Hands-On Sessions and

Completing a Sustainable Futures Summary Assessment Worksheet

Areas of a SF Assessment

- P/Chem & Environmental Fate
- Hazard Assessment
  - Aquatic Toxicity
  - Cancer Health Effects
  - Non-Cancer Health Effects
- Exposure Assessment
  - Occupational
  - Aquatic
  - General Population
- Risk Assessment

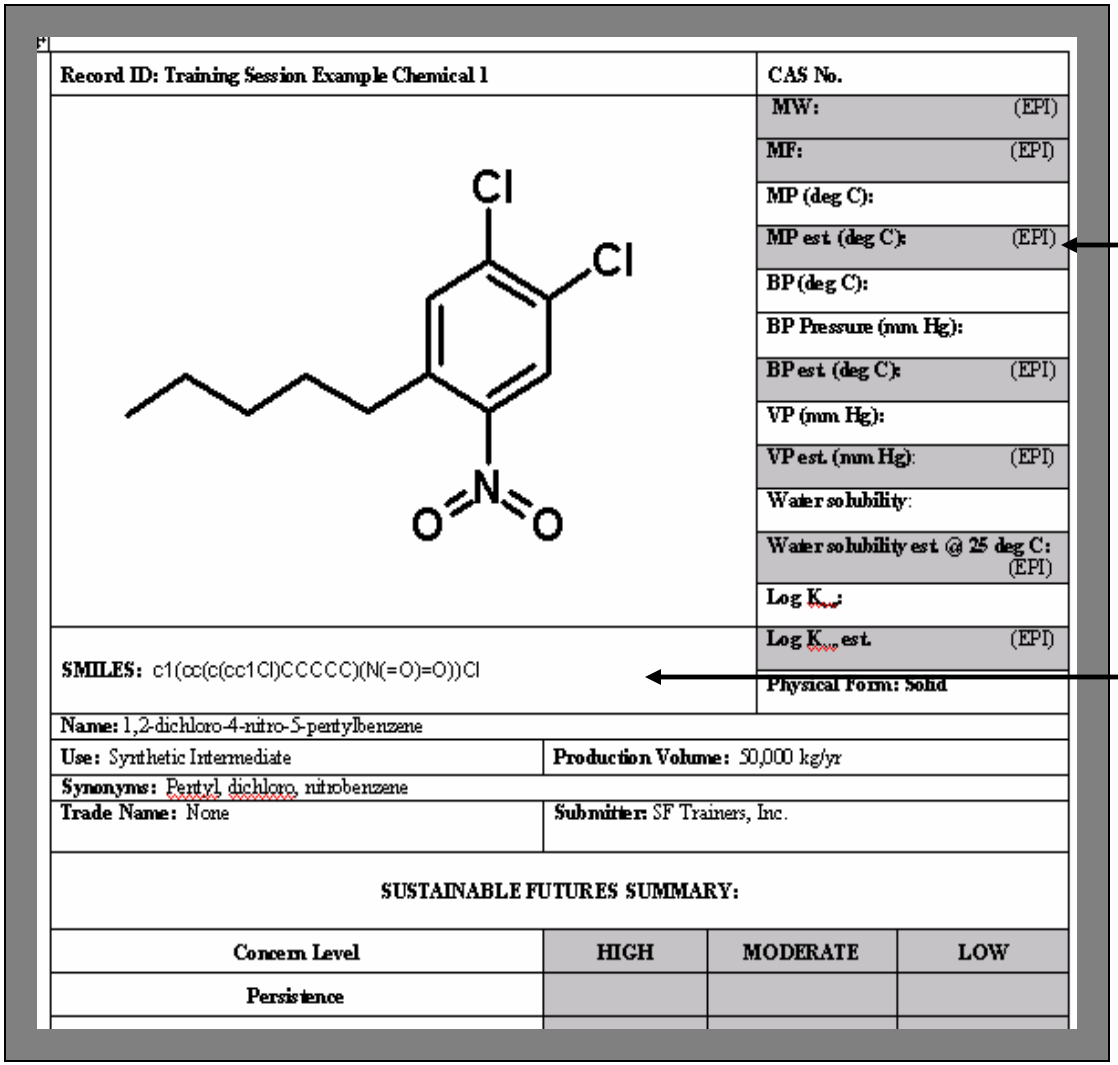
Areas of a SF Assessment

- P/Chem and Environmental Fate Properties [EPISuite™]
- Hazard Assessment
  - Aquatic Toxicity [ECOSAR]
  - Cancer Health Effects [OncoLogic™]
  - Non-Cancer Health Effects [Analog Analysis]
- Exposure Assessment
  - Occupational Exposure [ChemSTEER]
  - Aquatic Exposure [E-FAST]
  - General Population Exposure [E-FAST]
- Risk Assessment [Mathematical Calculations]

