-4)

- Dermal sensitization in laboratory animals (TSCA Section 8(e) submission, 8(e)-1572)

Octyl acrylate (CAS No. 2499-59-4) and decyl acrylate (CAS No. 2156-96-9) mixture

- Dermal sensitization in laboratory animals (TSCA Section 8(e) submission, 8(e)-11424)

Hexyl acrylate (CAS No. 2499-95-8)

- Dermal sensitization in human volunteers (TSCA Section 8(e) submission, 8(e)-3774)
- Negative in mutagenicity assay (CCRIS, 2004)

References for Health Effects Data Located

CCRIS. Chemical Carcinogenesis Research Information System. 2004. Available on-line at http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?CCRIS

Gordon, S.C.; Zimmerman, D.D.; and F.D. Griffith. 1991. Acute Toxicity, Genotoxicity, and Dermal Carcinogenicity Assessment of Isooctylacrylate. J Toxicol Environ Health. 34(3)297-308.

IUCLID 29590-42-9. IUCLID data sheet for isooctyl acrylate, CAS No. 29590-42-9.

TSCA Section 8(e) submission, 8(e)-1524. TSCATS Database. Teratology Screen in Rats (C190, C-181, C-183, C-236, C-253, C-254, C-255, C-256, C-257, C-258, C-259) (Final Report) with attachments and cover letter. U.S.EAP/OPTS Public Files: Fiche#: OTS0534620, Doc#: 88-920000170.

TSCA Section 8(e) submission, 8(e)-11424. TSCATS Database. Initial Submission: Mouse ear swelling test with octyl decyl acrylate with cover letter dated 102792; U.S. EPA/OPTS Public Files: Fiche#: OTS0571362, Doc#: 88-920009705.

TSCA Section 8(e) submission, 8(e)-14572. TSCATS Database. Initial Submission: Acrylate de n-octyle, Skin sensitization test in guinea pigs (Maximization method of Magnusson, B. and Kligman, A.M.), with cover letter dated 101599; U.S. EPA/OPTS Public files: Fiche#: OTS0559819, Doc#: 88-000000012.

TSCA Section 8(e) submission, 8(e)-3774. TSCATS Database. Initial Submission: Letter concerning information on the chemical substance hexyl acrylate with attachments (SANITIZED); U.S. EPA/OPTS Public Files: Fiche#: OTS0536468, Doc#: 88-9200024168.

Sustainable Futures

Summary Assessment

Using

P2 Framework Models

This document was developed to help compile estimation results from U.S. EPA OPPT's P2 Framework Models and is used by OPPT during Sustainable Futures (SF) training described at www.epa.gov/oppt/sf.
Participants in the voluntary SF Initiative are asked to submit the information contained in this assessment along with their SF PMNs in their choice of format.

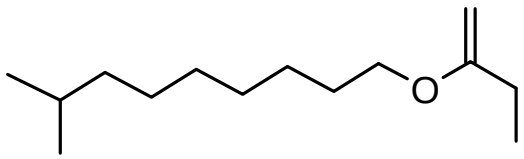
Use of this specific format is not mandatory.

Chemical Assessed:
Isodecyl acrylate, TN MyCure 3310™

CAS Registry Number:
1330-61-6

Participant Name:
The Green Chemical Company

Date of Assessment:
03/25/2005

Record ID: GCC001	**CAS No.** 1330-61-6
Chemical Structure  **Is this a representative structure? No**	**MW:** 212.34 **MF:** C13 H24 O2 **Physical Form:** Liquid **Submitter:** The Green Chemical Company **Trade Name:** MyCure 3310™ **Use:** Reactive diluent in radiation curable coatings and adhesives, etc. **Production Volume:** 11,200 kg
SMILES: O=C(C=C)OCCCCCCCCC(C)C	
Name: 2-Propoenic acid, isodecyl ester	
Synonyms: (1) Isodecyl alcohol, acrylate (2) Acrylic acid, isodecyl ester (3) Isodecyl propenoate (4) Isodecyl acrylate	

SUSTAINABLE FUTURES SUMMARY:

Concern Level	HIGH	MODERATE	LOW
Persistence			**X**
Bioconcentration			**X**
Cancer Health Hazard			**X**
Non-Cancer Health Hazard		**X**	
Aquatic Toxicity Hazard	**X**		
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard:** Moderate **Aquatic Hazard:** High		
Overall Risk	**Human Health Risk:** Low **Aquatic Risk:** Low		

