Tools and Approaches for Sustainable Chemicals Management

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Overview of presentation

- Moving towards safer chemicals and processes – Facility and chemicals planning
- Approaches to alternatives/substitution assessment
- Tools for understanding chemical risks and developing safer chemicals
- Challenges and lessons

Planning as a framework for chemicals management

- Implications of substitution or chemical reduction on process and product design.
  - Potential for significant changes in work organization and worker, community and environmental exposures.
  - Technical feasibility – substituting one multi-function chemical may result in the need for numerous replacements
- Important considerations that need thorough consideration.
- It's an important means to an end

The importance of planning

- Understanding materials flows and supply chain linkages
- Understanding production processes and product design – why and how chemicals are being used – the function of the chemical
- Understand options for reducing problem chemical use either in production process or product design – maintaining desired function.
- Understanding the performance, health safety and environmental trade-offs involved.
- Establishing priorities, performance targets and measuring progress towards more sustainable process and product design.

What planning can help achieve

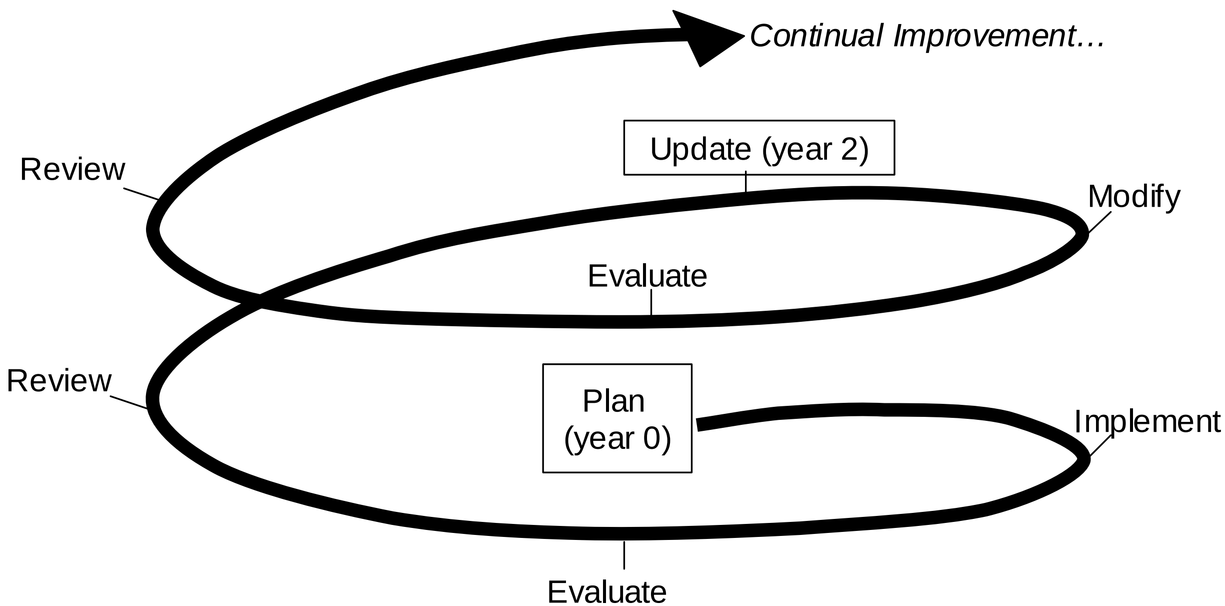
- Reorienting questions from quantifying problems to identifying solutions and opportunities
- Stimulating innovation
- Multi-risk reduction
- Greater multi-level involvement in firm in environmental/H&S activities

Steps of planning

- Problem identification
- Process/Product characterization and flows analysis
- Identification and development of a range of alternatives
- Identification of the consequences of the alternatives and comparison
- Decision
- Implementation
- Evaluation of results

TUR Planning Process

- Planning cycle when viewed as a continually improving



Defining substitution

- Substitution means the replacement or reduction of hazardous substances in products and processes by less hazardous or non-hazardous substances, or by achieving an equivalent functionality via technological or organizational measures (Okopol and Kooperationasstelle Hamburg)

What to consider in substitution/chemicals planning

- Substitution does not have to be chemical/chemical – trying to replace service or functionality (functional use approach)
- Risk trade-offs
  - Based on current data
  - Understand limits in data on alternatives
  - Clarity about uncertainties
- Focus on product is important
- Consider whole lifecycle – lifecycle thinking
- Understand supply chain
- What are most important criteria and how to compare?
  - Hazard, exposure, risk?

Goals of a substitution assessment method

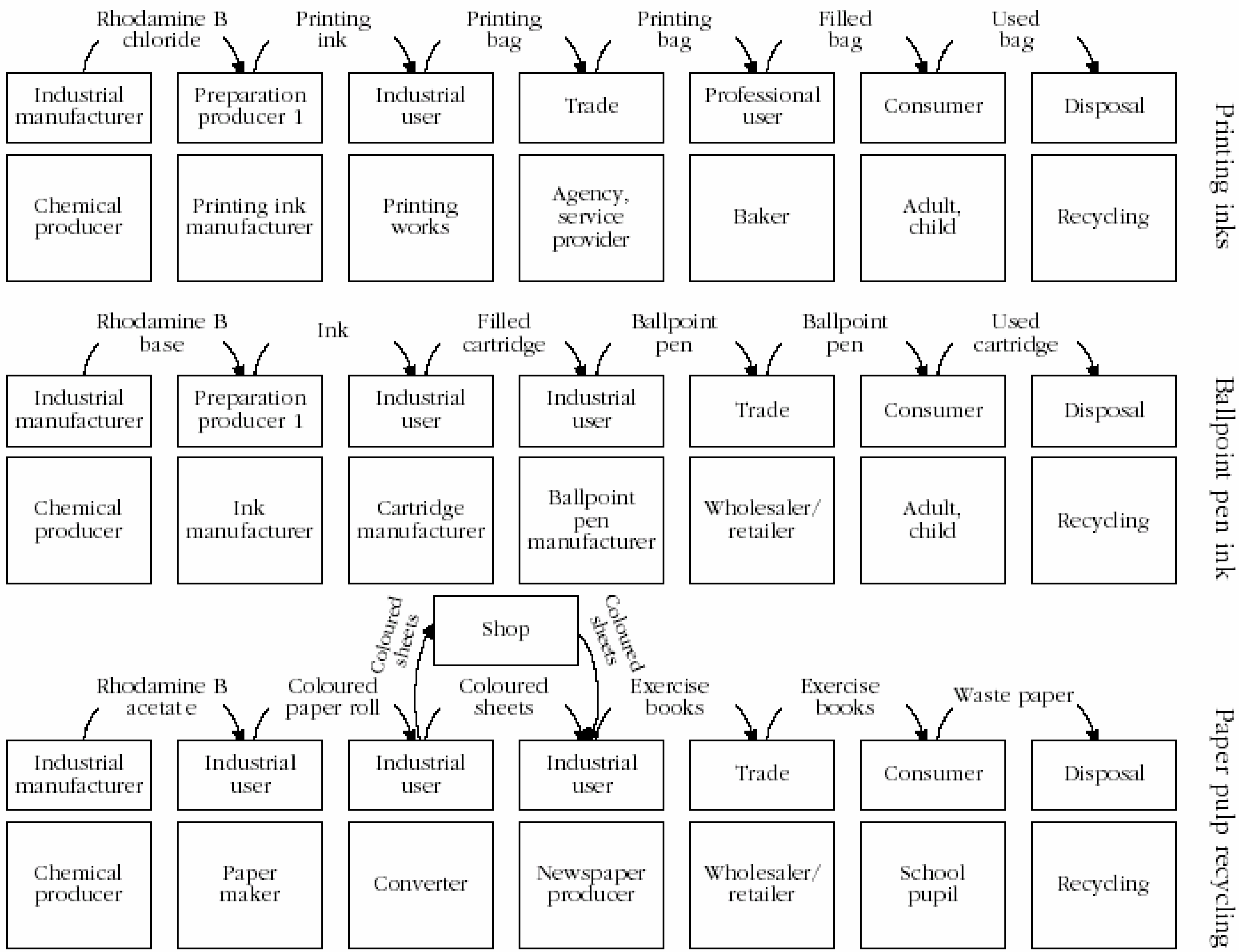
- Compare toxicity, physical hazards and other trade-offs at process and lifecycle levels
- Identify key criteria for avoidance or positive criteria (ie PBT)
- Allow flexibility to adapt to particular chemical, use
- Allow use of expert judgment
  - Number scores are easy but hide information
- Be simple and clear enough so that firms and regulators can use
- Outline a clear process/guidelines for “alternatives thinking” – link to design

Other goals

- Distinguish between whether a material is "inherently" toxic or not.
  - The toxic chemical used or generated as byproduct is intrinsic to the material's life cycle
- Identifying the inherent toxicity of a chemical helps to assess opportunities for reducing the toxicity profile of a material and opportunities for "greening"
- Example – perchloroethylene in cleaning