SF Training Hands-On Sessions

- Each model/method will be described in a technical SF presentation
- Following each of the presentations, there will be a “hands-on” session where participants will:
  - Use the models/methods to estimate endpoints
  - Begin to fill out a SF Assessment Worksheet for 3 sample chemicals

SF Summary Assessment Worksheets



Record ID: Training Session Example Chemical 1	**CAS No.**
	MW: (EPI)
	MF: (EPI)
	MP (deg C):
	MP est. (deg C): (EPI)
	BP (deg C):
	BP Pressure (mm Hg):
	BP est. (deg C): (EPI)
	VP (mm Hg):
	VP est. (mm Hg): (EPI)
	Water solubility:
	Water solubility est. @ 25 deg C: (EPI)
	Log K_{ow}:
SMILES: c1(cc(c(cc1Cl)CCCCC)(N(=O)=O))Cl	**Log K_{ow} est.** (EPI)
	Physical Form: Solid
Name: 1,2-dichloro-4-nitro-5-pentylbenzene	
Use: Synthetic Intermediate	**Production Volume:** 50,000 kg/yr
Synonyms: Pentyl, dichloro, nitrobenzene	
Trade Name: None	**Submitter:** SF Trainers, Inc.

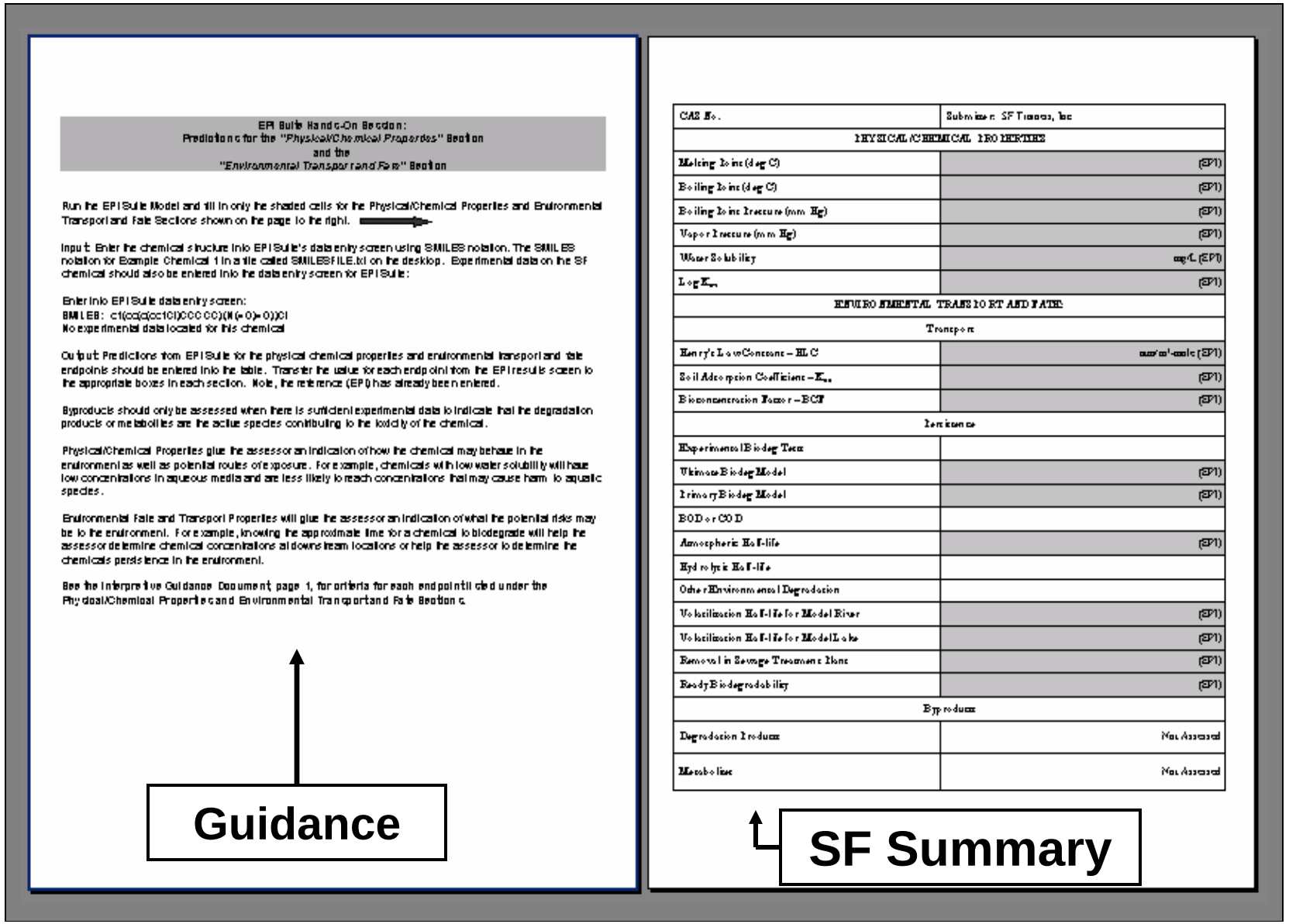
SUSTAINABLE FUTURES SUMMARY:

Concern Level	HIGH	MODERATE	LOW
Persistence			

Shaded sections of the assessment should be filled out during the hands-on portions of the training seminar

SMILES notations for each sample chemical are located on first page and in a text file on the desktop (exsmiles.txt)

SF Summary Assessment Worksheets



EPI Suite Hands-On Section:
Predictions for the "Physical/Chemical Properties" Section
and the
"Environmental Transport and Fate" Section

Run the EPI Suite Model and fill in only the shaded cells for the Physical/Chemical Properties and Environmental Transport and Fate Sections shown on the page to the right.

Input: Enter the chemical structure into EPI Suite's data entry screen using SMILES notation. The SMILES notation for Example Chemical 1 in a file called SMILESFILE.txt on the desktop. Experimental data on the SF chemical should also be entered into the data entry screen for EPI Suite:

Enter into EPI Suite data entry screen:
SMILES: c1(cc(c(cc1Cl)CCC CC)(N(=O)=O))Cl
No experimental data located for this chemical

Output: Predictions from EPI Suite for the physical chemical properties and environmental transport and fate endpoints should be entered into the table. Transfer the value for each endpoint from the EPI results screen to the appropriate boxes in each section. Note, the reference (EPI) has already been entered.

Byproducts should only be assessed when there is sufficient experimental data to indicate that the degradation products or metabolites are the active species contributing to the toxicity of the chemical.

Physical/Chemical Properties give the assessor an indication of how the chemical may behave in the environment as well as potential routes of exposure. For example, chemicals with low water solubility will have low concentrations in aqueous media and are less likely to reach concentrations that may cause harm to aquatic species.

Environmental Fate and Transport Properties will give the assessor an indication of what the potential risks may be to the environment. For example, knowing the approximate time for a chemical to biodegrade will help the assessor determine chemical concentrations at downstream locations or help the assessor to determine the chemicals persistence in the environment.

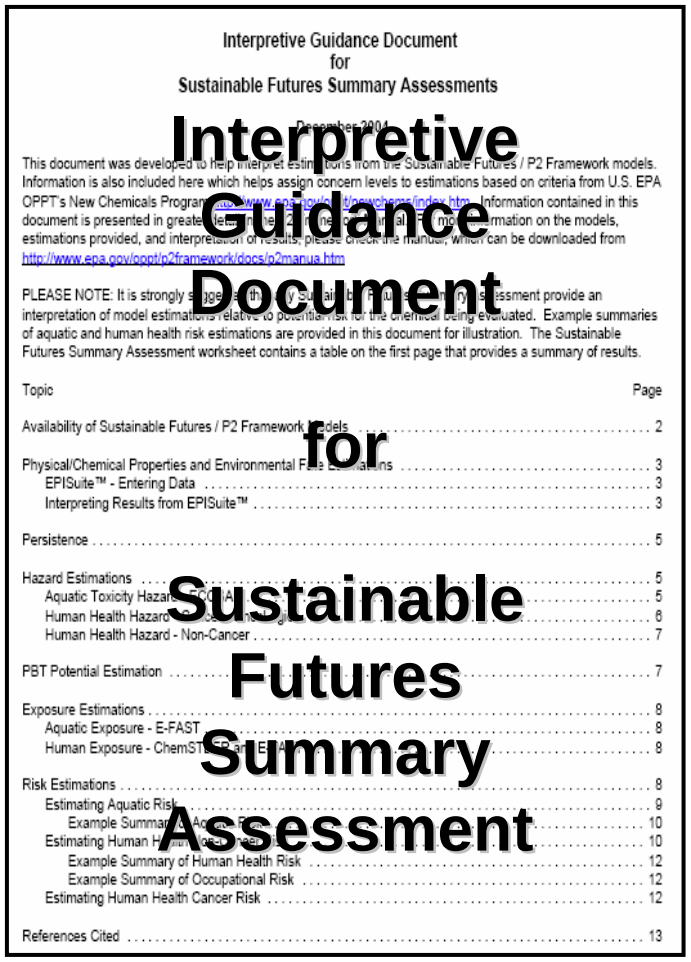
See the Interpretive Guidance Document page 1, for criteria for each endpoint listed under the Physical/Chemical Properties and Environmental Transport and Fate Sections.