CAS No. 1330-61-6	**Submitter:** The Green Chemical Company
PHYSICAL/CHEMICAL PROPERTIES:	
Melting Point (deg C)	– 100 (Experimental data from PhysProp database)
Boiling Point (deg C)	158 (Experimental data from PhysProp database)
Boiling Point Pressure (mm Hg)	50 (Experimental data from PhysProp database)
Vapor Pressure (mm Hg)	2.27E-02 (EPI v4.10, MPBPVP v1.43)
Water Solubility at 25 deg C (g/L)	3.034 (EPI v4.10, WSKOW v1.42)
Log K_{ow}	5.07 (EPI v4.10, KOWWIN v1.68)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC (atm-m^3/mol)	1.20E-03 (EPI v4.10, HENRYWIN v3.20 Group Method)
Soil Adsorption Coefficient – log K_{oc}	3.037 (EPI v4.10, KOCWIN v2.00)
Log Bioconcentration Factor – BCF	1.641 (EPI v4.10, BCFBAF v3.01)
Persistence	
Probability of Rapid Biodegradation	Likely to biodegrade rapidly (EPI v4.10, BIOWIN v4.10)
Ultimate Biodeg Model	Weeks (EPI v4.10, BIOWIN v4.10)
Primary Biodeg Model	Days (EPI v4.10, BIOWIN v4.10)
Ready Biodegradability (MITI Model)	Likely to biodegrade rapidly (EPI v4.10, BIOWIN v4.10)
Atmospheric Half-life	Reacts at moderate rate (5.8 hrs) w. OH radicals, slower rate (6.5 days) w. ozone, does not react with nitrate radicals (EPI v4.10, AopWin v1.92)
Hydrolysis Half-life	> 10 yrs at pH 7, > 1 year at pH 8 (EPI v4.10, HYDROWIN v2.00)
Volatilization Half-life for Model River	> 2 hours (EPI v4.10, WVOLNT)
Volatilization Half-life for Model Lake	> 6 days (EPI v4.10, WVOLNT)
Removal in STP (EPA Draft Method)	99% predicted, Recommended Max is 95% (EPI v4.10, STPWIN)
Experimental Data	Not available
Byproducts	
Degradation Products	Acrylic acid, isodecyl alcohol (Professional Judgment)
Metabolites	Not available

CAS No. 1330-61-6	**Submitter:** The Green Chemical Company
ECOTOXICITY:	
ECOSAR Class	Acrylates
Acute Toxicity	
Fish LC50	0.555 mg/L (ECOSAR)
Daphnid LC50	0.731 mg/L (ECOSAR)
Green Algae EC50	0.520 mg/L (ECOSAR)
Chronic Toxicity	
Fish ChV	0.0000955 mg/L (ECOSAR)
Daphnid ChV	0.10 mg/L (ECOSAR)
Green Algae ChV	0.91 mg/L (ECOSAR)
Hazard Concern for Aquatic Toxicity	High
Lowest Chronic Concern Concentration	1 ppb (see discussion)
CANCER HEALTH EFFECTS:	
Experimental data	Low by analogy to isooctyl acrylate (Gordon et al 1991)
OncoLogic Results	Marginal
Overall Hazard Concern for Carcinogenicity	Low
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low by analogy to isooctyl acrylate, based on acute LD50 >5000 mg/kg for rats by oral gavage (IUCLID 29590-42-9)
Irritation	Positive by analogy to isooctyl acrylate (Gordon et al. 1991)
Skin Sensitizer	Positive based on dermal sensitization of analogs in lab animals and humans (8e-11424, 8e-14572, 8e-3774)
Reproductive Effects	No relevant data identified
Developmental Effects	Moderate by analogy to isooctyl acrylate, which produced skeletal variations in the offspring of rats treated orally during pregnancy; LOAEL = 1,000 mg/kg-day (8e-1524)
Immune System Effects	No relevant data identified
Neurotoxicity	No relevant data identified
Genotoxicity	Negative by analogy to isooctyl acrylate and hexyl acrylate (CCRIS)
Mutagenicity	No relevant data identified
Systemic Effects	No relevant data identified
Overall Hazard Concern for Non-Cancer Health Effects	Moderate

