EPA's PBT Profiler

PBT Profiler Helps Identify Persistent, Bioconcentrating and Toxic Chemicals

Workshop on PBT Reduction Activities and Opportunities, NEWMOA Web Conference
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Ihab H. Farag, Sc.D., P.E.
Hamel Professor of Innovation and Technology
Chemical Eng Dept
University of New Hampshire (UNH)
Durham, NH 03824-3591,USA
Phone: 1-603-862-2313, fax: 1-603-862-3747
email:ihab.farag@unh.edu

1

What is the PBT Profiler?

- ✓ Estimate Persistence, Bioconcentration Potential, and Fish Chronic Toxicity of a Chemical From the Structure
- ✓ Compares predictions to EPA regulatory criteria for PBT-related action under TRI and TSCA New Chemical Program (PMNs), and to international criteria
- ✓ Provides PBT-related data previously unavailable
  - Measured data retrieved if available
  - Predictions when data are lacking
- ✓ Useful when data are lacking about the chemical

2

PBT Profiler: Helps Identify Persistent, Bioconcentrating and Toxic Chemicals

Agenda

- Chemicals and PBTs
- PBT Profiler
- PBT Profiler Demo
- Next steps

3

R&D Process - Status Quo

Chemicals Meeting All the Desired Criteria Will Be Evaluated Based on Additional Criteria:

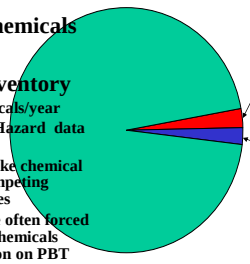
Market Research

Final Product Development

4

Chemicals in Commerce

Industrial Chemicals ~80,000
On TSCA Inventory
- ✓2,000 new chemicals/year
- ✓Relatively little Hazard data are available
- ✓Stakeholders make chemical choices among competing products / processes
- ✓Stakeholders are often forced to choose among chemicals without information on PBT tradeoffs.
- ✓Which chemicals are PBTs?



Pesticides ~2000

Drugs, Cosmetics, Food Additives ~2,000

5

Chemicals Are Considered PBTs If They Meet EPA and/or International PBT Criteria For

- ✓ Environmental Persistence AND
- ✓ Bioconcentration Potential AND
- ✓ Toxicity

6

EPA's PBT Profiler

Persistence (P) Criteria and Color scheme in PBT Profiler

Environmental Compartment	Half-Life (days)		
	Not Persistent	Persistent	Highly Persistent
Water (EPA NCP Program)	< 2 months	≥ 2 months	> 6 months
Soil	< 2 months	≥ 2 months	> 6 months
Air (TRI)	≤ 2 days		> 2 days
Sediment	< 2 months	≥ 2 months	> 6 months

Green Font | Orange Font | Red Font

7

Bioconcentration (B) Criteria and Color scheme in PBT Profiler

Bioconcentration Factor, Fish BCF		
No Regulatory Concern	Bioaccumulative	Highly Bioaccumulative
< 1,000	>= 1,000	>= 5,000

Green Font | Orange Font | Red Font

8

Fish Chronic Toxicity (T) Criteria and Color scheme in PBT Profiler

Toxicity Concern: Fish ChV (mg/l)		
Low	Moderate	High
> 10 mg/l or no effects at saturation	< 10 mg/l	< 0.1 mg/l

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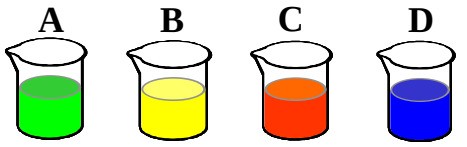
9

Which Chemical is a PBT?



Low	Green
Moderate	Orange
High	Red

10

Status of the PBT Profiler

- ✓ Created by EPA to address the PBT Initiative
- ✓ Developed as a collaborative effort with industry (ACC, SOCMA, CCC) and NGOs (ED)
- ✓ Beta tested by more than 100 participants from industry, academia, and government
- ✓ Peer Reviewed following EPA's Peer Review Guidelines and Peer Review is posted on EPA's E-Docket
- ✓ http://cascade.epa.gov/RightSite/dk_public_home.htm, "quick search" for "PBT Profiler"
- ✓ Released to the public in Sept 2002 and available at no cost at **www.pbtprofiler.net**

11

Why EPA Is Making The PBT Profiler Available to Industry?