Figure 5-I

The complexity of chemical supply chains: Rhodamine B



Flows of chemicals and flows of information

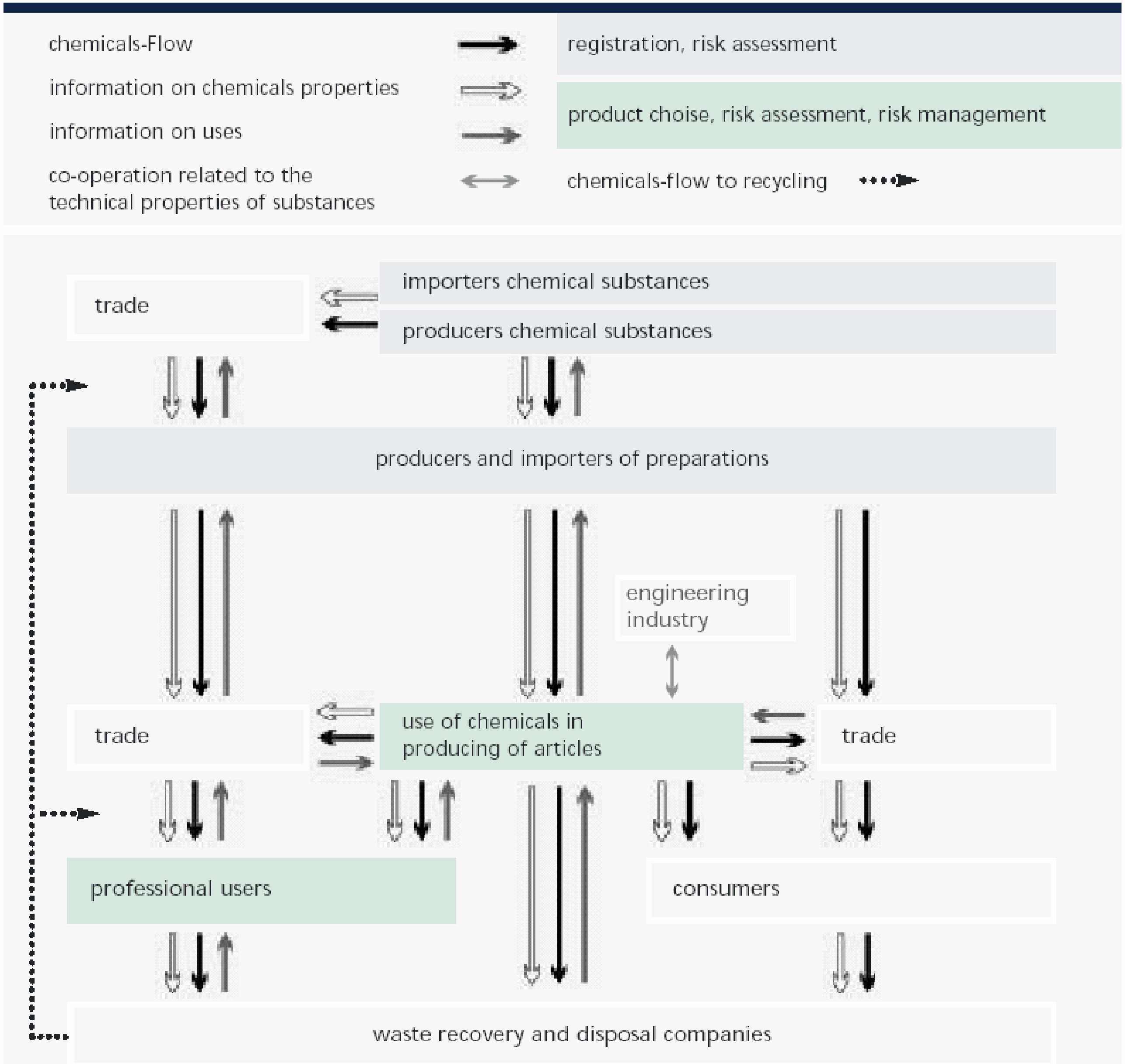


Fig. 1.1: Relevant players in the lifecycle of a chemical substance

Substitute Comparison tools

- Column Model
- COSHH Essentials
- GISBAU
- Swedish Guidance on Substitution
- EU Technical Guidance on Risk Reduction
- German Guidance for use of environmentally friendly substances
- Nordic Council Use of Decision-Aid Methods

Lowell Center Alternatives Assessment Framework

- Creating an open source framework for the relatively quick assessment of safer and more socially just alternatives. “Open source” means the collaborative development, sharing, and growth of methods, tools, and databases that facilitate decision making. “Relatively quick assessment” means that the process results in robust decisions informed by the best available science, while avoiding paralysis by analysis.

Parts of the Lowell Center Alternatives Framework

- Foundation, where values are made explicit by clearly articulating the Principles, Goals, and Rules that guide decisions made during the assessment of alternatives.
- Assessment Processes -- The methods, tools, and criteria used to evaluate which chemicals, materials, or products are safer and socially preferable. The Comparative Assessment Process and the Design Assessment Process are two separate yet overlapping tracks, varying depending on whether the subject of evaluation is an existing product or a product under development. For both having positive design criteria helps to set the stage and provide a benchmark for whether alternatives are moving towards safer materials/processes
- Evaluation Modules, which evaluate the economic feasibility, technical performance, human health and environment impacts, and social justice impacts of alternatives.

Figure 1. Alternatives Assessment Framework: Overview

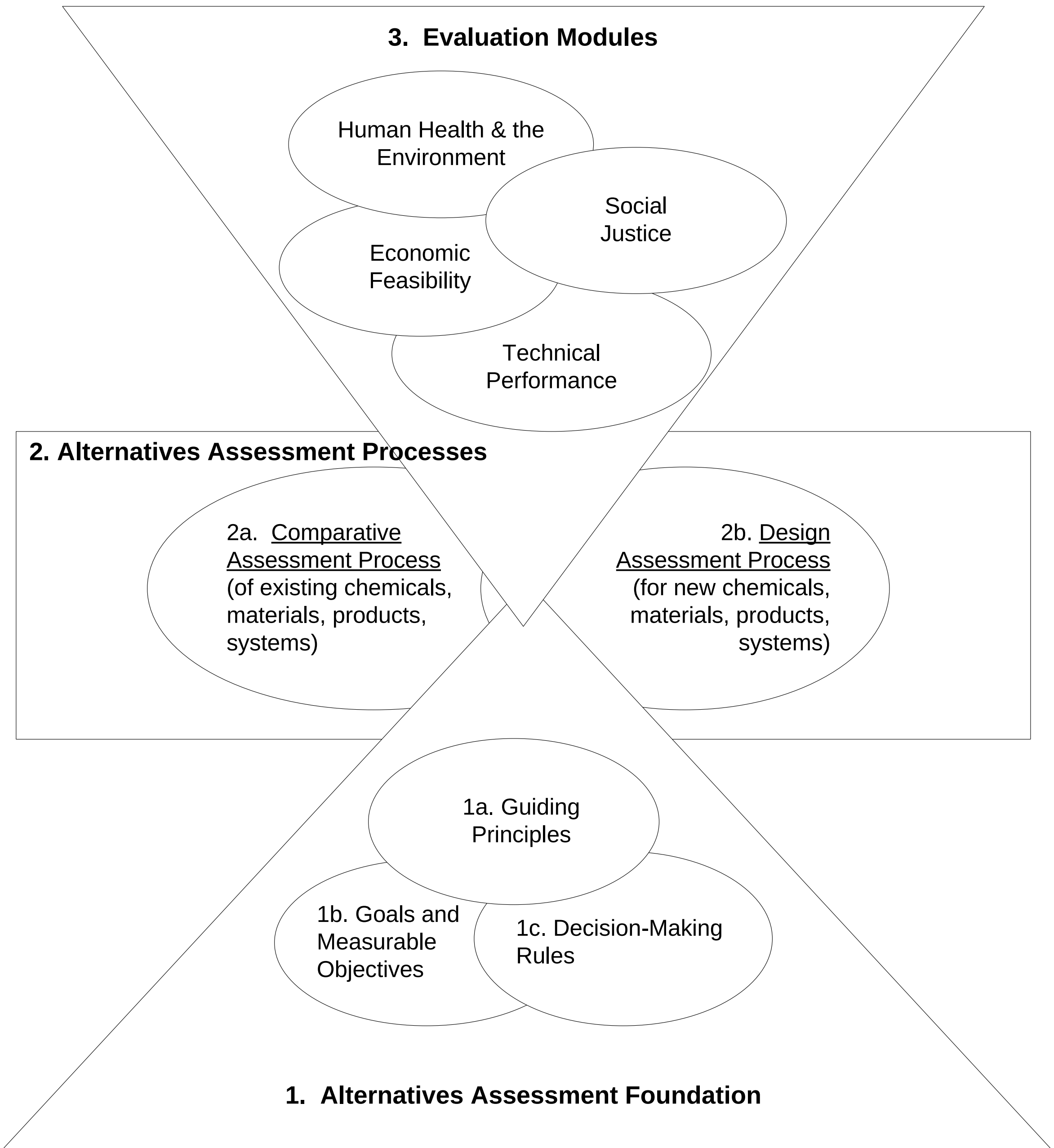
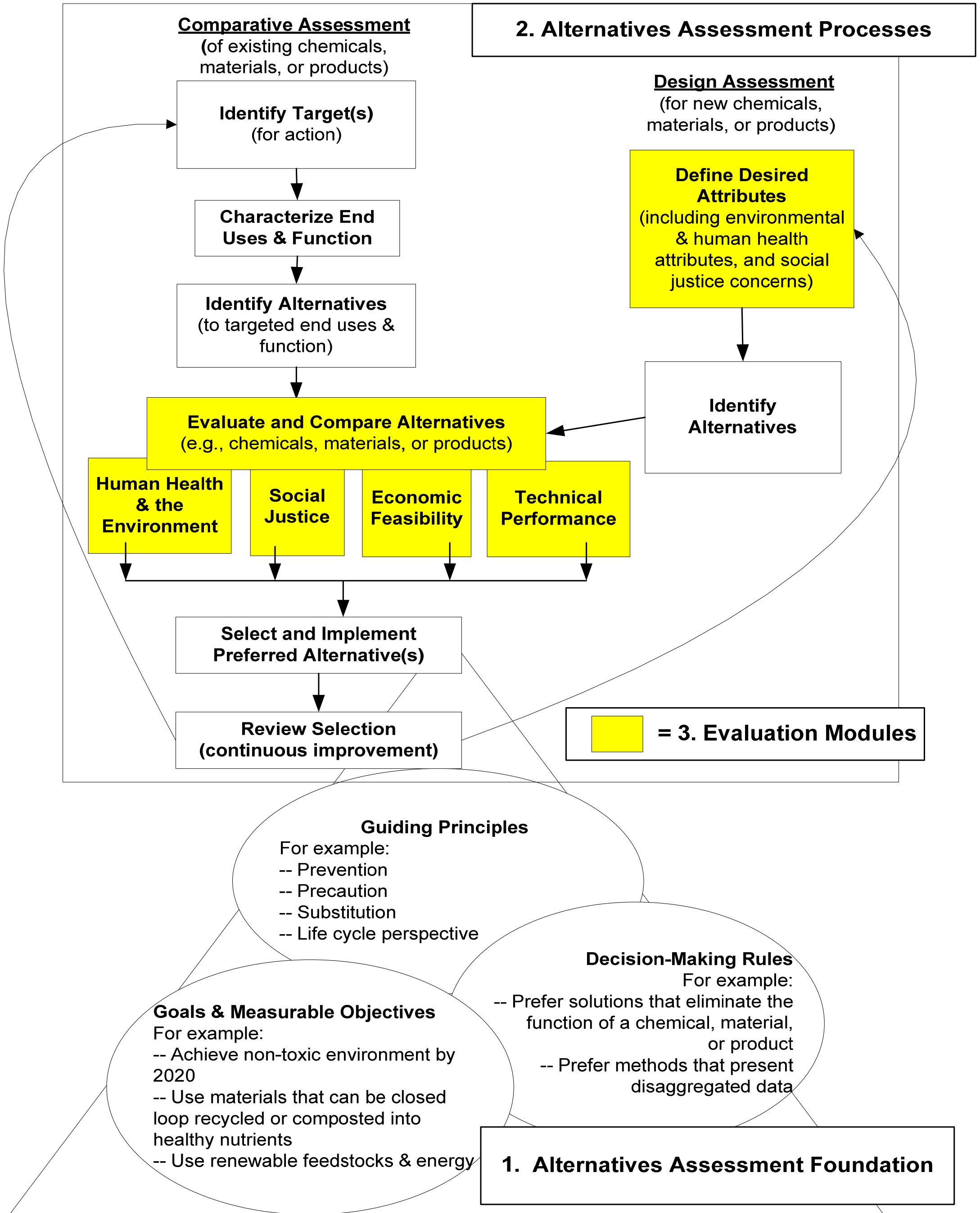