CAS No. 1330-61-6		**Submitter:** The Green Chemical Company	
EXPOSURE MODELS:			
INDUSTRIAL RELEASE AND EXPOSURE VALUES: CHEMSTEER			
Process	User-defined Processing	**Number of Release Days**	10
SIC Code / NPDES #	Adhesives & Sealants 2891	**Number of Facilities**	1
Occupational Exposure Values			
	Cancer LADD	**Chronic ADD**	**Acute APDR**
Dermal	0.118 mg/kg-day	0.207 mg/kg-day	7.56 mg/kg-day
Inhalation	3.12×10^{-3} mg/kg-day	5.45×10^{-3} mg/kg-day	0.199 mg/kg-day
Environmental Release Values			
Release to Water [Equipment cleaning]		11.2 kg/year over 1 day/yr	
Release to Air (Fugitive) [Equipment cleaning]		4.3040E-03 kg/site-day over 1 day/yr	
Release to Air (Fugitive) [loading liquid product into drums]		9.6848E-04 kg/site-day over 9 days/yr	
Release to Landfill			
Release from Incineration			
Other Release Activities			
GENERAL POPULATION EXPOSURE VALUES: E-FAST			
Aquatic Exposure:			
Lowest Acute COC – Aquatic Exposure		110/µg/L (fish LC50/5, rounded to 1 sig. digit)	
Lowest Chronic COC – Aquatic Exposure		1 µg/L (fish chronic value/10, rounded to 1 sig. digit)	
Predicted Environmental Concentration (PEC)		84 µg/L (ppb)	
PEC Exceeds Chronic COC (days / year)		0 day	
Human Exposure:			
	Cancer LADDpot	**Chronic ADDpot**	**Acute ADRpot**
Drinking Water	3.62×10^{-7} mg/kg-day	6.79×10^{-7} mg/kg-day	7.02×10^{-3} mg/kg-day
Fish Ingestion	6.83×10^{-8} mg/kg-day	1.28×10^{-7} mg/kg-day	1.34×10^{-3} mg/kg-day
Fugitive Emissions [drumming]	1.92×10^{-8} mg/kg-day	3.6×10^{-8} mg/kg-day	2.43×10^{-5} mg/kg-day
Fugitive Emissions [reactor cleaning]	7.27×10^{-9} mg/kg-day	1.36×10^{-8} mg/kg-day	8.29×10^{-5} mg/kg-day
Incineration Emissions			
Landfill Leaching			
Dermal – Consumer Use			
Inhalation – Consumer Use			
RISK ASSESSMENT CALCULATIONS:			
MOE – Acute Occupational Exposure		N/A	
MOE – Chronic Occupational Exposure		5025	
MOE – Acute General Population Exposure		N/A	
MOE – Chronic General Population Exposure		1.2×10^{5}	

CAS No. 1330-61-6	**Submitter:** The Green Chemical Company

SUMMARY CONCLUSIONS:

Occupational Risk:

Risk of Non-Cancer Acute Effects from Occupational Exposure: Low potential for risk due to low hazard since mammalian LD50 >50 mg/kg.

Risk of Non-Cancer Chronic Effects from Occupational Exposure: Low potential for chronic risk because MOE >1000.

Risk of Cancer Effects from Occupational Exposure: Low potential for risk since there is low hazard concern.

General Population Risk:

Risk of Non-Cancer Acute Effects to General Population: Low potential for risk due to low hazard since mammalian LD50 >50 mg/kg.

Risk of Non-Cancer Chronic Effects to General Population: Low potential for chronic risk because MOE > 1000.

Risk of Cancer Effects to General Population: Low potential for risk since there is low hazard concern.

Aquatic Risk:

Acute Risk to the Aquatic Environment: Low potential for acute risk because PEC does not exceed any acute COC.

Chronic Risk to the Aquatic Environment: Low potential for chronic risk because PEC does not exceed any chronic COC more than 20 days per year.

WRITE-UP SECTIONS:

Physical/Chemical Properties

GCC00 I is a liquid at room temperature with a measured melting point of -100 °C and a measured boiling point of 158 °C at 50 mm Hg (PhysProp Database). This melting point was input into EPISuite, but the boiling point was not, since it was measured at a reduced pressure. All of the remaining physical properties were estimated by EPISuite. GCC00 1 is expected to be slightly soluble in water, estimated at about 3 mg/L. The estimated vapor pressure of 0.023 mm Hg indicates that the material will exist primarily in the vapor phase in the atmosphere. Due to the relatively high vapor pressure and low water solubility, material is estimated to volatilize readily from water with a Henry's Law constant of 1.2×10^{-3} atm-m^3/mole.