- ✓ **Help Industry Pre-Screen Chemical Alternatives**
- ✓ **Understand Potential PBT Characteristics Of Product Alternatives Under Consideration at R&D**
- ✓ **Understand Potential PBT Trade-offs of Alternatives Under Consideration**
- ✓ **Reduce Product Development Costs**
- ✓ **Stimulate the Development of Environmentally Preferable Products and Processes**

12

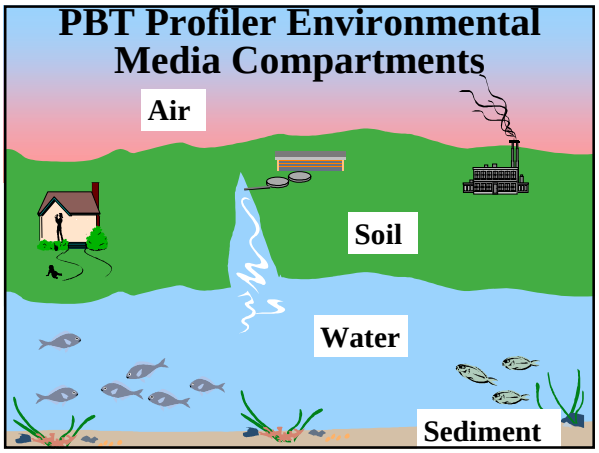
EPA's PBT Profiler

Hazard-related Information from PBT Profiler

- ✓Once released, will chemical go to air, water, soil, sediment?
- ✓How long will chemical stay in media?
- ✓Will chemical present a hazard?

13

PBT Profiler Environmental Media Compartments



www.pbtprofiler.net

15

Purpose of the PBT Profiler:

To identify materials that may need additional technical evaluation for Persistence, Bioaccumulation and Toxicity characteristics.

1. The PBT Profiler is a predictive screening tool to be used when data are not available. More information
2. For technical reasons, there are certain chemicals (or chemical classes) that should not be profiled with the PBT Profiler. More information
3. PBT Profiler predictions are not sufficient to definitively label a material a PBT chemical. The PBT Profiler is a research, not regulatory, tool to identify chemicals that may need further characterization. More information

I have read and understand the issues and considerations discussed above

Return to Home Page

Developed by the Environmental Science Center under contract to the Office of Pollution Prevention and Toxics, U.S. Environmental Protection Agency

16

PBT Profiler

Before running the PBT Profiler:

1. Determine the structure of the chemical you want to profile. Also have a chemical name and ID number (preferably a CAS Registry number) available.
2. Establish if any persistence, bioaccumulation, and toxicity data are available for your chemical. Chemicals with experimental data should not be profiled - the PBT Profiler is a screening-level predictive tool.
3. Read and acknowledge the PBT Profiler Terms of Use

Start the PBT Profiler

17

PBT Profiler

Methodology · Criteria · Definitions · Chemicals That Should Not be Profiled
Home · Start a New Profile · Results · Terms of Use · Security

Start a New Profile

Users of the PBT Profiler acknowledge that they have read and accept the Terms of Use

To start using the PBT profiler, enter a CAS Registry number or other identifier. 95-47-6 Lookup
Then, click on the 'Lookup' button to continue.

Need Help? Examples
Registry numbers and other identifiers
SMILES Notations
What the PBT Profiler lookup function does
Draw your chemical

18

EPA's PBT Profiler

PBT Profiler (o-Xylene, CAS 95-47-6)

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

Estimate the persistence, bioaccumulation, and toxicity of Benzene, 1,2-dimethyl- by starting the PBT Profiler [Start the PBT Profiler]

Or

Build the list of chemicals to be profiled by adding another CAS Registry number or other identifier: [ ] [Lookup]

Draw your chemical

List of Chemicals to be Profiled

#	CAS Number	Name	SMILES
1	95-47-6	Benzene, 1,2-dimethyl-	c(c(ccc1)C)(c1)C

[Update Name]

Black-and-white version

19

PBT Profiler (o-Xylene, CAS 95-47-6)

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Or

Build the list of chemicals to be profiled by adding another CAS Registry number or other identifier: [ ] [Lookup]

Draw your chemical

List of Chemicals to be Profiled

#	CAS Number	Name	SMILES
1	95-47-6	o-xylene	c(c(ccc1)C)(c1)C

[Update Name]