Figure 5. Alternatives Assessment Framework: Detailed Summary



Analysis Strategies

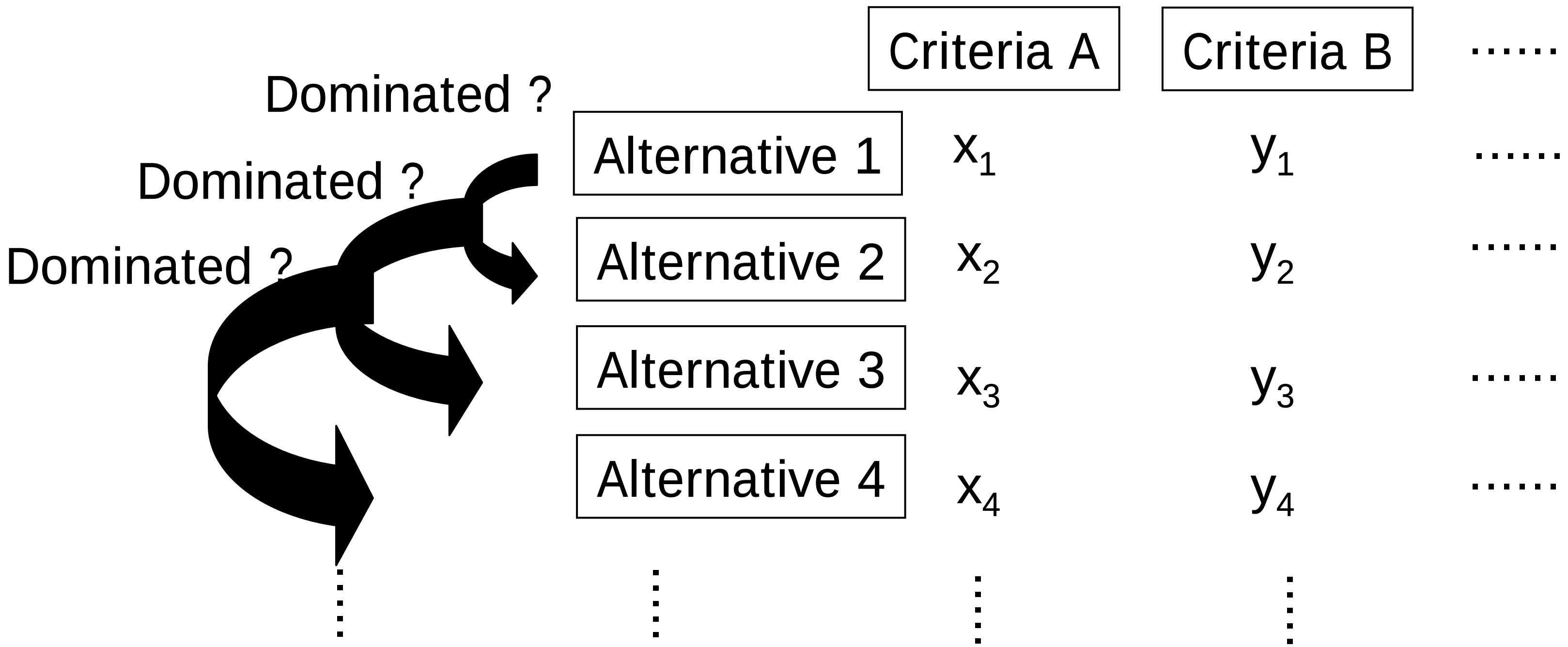
- Aggregated
  - Dominance Analysis
  - Position Analysis
  - Elimination by Aspects
  - Semi-Quantitative comparative analysis
- Disaggregated
  - Risk Benefit Quantification
  - Lifecycle assessment
- From (Okopol, 2003 and Nordic Council 1997)

Decision Matrix for Multi-Criteria problems

|—— Disaggregative ——| |— Aggregative —|

	Criteria A	Criteria B	Criteria C	......	
Alternative 1	x_1	y_1	z_1	......	⇨ K_1
Alternative 2	x_2	y_2	z_2	......	⇨ K_2
Alternative 3	x_3	y_3	z_3	......	⇨ K_3
Alternative 4	x_4	y_4	z_4	......	⇨ K_4
⋮	⋮	⋮	⋮		