Environmental Fate

No references to the environmental fate of GCC001 were located in the available literature, and its environmental fate is based on EPI estimates. If released to the environment, GCC001 is not expected to be persistent. In air, the estimated half-life for the gas-phase reaction with hydroxyl radicals is 17 hours. The gas-phase reaction with ozone will also contribute to its atmospheric destruction. GCC001 is not expected to undergo hydrolysis under conditions typically found in the environment, with an estimated half-life of 1 year at pH 8 and over 10 years under neutral conditions based on HYDROWIN estimates. Biodegradation is expected to be the predominant degradation process in water and soil, with ultimate biodegradation occurring within weeks, as estimated by the expert survey biodegradation model. Volatilization from water to the atmosphere is expected to be a competing process for its removal from streams based on EPI estimates. Its soil adsorption coefficient (log Koc = 3.1) indicates moderate adsorption to soil and slow migration to groundwater. The Koc also indicates potential for adsorption to sediment and suspended organic matter in surface waters. Consistent with this assessment, the Level III fugacity model indicates that it will partition predominantly to soil, with lesser amounts to water and sediment. An estimated BCF of 161 indicates low potential to bioconcentrate in fish and aquatic organisms. GCC001 is not estimated to be a PBT based on the results of the PBT Profiler.

Overall, GCC001 is expected to partition mainly to soil and have low persistence.

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Aquatic Hazard

The ecotoxicity estimates are based on structure activity relationship (SAR) equations in the ECOSAR software. In the case of GCC001, the estimates are based on the "Acrylates" SAR, and the software was able to estimate values for all three acute endpoints (fish, daphnid, and green algae) and all three chronic endpoint (also fish, daphnid, and green algae); An acute effect level value <1 mg/L indicates a high hazard concern, a value between 1 and 100 mg/L indicates a moderate hazard concern, and a value> 100 mg/L indicates a low hazard concern. A chronic endpoint value <0.1 mg/L indicates a high hazard concern, between 1 and 10 indicates a moderate hazard concern, and >10 mg/L indicates a low hazard concern.

Overall, for GCC001 all three acute effect level estimates are <1 mg/L and all three chronic effect level estimates are <0.1 mg/L, indicating a high aquatic hazard concern for this chemical.

Human Health Cancer Hazard

No data were identified either on the GCC001 (isodecyl acrylate) or structural analogs that indicate a concern for carcinogenicity. Overall, there appears to be a low carcinogenicity concern for the submitted substance based on three factors: (1) OncoLogic predicted a "Marginal" concern for cancer effects; (2) an analog of the submitted substance (isooctyl acrylate) was not carcinogenic when applied dermally to male mice in an adequately conducted lifetime bioassay (Gordon et al 1991); and (3) isooctyl acrylate and hexyl acrylate produced negative results in adequately conducted mutation assays.

Based on analog data and OncoLogic predictions, GCC001 is estimated to pose a low concern for human health cancer hazard.

Human Health Non-Cancer Hazard

No relevant toxicity data for GCC001 were identified and the assessment was based on data identified for analogs. A close structural analog, isooctyl acrylate (CAS No. 29590-42-9) had low acute toxicity with a reported LD50 of >5000 mg/kg for rats by oral gavage (IUCLID 29590-42-9). In a separate study, isooctyl acrylate produced skeletal variations in offspring at 1000 mg/kg-day (the only dose tested) when administered to pregnant rats via oral gavage. However, isooctyl acrylate did not induce developmental toxicity when dermally administered to rats in an adequately conducted study; therefore, there does not appear to be a developmental toxicity concern when dermal exposure is expected. Dermal sensitization was also identified as a potential concern based on analogy to octyl acrylate, octyl and decyl acrylate mixture, and hexyl acrylate, all of which induced dermal sensitization reactions in either laboratory animals or human volunteers. Table 1 reports the potential hazard concerns identified for selected analogs of the submitted substance.

Based on developmental effects for a close structural analog at 1000 mg/kg-day, an overall non-cancer hazard concern of moderate was estimated for GCC001.

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Environmental (Aquatic) Exposure

Environmental exposure may result from releases of GCC001 to surface water from a single site during cleaning of the reactor, which occurs 1 day/year. ChemSTEER estimates a release of 11.2 kg/site-day to surface waters, with total releases of 11.2 kg/year. The aquatic exposure estimates indicate a predicted environmental concentration (PEC) of 84 µg/L (E-FAST). The PEC and the days per year of release will be used to determine risk potential to the aquatic environment resulting from releases of GCC001.