Black-and-white version

20

PBT Profiler (Output o-Xylene, CAS 95-47-6)

Results

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

Persistence | Bioaccumulation | Toxicity

95-47-6 o-xylene

PBT Profiler Estimate = PBT

Media	Half-Life (days)	Percent in Each Medium	BCF	Fish ChV (mg/l)
Water	15	32%	50	1.1
Soil	30	57%		
Sediment	140	1%		
Air	1.2	10%		

P2 Considerations

[Start a New Profile] [Add More Chemicals to Your Profile]

21

Pollution Prevention (P2) Considerations for o-xylene

PBT Profiler Estimate = P B T

Return to PBT Profiler Results

Chemicals that are persistent, bioaccumulative, and toxic have the potential to concentrate to levels that may cause significant averse impact on human health and the environment. Orange or red highlights for the above "PBT Profiler Estimate" indicates the EPA criteria have been exceeded for persistence (P), bioaccumulation (B), or toxicity (T) . The PBT Profiler estimates are designed for **screening-level** assessments to help identify Pollution Prevention (P2) opportunities for chemical substances when no experimental data are available. Experimental data should always be used in preference to the results of the PBT Profiler.

PBT Profiler Physical/Chemical Property Estimates

Molecular Weight	110	
Melting Point	-40	degrees C
Vapor Pressure	4.3	mm Hg at 25 degrees C
Log K_{ow}	3.1	at 25 degrees
Water Solubility	240	mg/L at 25 degrees C
Henry's Law Constant	0.0066	atm/m^3 mole at 25 degrees
Hydroxyl Radical Reaction Rate Constant	0.000000000013	cm^3/molecule-sec at 25 degrees C

22

Persistence Summary

Partitioning

The PBT Profiler uses three environmental compartments (water, soil, and sediment) to determine the persistence of a chemical in the environment. If released to the environment, o-xylene is expected to be found predominately in soil. It is also expected to be found in water and sediment .

The PBT Profiler does not explicitly consider a chemical's fate in the atmosphere in its persistence estimate. It also does not consider a chemical's potential to enter groundwater. Important P2 considerations in these media may be discussed on a chemical by chemical basis in the sections that follow.

Transformation and Persistence

The PBT Profiler has estimated that o-xylene 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, 30 days, does not exceed the EPA criteria. Therefore, o-xylene is estimated not to be persistent in the environment.

Pollution Prevention Considerations

The PBT Profiler estimates persistence in sediment by its potential for biodegradation in anaerobic (oxygen free) environment. Groundwater is also an anaerobic compartment. Chemicals may leach through soil and enter groundwater depending on thier physical and chemical properties. The PBT Profiler has estimated that the physical and chemical properties of o-xylene indicate that it may have the potential to leach through soil and enter groundwater. Pollution Prevention (P2) opportunities for this compound should also consider its potential transport to and persistence in groundwater. The PBT Profiler does not explicitly consider groundwater in its persistence estimate.

Long-Range Transport (CTD)

The Characteristic Travel Distance (CTD) is an expression of a chemical's potential for Long Range Transport (LRT), or its potential to be transported long distances. If a chemical travels long distances, it may become widely distributed in regions far from where the chemical was produced or used. The PBT Profiler considers a chemical's CTD in air, which provides insight into its potential widespread distribution through deposition from the atmosphere onto soil or water.

The PBT Profiler has estimated that o-xylene has a CTD in air of 580 Km. Using a published set of criteria, this value is considered relatively low, and o-xylene has limited potential to travel long distances in air. It is important to note that there are currently no generally recognized criteria for the CTD in air although International efforts to develop these critieria have been initiated. The PBT

23

Overall Persistence

The overall persistence is a calculated term that allows the persistence of different chemicals to be compared using a single value. Even though the units of the overall persistence are the same as those used for a chemical's half-life (hrs), these two terms are not inter-convertible. The overall persistence takes into account both a chemical's media-specific half-life *as well as* its rate of transport into (and out of) that compartment. Because the overall persistence takes into account transport, its value can be greater than (or less than) any of the media-specific half-lives.

The overall persistence can only be calculated in a mass-balance multimedia model. These models calculate the overall persistence by determining the the weighted average of the residence time in each compartment.

The overall persistence for o-xylene is 9.2 days using the default emission scenario of the level III multimedia model. The overall persistence using different release scenarios is provided in the following section.