Concept of Dominance Analysis

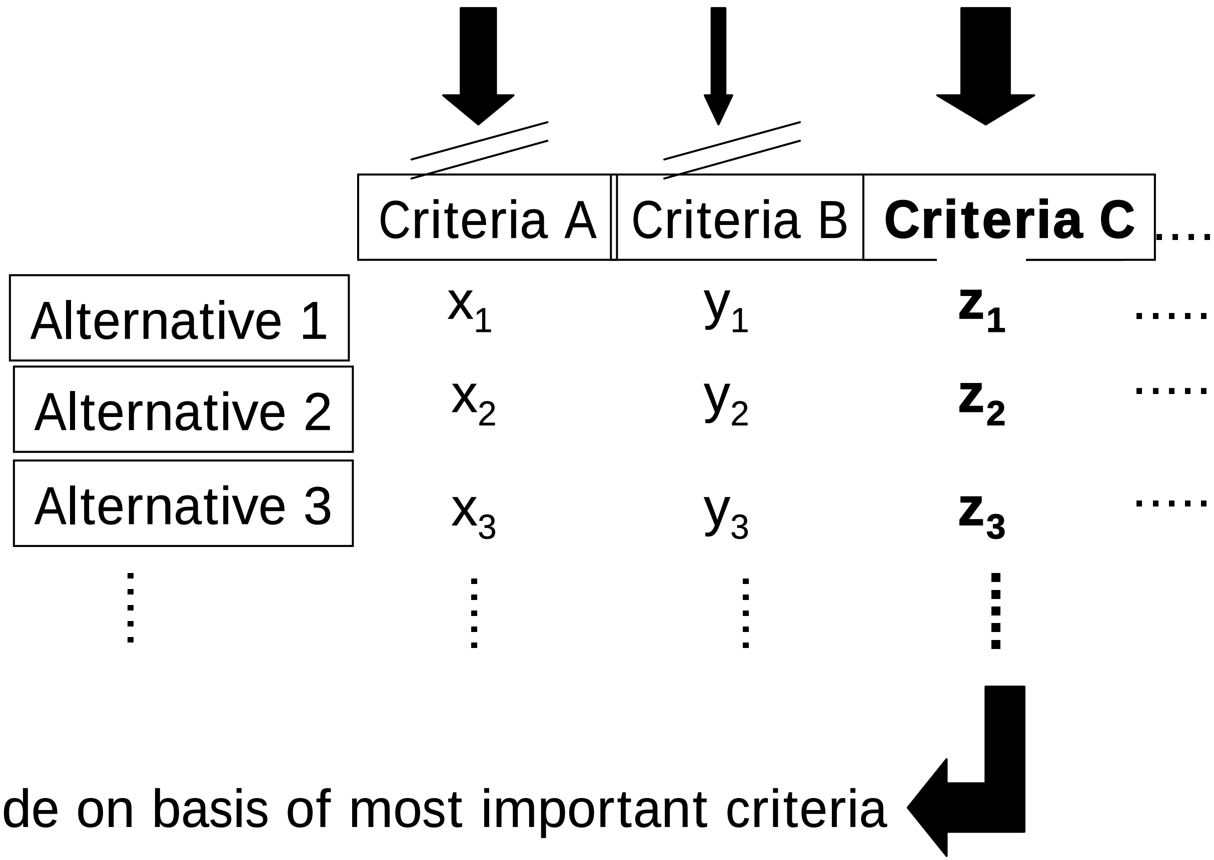


A number of non-dominated alternatives remain

Concept of Positional Analysis

Rank criteria in order of importance

Select most important criteria



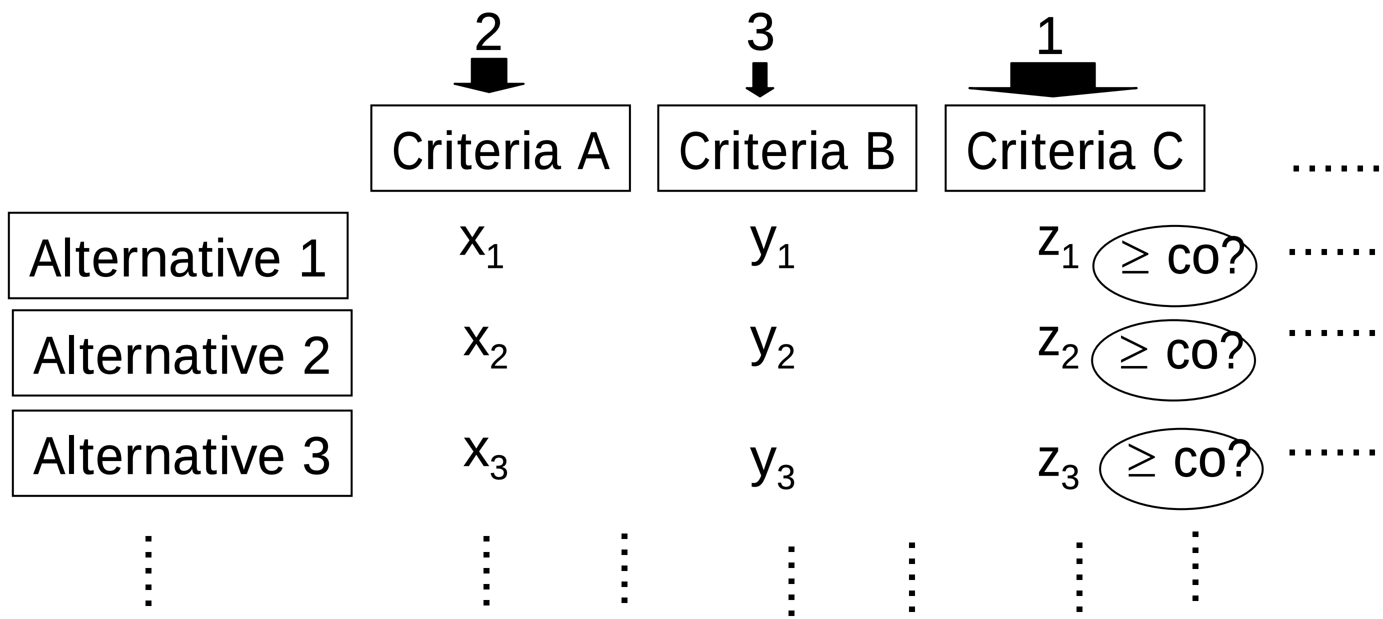
Decide on basis of most important criteria

Concept of Elimination by Aspects (EbA)

Establish cut-off values for each criterion

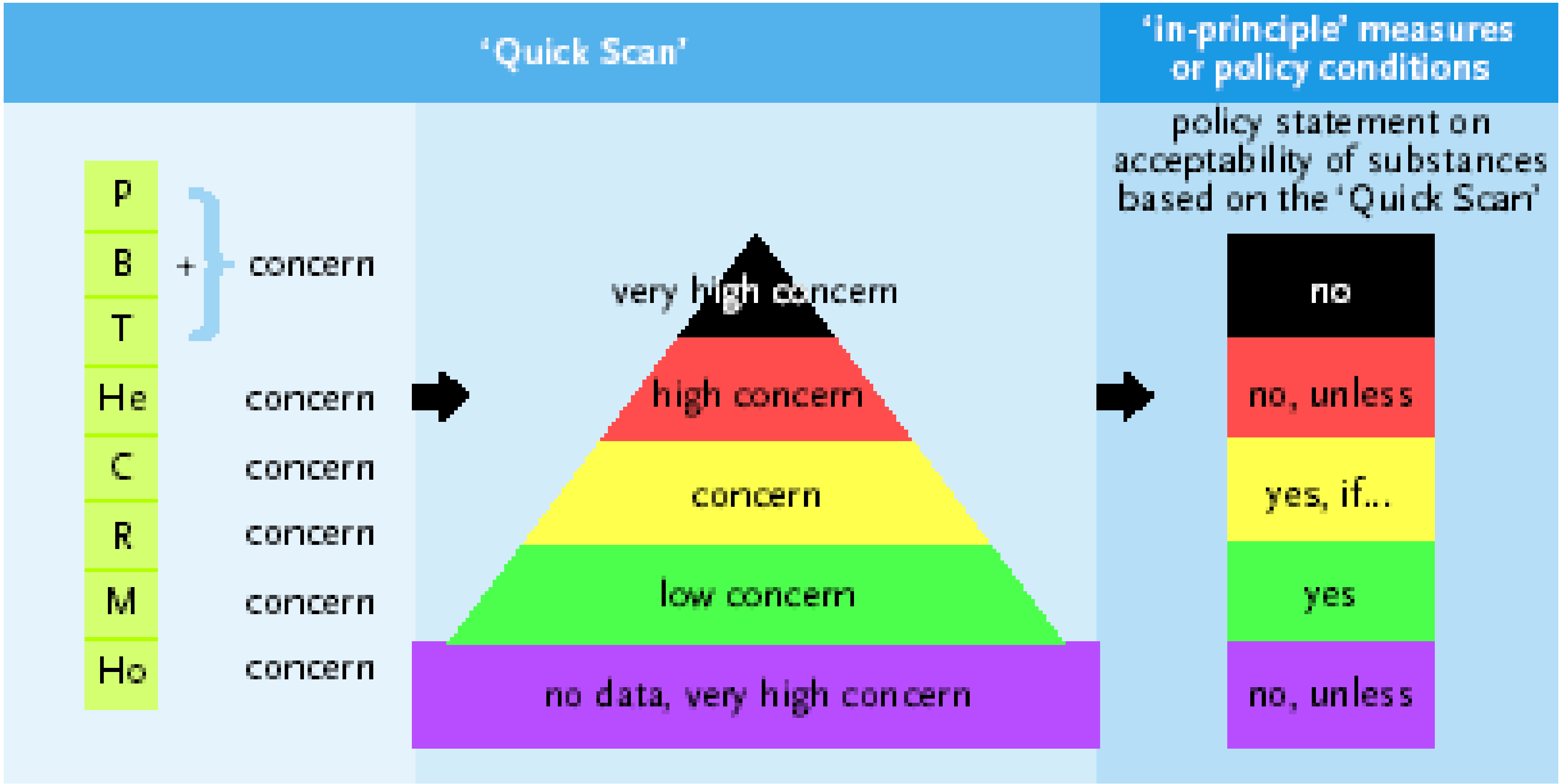
Start with most important criterion

Eliminate alternatives not meeting cut-off values (co)



Remaining alternatives fulfil most important cut-off values

Screening Method: Quick Scan



*Dutch Strategy on Management of Substances, 2001

Dutch Quick Scan - 2002

Substances in concern category on basis of hazard and use[22)]

CONCERN ON BASIS OF HAZARD / EXPOSURE ON BASIS OF USE	Use of substances as indication of exposure Site limited intermediate substances Low Exposure	Substances in industrial applications Exposure	Open professional use of substances High exposure	Substances in consumer applications Very high exposure
Very high concern	High concern	High concern	Very high concern	Very high concern
High concern	Concern	Concern	High concern	High concern
Concern	Concern	Concern	Concern	High concern
Low concern	Low concern	Low concern	Low concern	Concern
No data, very high concern	Very high concern	Very high concern	Very high concern	Very high concern

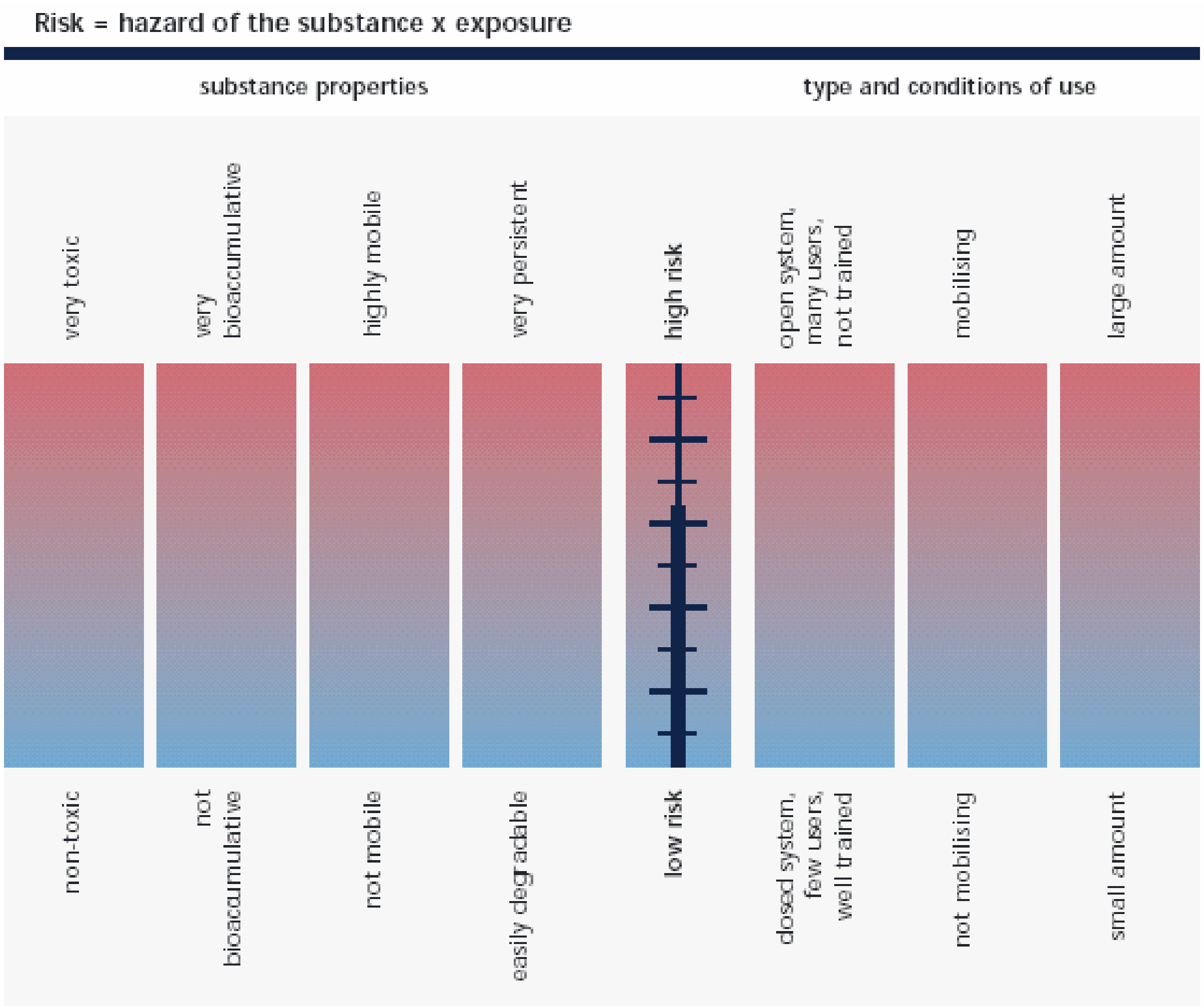


Fig. 1.3: Risk factors

German Guidance for the use of environmentally sound chemicals

Table 2.12: Risk profile TBBA in circuit boards

Five-step evaluation matrix

Contribution to risk	Persistence	Bioaccumulation	Aquatic toxicity	Chronic toxicity for vertebrates	Inherent mobility	Amount	Mobilising conditions of use	Indirect releases	Risk-index
very high									
high									
medium									
low									
very low									
weighting									