Guidance

CAS No.	Submitter: SF Tissues, Inc
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	(EPI)
Boiling Point (deg C)	(EPI)
Boiling Point Pressure (mm Hg)	(EPI)
Vapor Pressure (mm Hg)	(EPI)
Water Solubility	mg/L (EPI)
Log K_{ow}	(EPI)
ENVIRONMENTAL TRANSPORT AND FATE	
Transport	
Henry's Law Constant – HLC	atm-m³-mole (EPI)
Soil Adsorption Coefficient – K_{oc}	(EPI)
Bioconcentration Factor – BCF	(EPI)
Persistence	
Experimental Biodeg Test	
Ultimate Biodeg Model	(EPI)
Primary Biodeg Model	(EPI)
BOD or COD	
Atmospheric Half-life	(EPI)
Hydrolysis Half-life	
Other Environmental Degradation	
Volatilization Half-life for Model River	(EPI)
Volatilization Half-life for Model Lake	(EPI)
Removal in Sewage Treatment Plant	(EPI)
Ready Biodegradability	(EPI)
Byproducts	
Degradation Products	Not Assessed
Metabolites	Not Assessed

SF Summary

Interpretive Guidance Document



Interpretive Guidance Document
for
Sustainable Futures Summary Assessments

December 2004

This document was developed to help interpret estimations from the Sustainable Futures / P2 Framework models. Information is also included here which helps assign concern levels to estimations based on criteria from U.S. EPA OPPT's New Chemicals Program (see http://www.epa.gov/oppt/newchems/tools.htm). Information contained in this document is presented in greater detail in the P2 Framework Manual. More information on the models, estimations provided, and interpretation of results, please check the manual, which can be downloaded from http://www.epa.gov/oppt/p2framework/docs/p2manua.htm

PLEASE NOTE: It is strongly suggested that Sustainable Futures Summary Assessment provide an interpretation of model estimations relative to potential risk for the chemical being evaluated. Example summaries of aquatic and human health risk estimations are provided in this document for illustration. The Sustainable Futures Summary Assessment worksheet contains a table on the first page that provides a summary of results.

Topic Page

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Interpreting Results from EPISuite™ 3
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Human Health Hazard - [illegible] 6
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Exposure Estimations 8
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Estimating Human Health Risk 10
Example Summary of Human Health Risk 12
Example Summary of Occupational Risk 12
Estimating Human Health Cancer Risk 12
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Interpretive Guidance Document for Sustainable Futures Summary Assessment

Assists assessors with:

- Interpreting P/Chem and Fate properties
- Interpreting experimental toxicity data
- Assigning hazard criteria
- Understanding terminology
- Performing Risk Calculations

Risk Assessment

Risk = Hazard x Exposure

If Hazard = 0, (Low Toxicity Concern)

or

If Exposure = 0, (Minimal Exposure Expected)

Then LOW Potential for Risk!

Risk Assessment

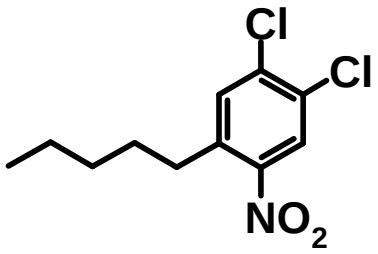
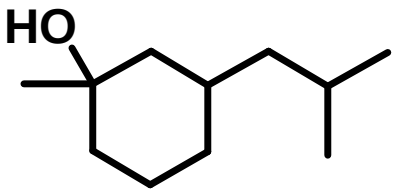
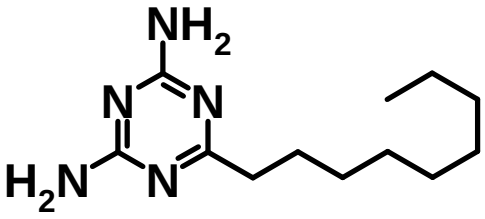
Examples:

Hazard (High Concern) x Exposure (Minimal) = Low Risk

Hazard (Low Concern) x Exposure (High) = Low Risk

Hazard (Moderate Concern) x Exposure (High) = Potential for Risk Exists

SF Sample Chemicals

Chemical Structure	Identity	Use	Production Volume (kg/yr)
	Example 1	Intermediate	50,000
	Example 2	Fragrance	10,000
	Example 3	Component of soldering flux	10,000