Occupational Exposure

Occupational exposures were estimated using ChemSTEER. Based on the expected use and manufacturing of GCC001, workers may be exposed to vapors (inhalation exposure) at up to 2.59 mg/day (10 days/year) and to liquid (dermal exposure) at up to 441 mg/day (10 days/year) from loading liquid product into drums. These daily exposures are used by ChemSTEER to estimate lifetime average daily dose rates (LADD), average daily dose rates (ADD), and acute potential dose rates (APDR) for both inhalation and dermal exposure to GCC001. The calculated dose rates are listed on the exposure models page above. Potential risk to workers will be calculated by comparison of the appropriate exposure value, assuming that no protective gear is used, to the estimated LOAEL of 1000 mg/kg-day and is discussed in the following section.

General Population Exposure

Occupational exposures were estimated using ChemSTEER. Based on expected processing of the submitted chemical, workers may be exposed to vapors (inhalation exposure), at up to 13.9 mg/day, and to liquid (dermal exposure), at up to 529 mg/day, from loading liquid product into drums, which occurs 10 days/year. These daily exposures are used by ChemSTEER to estimate lifetime average daily dose (LADD), average daily dose rates (ADD), and acute potential dose rates (APDR) for both inhalation and dermal exposure to GCC001. The calculated dose rates are listed on the exposure models page above. Potential risk to workers will be calculated by comparison of the appropriate exposure value, assuming that no protective gear is used, to the estimated LOAEL of 1000 mg/kg-day and is discussed in the following section.

Environmental (Aquatic) Risk Assessment

Acute risk to the aquatic environment is estimated by comparison of the acute COC for each species to the estimated PEC (see Appendix 1 below). If the PEC **>** the acute COC estimated for a species, then the potential for acute risk exists for that species. For GCC00l, the PEC < the acute COC, indicating a low potential for acute risk to aquatic organisms. Chronic risk to the aquatic environment is evaluated by estimating the number of days the PEC exceeds the chronic COC for each species (see Appendix 1 below). This estimation is done by E-FAST and is based on the PEC, the number of days of release per year, and estimated stream flow rates. If the PEC is estimated to exceed the relevant chronic COC for 20 days/year or more, a potential for chronic risk exists for the species being evaluated. GCC00l is estimated to have releases to the aquatic environment for 1 day/year and, in all cases, the PEC exceeds the COC for **<** 20 days/year, indicating a low potential for chronic risk to the aquatic environment.

A concentration of concern (COC) is estimated for both acute and chronic endpoints for each species by dividing the relevant endpoint by a factor and rounding the result to one significant digit; all results <1 µg/L (ppb) are rounded up to 1 µg/L. These COCs are used to determine risk (see below).

Overall, GCC00l is estimated to pose a low potential for acute and chronic risk to the environment.

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Human Health Risk Assessment

Risk is assessed by establishing a margin of exposure (MOE) for both occupational exposure and general population exposure for each relevant effect estimated for the chemical. This is done by dividing the effect level, either a lowest-observed-adverse-effect level (LOAEL) or a no-observed-adverse-effect level (NOAEL), by the estimated exposure dose. In the case of a LOAEL, a MOE <1000 indicates a potential for risk for that effect from that exposure; in the case of an NOAEL, a MOE <100 indicates potential for risk. For GCC001, developmental toxicity is based on analogy to isooctyl acrylate, which induced skeletal variations at 1,000 mg/kg-day; a NOAEL was not observed. Developmental effects are systemic or chronic effects that are caused by acute exposure of a pregnant female. The LOAEL for this effect is compared to the highest relevant acute dose rate (APDR and ADRpot) for both occupational exposure and general population exposure. In the case of occupational exposure, the inhalation APDR is used, even though the dermal APDR is higher, since the study specifically showed that dermal exposure does not induce developmental effects. If effect levels, either LOAELs or NOAELs, were estimated for multiple effects shown in the table above, each would be subject to risk assessment, as described, using the relevant potential exposure levels.

Cancer human health risk assessment is not currently performed for a Sustainable Futures summary assessment; however, in cases where there is low hazard concern for human health cancer effects, there will be low risk for cancer effects also.

Risk from occupational exposure is estimated by dividing the estimated LOAEL of 1000 mg/kg-day by the inhalation APDR of 0.199 mg/kg-day to get the MOE (see Appendix 2 below). The MOE from this calculation is >1000 (5025), indicating a low potential for risk from occupational exposure to GCC001.