German Guidance for the use of environmentally sound chemicals

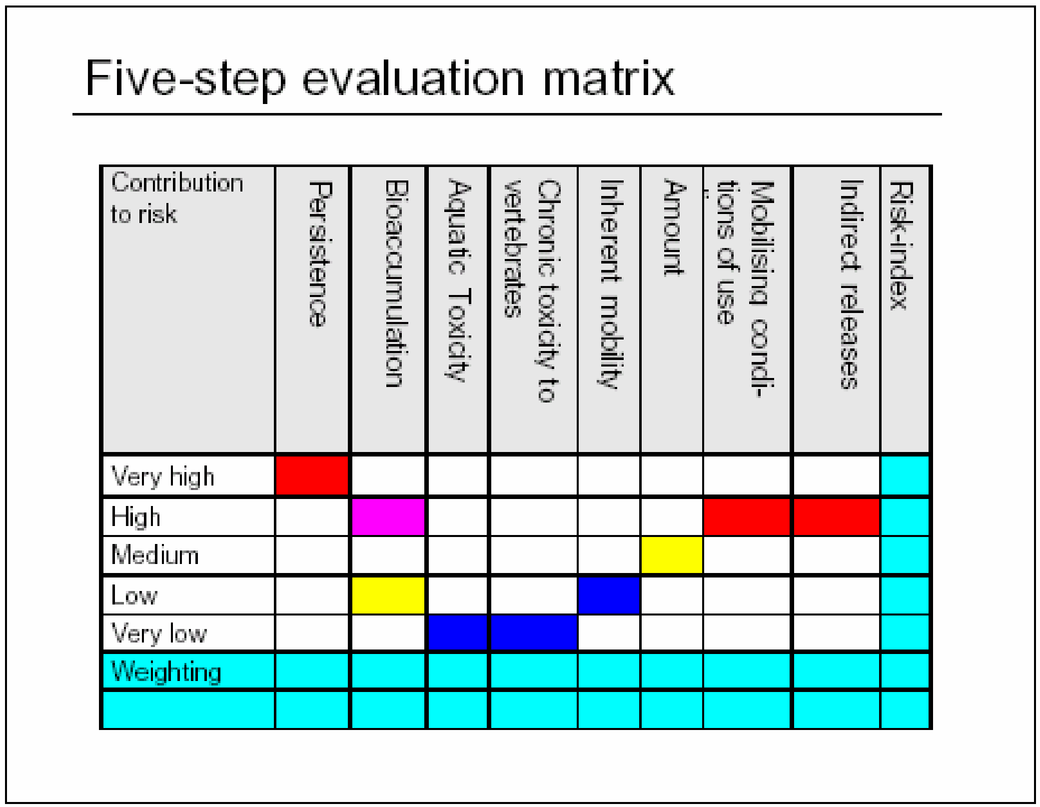


Table 2.11: Risk profile DECA in textiles

Column Model – to inventory and compare substances

<- To Alternative 3

Help !!!

Hazard -> Table

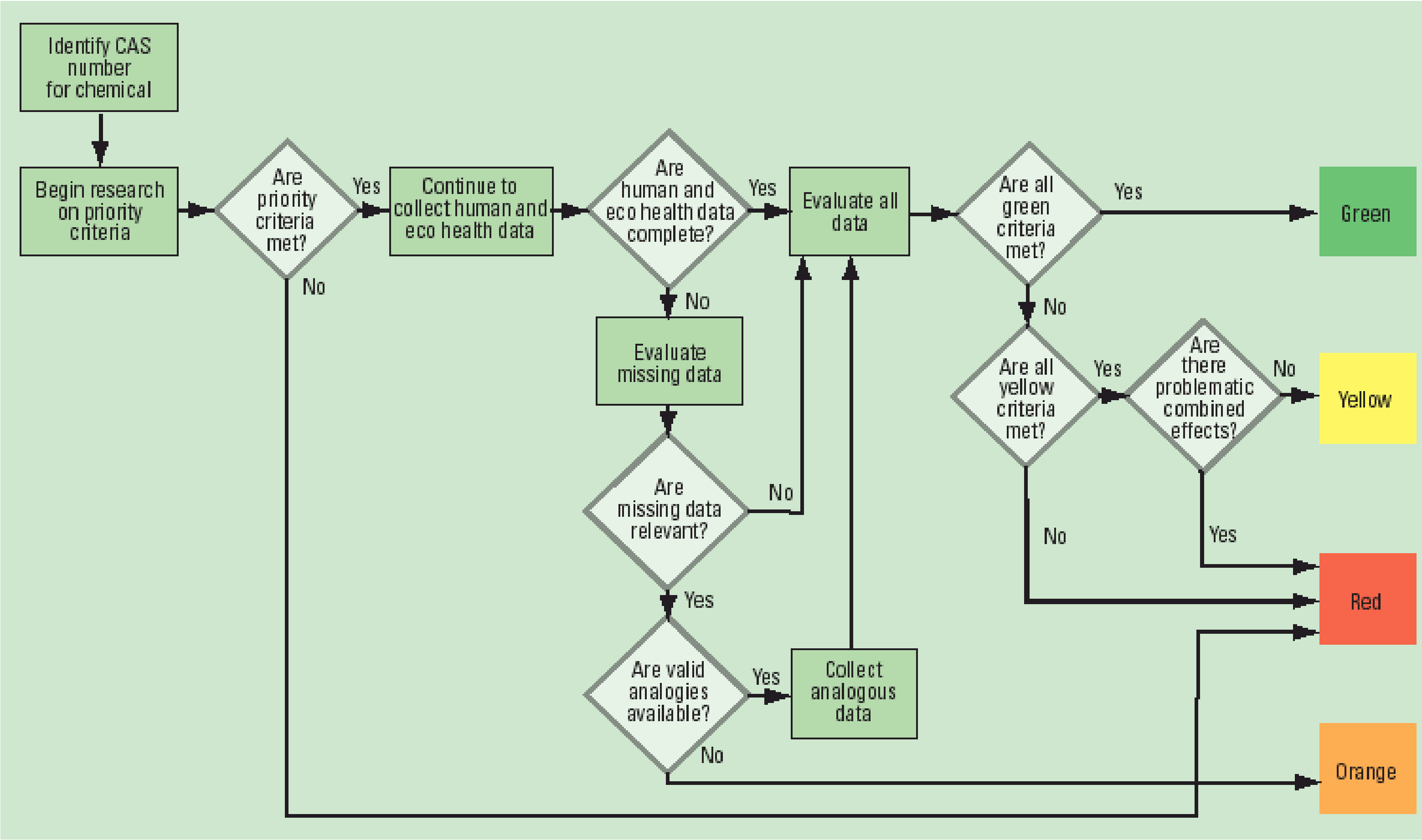
To Hazard Score Data Base

Comparative Scores

Category		Current		Alternative 1		Alternative 2		Alternative 3	
Acute human effects	**Units**	**Score**	**Cert.**	**Score**	**Cert.**	**Score**	**Cert.**	**Score**	**Cert.**
Inhalation LC50	ppm								
PEL/TLV	ppm								
PEL/TLV (dusts/particles)	mg/m3								
IDLH	ppm								
Respiratory irritation	L/M/H								
Oral LD50	mg/kg								
dermal irritation	L/M/H								
skin absorption	L/M/H								
dermal LD50	mg/kg								
ocular irritation	L/M/H								
Chronic human effects		**Score**	**Cert.**	**Score**	**Cert.**	**Score**	**Cert.**	**Score**	**Cert.**
Reference Dose RfD	mg/kg/day								
carcinogen	IARC/EPA Class								
mutagen	L/M/H								
reproductive effects	L/M/H								
neurotoxicity	L/M/H								
developmental effects	L/M/H								
respir. sensistivity/disease	L/M/H								
other chronic organ effects	L/M/H								
Physical hazards		**Score**	**Cert.**	**Score**	**Cert.**	**Score**	**Cert.**	**Score**	**Cert.**
heat	WBGT, °C								
noise generation	dBA								
vibration	m/S^2								
ergonomic hazard	L/M/H								
psychosocial hazard	L/M/H								

Preliminary chemical assessment steps from MBDC's materials assessment protocol

This flow chart describes how each chemical in a process is evaluated. A green rating indicates that a chemical presents little or no risk and is acceptable for the desired application. A yellow rating indicates low to moderate risk, and this chemical can be used acceptably until a green alternative is found. An orange rating means that the chemical is not necessarily high risk, but a lack of information prevents a complete assessment. A red rating means high risk. Chemicals with a red rating include all known or suspected carcinogens, endocrine disrupters, mutagens, reproductive toxins, teratogens, and chemicals that do not meet other human health or environmental relevance criteria.



Parameters for MBDC's materials assessment protocol

Human health criteria	Ecological health criteria
Carcinogenicity	Algae toxicity
Teratogenicity	Bioaccumulation
Reproductive toxicity	Climatic relevance
Mutagenicity	Content of halogenated organic compounds
Endocrine disruption	Daphnia toxicity
Acute toxicity	Fish toxicity
Chronic toxicity	Heavy metal content
Irritation of skin/mucous membranes	Persistence/biodegradation
Sensitization	Other (water danger list, toxicity to soil organisms, etc.)
Other relevant data (e.g., skin penetration potential, flammability, etc.)	

Herman Miller design for environment assessment criteria

Human health and eco-toxicological assessment

No problems identified or expected, or extremely low risk.
Low to moderate risk.
Lacking sufficient data to make a determination.
Severe problems or high risks identified or expected.

Human criteria

Carcinogenicity
Disruption of endocrine system
Mutagenicity
Reproductive toxicity
Teratogenicity
Acute toxicity
Irritation of skin/mucous membranes
Chronic toxicity
Sensitization
Others (e.g., carrier function, skin penetration potential)

Ecological criteria

Fish toxicity
Daphnia toxicity
Algae toxicity
Toxicity to soil organisms
Persistence/biodegradation

Bioaccumulation

Content of halogenated organic compounds
Heavy metal content
Climatic relevance/ozone depletion potential

Recyclability

Material is a technical or biological nutrient, and a commercial infrastructure exists.
Material can be down-cycled, and a commercial infrastructure exists.
Material can be incinerated for energy recovery.
Material is normally landfilled.

Recycled/renewable content

Percentage of total product weight
Post-industrial recycled content
Post-consumer recycled content
Renewable content

Disassembly

Can the component be separated with no dissimilar materials attached?
Can common disassembly tools be used (pry-bar, hammer, drivers, utility knife, pliers)?
Can one person disassemble the component in 30 seconds or less?
Can the material type be identified through markings, magnets, and so on?

So what to do when data for evaluation are scarce?

- Most chemicals in commerce lack some basic toxicity information
  - Situation is improving for High Production Volume Chemicals
  - REACH will solve some of the data gap problems
- Large quantity users can demand from suppliers
- Smaller quantity can use a series of tools
- Don’t need perfect data, just enough to make informed decisions and to understand hazards, exposures, and potential trade-offs
- How to integrate toxicity considerations at design stage?

Toxicity databases

- Commercial sources – ie Micromedix, Lifeline group, consultancies, other
- Public Sources:
  - Iris Database – Database of health effects of some 300 chemicals
  - The High Production Volume Information System (HPVIS) – EPA Database of information from HPV challenge
  - Toxnet – National Library of Medicine databases
  - Scorecard – put together by Environmental Defense
  - EU European Chemicals Bureau Databases

Framework Models

Phys/Chem Properties: EPI Suite™

MP, BP, VP; KOW; WS; KOC; Henry's law constant

Environmental Fate: EPI Suite™

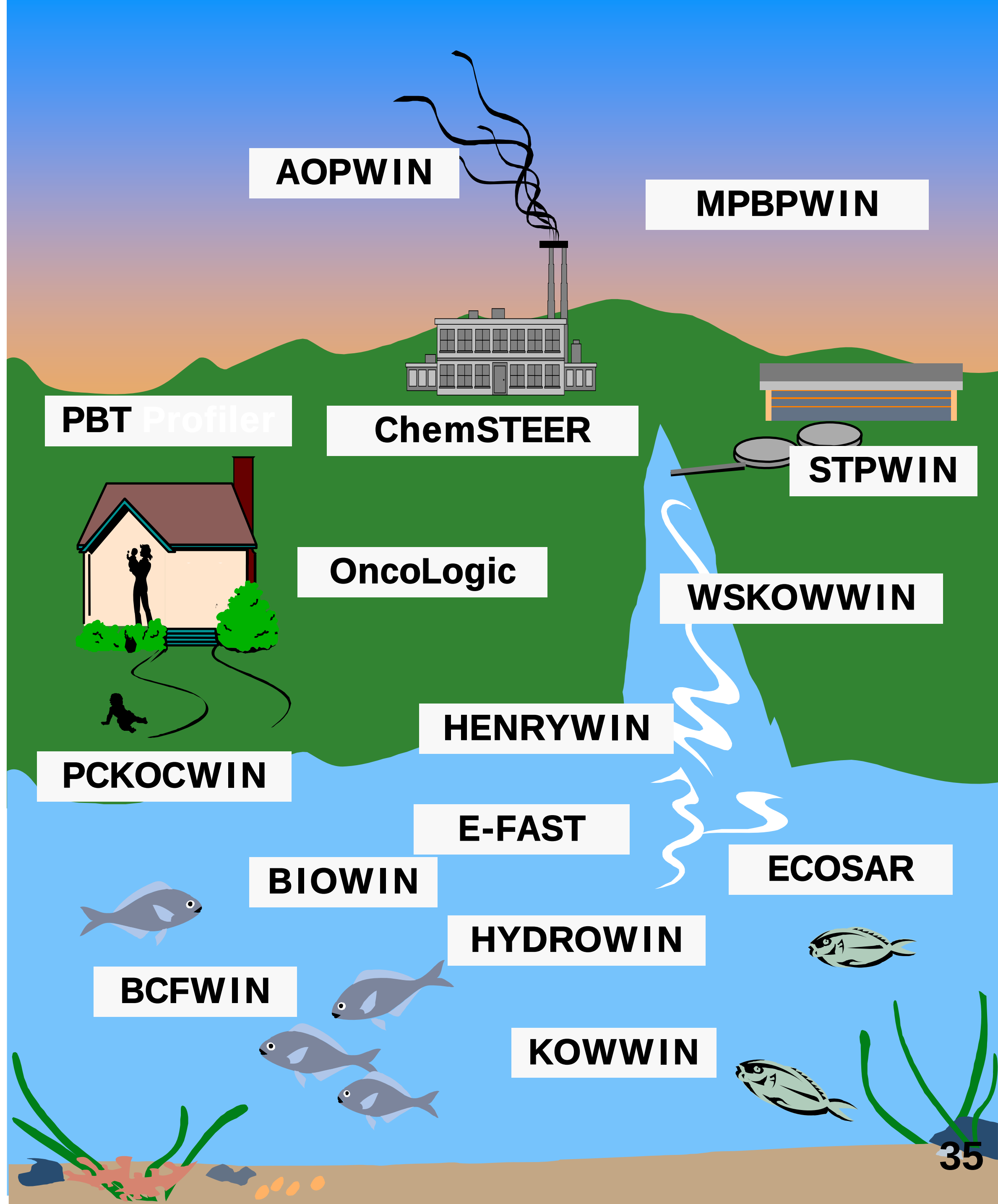
AOP; Fish BCF; Biodegradation; Hydrolysis; Removal in WWTP

Hazard

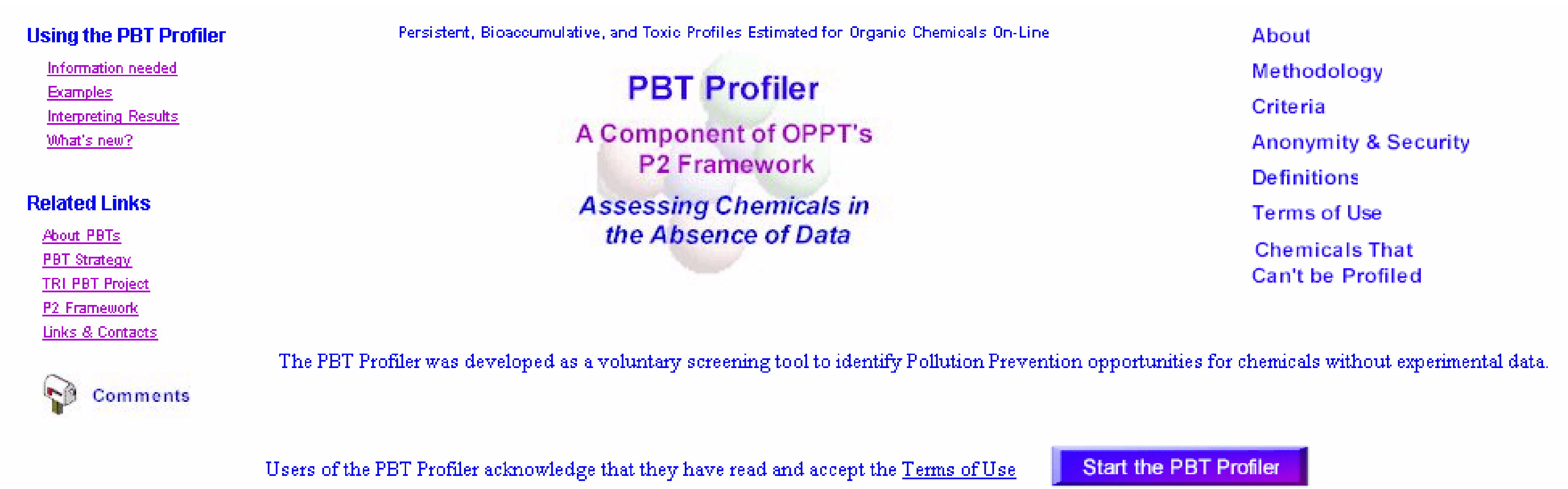
- ECOSAR Aquatic Toxicity
- OncoLogic - Carcinogenicity
- PBT Profiler PBT potential

Exposure / Risk

- ChemSTEER
  - Release amounts
  - Worker exposure
- E-FAST Human Risk: Consumer dermal & inhalation exposure, Human PDRs. Aquatic risk



The PBT Profiler Estimates Persistence, Bioconcentration potential, and fish chronic Toxicity <u>from chemical structure</u>



How Does the PBT Profiler Work?