Risk to the general population is estimated by dividing the LOAEL of 1000 mg/kg-day by the acute fish ingestion, drinking water, and inhalation rates combined (worst case via applicable routes). The MOE from this calculation is >1000 (1.2×10^5), indicating a low potential for risk to the general population from exposure to GCC001.

Overall, GCCOOI has a low potential for risk to human health from occupational exposure and general population Exposure.

Abbreviations Used
GCC001 - Chemical and assessment ID (isodecyl acrylate)
SAR - Structure activity relationship
ACR - Acute-to-chronic ratio
COC - Concentration of concern
PEC - Predicted environmental concentration
LADD/LADDpot - Lifetime average daily dose (potential)
ADD /ADDpot - Average daily dose (potential)
APDR/ADRpot - acute potential dose rate
MOE - margin of exposure

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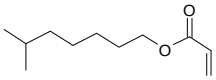
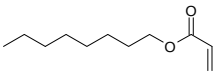
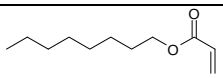
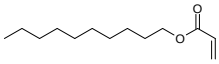
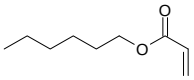
Table I - Selected Analogs

Analog	Structure	Concern Identified	Basis of Concern	Concern Level
Isooctyl acrylate (29590-42-9) TSCATS 8-e-1524, 8e-3774; (IUCLID 29590-42-9)		Positive: Developmental toxicity (oral), dermal sensitization, dermal irritation Negative: Developmental toxicity (dermal), genotoxicity, cancer (dermal), acute toxicity	Induced skeletal variations at 1000 mg/kg-day (only dose tested) in rats by oral gavage. Acute LD50 of >5000 mg/kg in rats by oral gavage. Skin irritation in rabbits.	Moderate for developmental effects; Low for acute toxicity; N/A for skin irritation
Octyl acrylate (2499-59-4) TSCATS 8(e)-1572		Positive: Dermal sensitization	Induced skin sensitization in laboratory animals	N/A
Octyl and decyl acrylate mixture TSCATS 8(e)-11424	 and 	Positive: Dermal sensitization	Produced positive results in mouse ear swelling test	N/A
Hexyl acrylate (2499-95-8) TSCATS 8(e)-3774 CCRIS		Positive: Dermal sensitization (6% solution) Negative: Genotoxicity	Induced skin sensitization in human volunteers	N/A

References

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Appendix 1: Determination of Aquatic Risk

Chemical Identifier: GCC001 **CAS Number:** 1330-61-6

Release Activity 1: User-defined Processing **Site Information:** Adhesives and Sealants Processing

	Endpoint	Effect Level (ppb)	Assessment Factor	Acute COC (ppb)	PEC (ppb)	Potential for Risk?
Acute Profile	Fish	555	5	111	84	No
	Daphnid	731	5	146	84	No
	Green Algae	520	4	130	84	No
Chronic Profile	**Endpoint**	**Effect Level (ppb)**	**Assessment Factor**	**Chronic COC (ppb)**	**Days/Year PEC Exceeds COC**	**Potential for Risk?**
	Fish	0.1	10	1	< 1	No
	Daphnid	10	10	1	< 1	No
	Green Algae	91	10	9.1	< 1	No

Appendix 2: Determination of Human Health Risk from Occupational Exposure

Chemical Identifier: GCC001 **CAS Number:** 1330-61-6

Exposure Activity 1: User-defined Processing **Site Information:** Adhesives and Sealants Processing

	Endpoint (Concern Effect)	NOAEL (mg/kg-d)	LOAEL (mg/kg-d)	Exposure Dose and Source (mg/kg-d)	MOE*	Potential for Risk?
Occupational Exposure	1. Developmental Effects		1000	0.199 (inhalation APDR)	5000	No

*MOE < 100 indicates potential for risk when using a NOAEL value; MOE < 1000 indicates potential for risk when using a LOAEL value.

Appendix 3: Determination of Human Health Risk to the General Population

Chemical Identifier: GCC001 **CAS Number:** 1330-61-6

Exposure Activity 1: User-defined Scenario **Site Information:** Adhesives and Sealants Processing

	Endpoint (Concern Effect)	NOAEL (mg/kg-d)	LOAEL (mg/kg-d)	Exposure Dose and Source (mg/kg-d)	MOE*	Potential for Risk?
General Population Exposure	1. Developmental Effects		1000	0.00847	1.2×10^5	No

*MOE < 100 indicates potential for risk when using a NOAEL value; MOE < 1000 indicates potential for risk when using a LOAEL value.