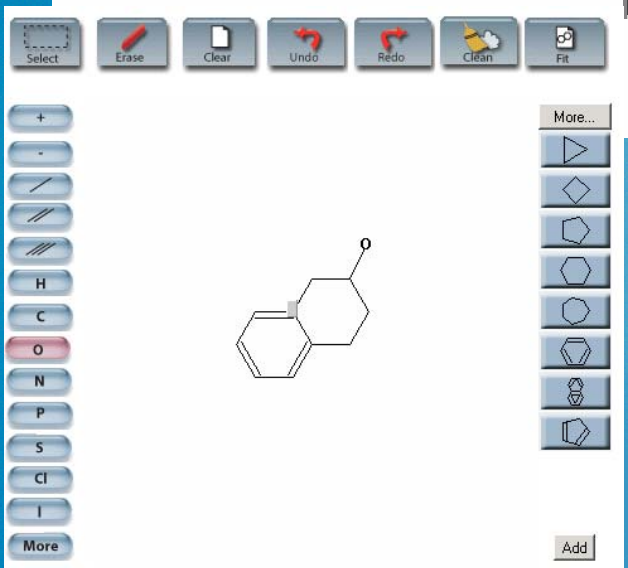
- Estimates physical/chemical and fate properties
  - Persistence: WS, K_{ow}, VP, Henry's Law constant, OH• and O_3 reaction rates, MP, MW, and ultimate biodegradation
  - Bioaccumulation: BCF
  - Toxicity: fish chronic value (ChV) from ECOSAR
- Uses a level 3 multi-media model to estimate distribution in water, soil, sediment, and air
- Compares P, B, and T estimates to EPA criteria and formats results in color-coded output (Level I)
- Provides quantitative results (Level II) and additional information for P2 assessments (Level III)

Data Entry – Chemical Information

CAS Registry Number:
(or other unique identifier) ACME 2323

Name: My compound

Smiles: c12c(CCC(O)C1)cccc2
120 characters or less



Continue Cancel

Results for a Non-PBT Chemical
Three Tiers of Results are

Methodology · Criteria · Definitions · Chemicals That Should Not be Profiled

Home · Start a New Profile · Results · Terms of Use · Security

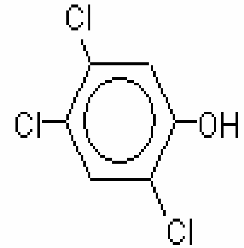
95-95-4 Phenol, 2,4,5-trichloro-

(1) Summary Results

PBT Profiler Estimate = PBT

Media	Half-Life (days)	Percent in Each Medium	BCF	Fish ChV (mg/l)
Water	60	11%	36	0.053
Soil	120	87%		
Sediment	540	2%		
Air	7.5	1%		

(2) Detailed Results



P2 Considerations and more information

(3) P2 Information

PBT Profiler Results – All 3 Criteria Exceeded

Results

Orange or red highlights indicate that the EPA criteria have been exceeded.
Black-and-white version

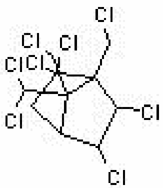
Persistence	Bioaccumulation	Toxicity

8001-35-2 Toxaphene

PBT Profiler Estimate = PBT

Screening estimates indicate this chemical may be a PBT - a P2 Assessment may allow further evaluation

Media	Half-Life (days)	Percent in Each Medium	BCF	Fish ChV (mg/l)
Water	180	1%	34,000	0.003
Soil	360	42%		
Sediment	1,600	57%		
Air	7.1	0%		



P2 Considerations and more information

“P2 Considerations” Information to Manage Risk

Pollution Prevention (P2) Considerations for “Phenol, 2,4,5-trichloro-”

PBT Profiler Estimate = P B T

Persistence Summary

Partitioning The PBT Profiler has estimated that if released to the environment, 'Phenol, 2,4,5-trichloro-' is expected to be found predominately in soil. It is also expected to be found in water and sediment.

Transformation and Persistence The PBT Profiler has estimated that 'Phenol, 2,4,5-trichloro-' is expected to be found predominately in soil and its persistence estimate is based on its transformation in this medium. Its half-life in soil, 120 days, exceeds the PBT Profiler criteria of >= 2 months (and <= 6 months). Therefore, 'Phenol, 2,4,5-trichloro-' is estimated to be persistent in the environment.

Pollution Prevention Considerations The PBT Profiler has estimated that the physical and chemical properties of 'Phenol, 2,4,5-trichloro-' indicate that it may have the potential to leach through soil and enter groundwater.

Long-Range Transport distances (CTD) The PBT Profiler has estimated that 'Phenol, 2,4,5-trichloro-' has a CTD in air of 2,400 Km. Using a published set of criteria, this value is considered relatively high, and 'Phenol, 2,4,5-trichloro-' has the potential to travel long from its original point of release.

Release Scenarios The following table provides the percent estimated in each environmental media using different release scenarios. The color of the estimates indicates if the PBT Profiler criteria have been exceeded in each medium, based on the following estimated half-lives for 'Phenol, 2,4,5-trichloro-': Water 60 days, Soil 120 days, Sediment 540 days, Air 7.5 days

Release to each Medium (Kg)			Percent in each medium			
Air	Water	Soil	Air	Water	Soil	Sed
1,000	1,000	1,000	1	13	84	2
1,000	1	1,000	1	1	98	0
1,000	1	1	13	6	80	1
1,000	1,000	1	5	55	31	8
1	1,000	1,000	0	14	84	2
1	1,000	1	0	86	1	13
1	1	1,000	0	0	100	0

Bioaccumulation Summary

Bioconcentration The estimated bioconcentration factor (BCF) for 'Phenol, 2,4,5-trichloro-' , 58, does not exceed the PBT Profiler criteria.

Bioaccumulation Estimate The PBT Profiler estimates that 'Phenol, 2,4,5-trichloro-' is not expected to bioaccumulate in the food chain.

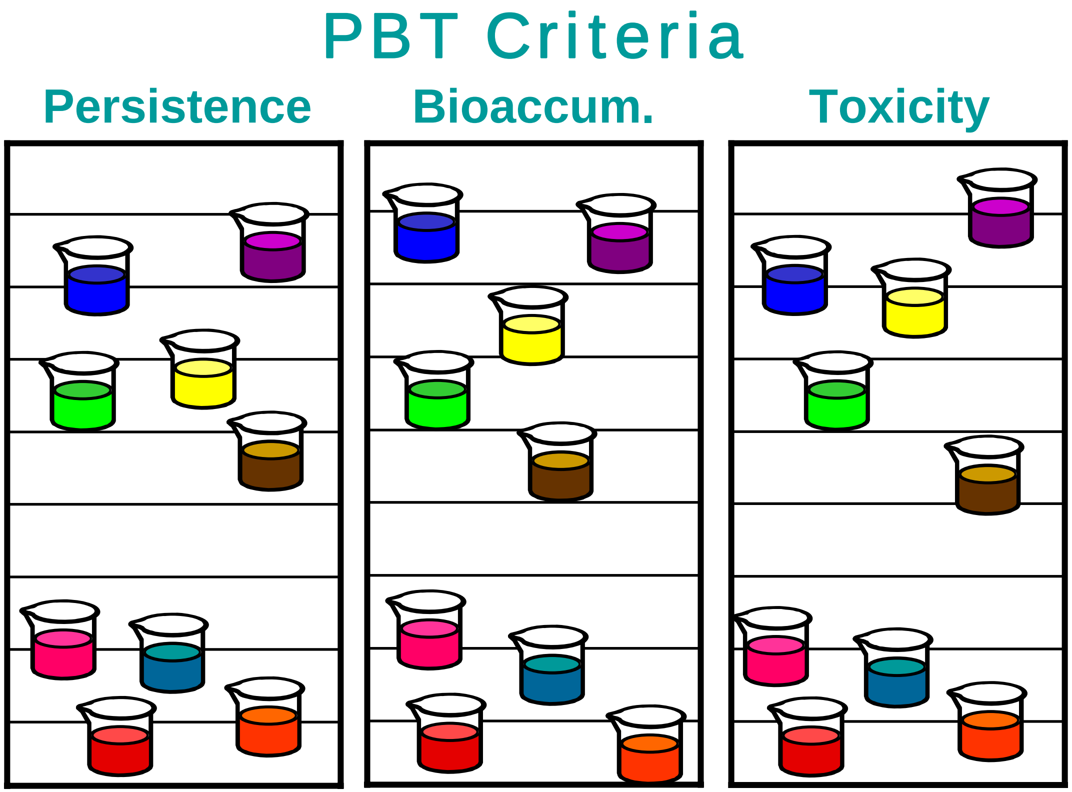
Toxicity Summary

Fish Chronic Toxicity The estimated fish chronic toxicity value (ChV) for 'Phenol, 2,4,5-trichloro-' , 0.053 mg/l, exceeds the PBT Profiler criteria (<0.1 mg/l).

Toxicity Estimate The PBT Profiler estimates that 'Phenol, 2,4,5-trichloro-' is estimated to be toxic to fish.

Bayer's PBT Profiler Case Study

Nine candidate chemicals were evaluated for PBT potential.

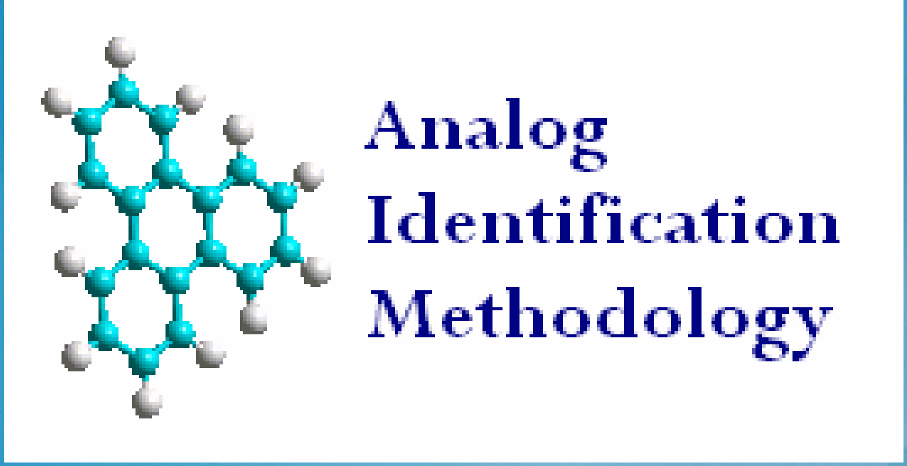


None exceeded PBT criteria, however, candidates with the most favorable characteristics were commercialized, and problematic chemicals were dropped.

Chemicals That Can Not be Profiled

- Chemicals With Experimental Data
- Inorganic Chemicals
- Reactive Chemicals
- Salts (Organic Salts)
  - Sodium (Na), Potassium (K), and ammonium (NH_4+) salts can be Profiled
- High Molecular Weight Compounds (MW > 1000)
- Chemicals with Unknown or Variable Composition
- Mixtures
- Surfactants
- Highly Fluorinated Compounds

Analog Identification Methodology (AIM)



Beta Test
Begins December 2004

Office of Pollution Prevention and Toxics
U.S. Environmental Protection Agency

AIM Methodology

- The AIM database contains 31,031 potential analogs with publicly available toxicity data
- Enter chemical by CAS, SMILES, or Drawing structure
- Experimental data sources Indexed
  - On-Line Databases

    TSCATS, HSDB, IRIS
  - U.S. Government Documents

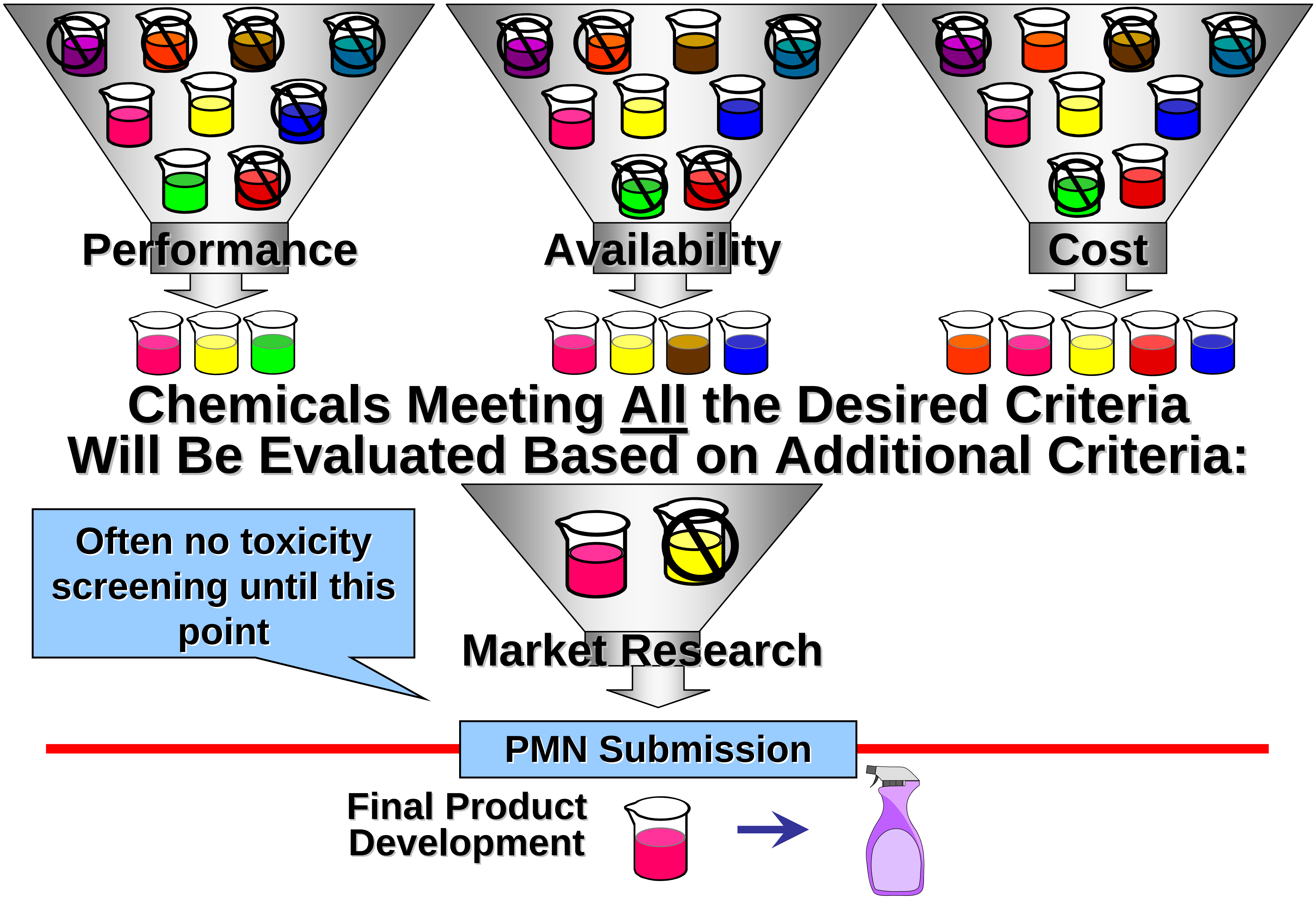
    NTP, ATSDR, HPV Challenge Program
  - Other Sources

    DSSTox, RTECS, IUCLID, AEGLS
- Uses a chemical fragment-based approach with 645 individual chemical fragments to identify potential analogs.

Other estimation tools

- Danish advisory list for self-classification of dangerous substances
- Swedish PRIO system
- US EPA Green chemistry expert system - Synthetic Methodology Assessment for Reduction Techniques (SMART)
- EPA Sustainable Futures Program http://www.epa.gov/oppt/newchems/pubs/sustainablefutures.htm
- Tools need to be used in conjunction with professional judgment, etc.

R&D Process - Status Quo



Moving toward safer design

- Green Chemistry is the utilization of a set of principles that reduces or eliminates the use or generation of hazardous substances in the design, manufacture and application of chemical products.
- Green chemistry is a revolutionary philosophy that seeks to unite government, academic and industrial communities by placing more emphasis on tending to environmental impacts at the earliest stage of innovation and invention. This approach requires an open and interdisciplinary view of materials design, applying the principle that it is better to not generate waste in the first place, rather than disposing or treating it afterwards.
- Green Engineering is the development and commercialization of industrial processes that are economically feasible and reduce the risk to human health and the environment.
- The principles of green chemistry and green engineering provide a framework for scientists and engineers to use when designing new materials, products, processes and systems.
- http://www.chemistry.org/portal/a/c/s/1/acsdisplay.html?DOC=greenchemistryinstitute\index.html

Principles of Green Chemistry – materials design principles

- It is better to prevent waste than to treat or clean up waste after it is formed.
- **Synthetic methods should be designed to maximize the incorporation of all materials used in the process into the final product.**
- Wherever practicable, synthetic methodologies should be designed to use and generate substances that possess little or no toxicity to human health and the environment.
- **Chemical products should be designed to preserve efficacy of function while reducing toxicity .**

More principles of Green Chemistry

- The use of auxiliary substances (e.g. solvents, separation agents, etc.) should be made unnecessary whenever possible and, innocuous when used.
- Chemical products should be designed so that at the end of their function they do not persist in the environment and break down into innocuous degradation products.
- **Analytical methodologies need to be further developed to allow for real-time in-process monitoring and control prior to the formation of hazardous substances.**
- **Substances and the form of a substance used in a chemical process should chosen so as to minimize the potential for chemical accidents, including releases, explosions, and fires.**

Design for Environment

- DfE is a recognized approach that companies first adopted in the late 1980s that involves thinking in terms of "design for" qualities or traits in products and process design. In the environmental field this involves approaches that promote reducing risks to human health and the environment through pollution prevention or source reduction instead of relying on end-of-the-pipe pollution control.
- Through the DfE approach, businesses can bring together performance, cost, and environmental considerations.
- http://www.epa.gov/oppt/dfe/

Challenges

- Identifying materials of concern
  - Which are they?
  - How do we know?
  - What data are available and how to get it?
- Inventorying materials of concern in supply chain
  - How do I find out what chemicals are in my final product or in the supply chain (either as a process chemical or part of the product?
  - How do I set up a materials accounting framework in the firm?
- Identifying toxicity/exposure data on current substance and alternatives
  - How do I determine what is safer?
  - What criteria are the most important with which to judge a chemical and alternatives?

More challenges

- Getting to zero – is it possible?
  - How do I set realistic goals for materials of concern and reward efforts to address the most important uses?
  - How do I measure progress towards those goals?
- Actual implementation
  - How will I ensure the alternatives actually provide sufficient functionality?
  - Will the alternatives be cost effective and will I be able to recoup that cost?
  - Can I market the change as more “environmentally-friendly?”

Lessons: the importance of planning

- First step is to understand “functions” a chemical/chemicals provide and whether that function can be provided through a chemical, process or product change.
- Need to understand materials flows and supply chain linkages
- Develop and Understand options for reducing problem chemical use either in production process or product design – maintaining desired function.
- Understanding the performance, health safety and environmental trade-offs involved.
- Establishing priorities, performance targets and measuring progress towards more sustainable process and product design.
- How options are evaluated/compared and progress is measured will depend on the firm.

Design and implementation of safer chemistry is not always easy

- Need for assistance in getting good data for analysis
- Need for research and development support to firms
  - Training in planning
  - Demonstration projects/sites
  - Networking of firms
  - Research support
  - Technical assistance to firms
- Need networking of supply chains and firms in sectors
- Rewarding leaders for their efforts

Lessons Learned – rapid screening and assessment tools

- Need for tools to rapidly characterize chemical hazards, exposures and risks
  - Data are limited and estimation tools have their limits
  - BUT: Comparative assessment, understanding trade-offs may be easier than absolute quantification
  - Mistakes may be made so need to be ready to change course.
- Need effective prioritization schemes
- Tools that identify positive criteria in chemicals.
- Need for good tools to compare alternative chemicals/processes but likely to be firm specific

Conclusion

- Need to go beyond next regulation to examining how to design and implement safer and cleaner processes and products
- Tools, approaches and support exist to help firms move forward though they have their limits
- More and more companies, academic institutions, and government agencies are moving in these directions.