Release Scenarios

The PBT Profiler estimates persistence based on a standard release scenario emitting equal amounts to soil, water, and air. A more in-depth P2 assessment may utilize a release scenario that is more representative of an individual chemical's life cycle. This section of the PBT Profiler provides seven different release scenarios to help identify P2 opportunities for o-xylene. The seven release scenarios are based on a total release of 300 kg/hr to the environment. Since the fugacity model is linear, the percent in each medium and overall persistence is dependent on the relative amounts released to each compartment and not the total amount released to the

Release to each medium (Kg/hr)			Percent in each medium				P_o
Air	Water	Soil	Air	Water	Soil	Sed	
100	100	100	11	32	57	1	9.2
150	0	150	13	0	87	0	8.4
300	0	0	99	0	1	0	1.7
150	150	0	18	80	0	2	6.3
0	150	150	6	34	60	1	13
0	300	0	6	92	0	2	11
0	0	300	6	0	94	0	15

24

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directly to the default persistence value, P, estimated by the PBT Profiler.

The overall persistence, P_o (days), calculated for each release scenario is also provided.

Bioaccumulation Summary

Bioconcentration The estimated bioconcentration factor (BCF) for o-xylene , 50, does not exceed the EPA criteria. Therefore, bioconcentration is not expected to be important.

Bioaccumulation Estimate The PBT Profiler estimates that o-xylene is not expected to bioaccumulate in the food chain.

Toxicity Summary

Fish Chronic Toxicity The estimated fish chronic toxicity value (ChV) for o-xylene , 1.1 mg/l, exceeds the EPA criteria (< 10 mg/l) .

Toxicity Estimate The PBT Profiler estimates that o-xylene is estimated to be toxic to fish.

Return to PBT Profiler Results

25

Flag for Chemicals on PBT Lists Benz(a)anthracene (CAS 56-55-3)

Data Entry

Benz a anthracene is listed as a PBT chemical in EPA's final rule on Persistent, Bioaccumulative, and Toxic Substances and/or as a Persistent Organic Pollutant (POP) by the United Nations Environment Programme (UNEP)

Estimate the persistence, bioaccumulation, and toxicity of Benz a anthracene by starting the PBT Profiler [Start the PBT Profiler]

Or

Build the list of chemicals to be profiled by adding another CAS Registry number or other identifier: [ ] [Lookup]

Draw your chemical [ ]

List of Chemicals to be Profiled

#	CAS Number	Name	SMILES
1	56-55-3	Benz a anthracene	c(c(c(c(c1)ccc2)c2)cc(c3ccc4)c4)(c1)c3

Benz(a)anthracene (CAS 56-55-3)

Methodology · Criteria · Definitions · Chemicals That Should Not be Profiled
Home · Start a New Profile · Results · Terms of Use · Security

Results

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

Persistence | Bioaccumulation | Toxicity

56-55-3 Benz a anthracene

PBT Profiler Estimate = PBT

Media	Half-Life (days)	Percent in Each Medium	BCF	Fish ChV (mg/l)
Water	60	4%	5,400	0.019
Soil	120	42%		
Sediment	540	54%		
Air	0.32	0%		

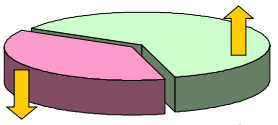
P2 Considerations

27

Limitations of the PBT Profiler

Over 60% of the 80,000 Chemicals on the TSCA Inventory Can Be Profiled using the PBT Profiler

Chemicals That Can Be Profiled (62%)
- Discrete organics
- Mixtures with representative component



Chemicals That Should Not Be Profiled (38%)
- Complex products (e.g., distillates and rosin)
- Natural products (e.g., oils, tallow, and enzymes)
- Chemicals of unknown structure (e.g., reaction products, ores)
- Metals and metal salts
- Polymers

28

Chemicals That Should Not be Profiled Using the PBT Profiler

- ✓ **Chemicals With Experimental Data** - Don't use predicted data when measured data exist!
- ✓ **Inorganic Chemicals**
- ✓ **Chemicals that Rapidly Hydrolyze** - Acid Halides; Isocyanates; Sulfonyl Chlorides; Siloxanes; alpha-Chloro ethers. Note: hydrolysis products can be evaluated.
- ✓ **Cationic salts** of Group I, Group II, Transition metals, Actinide, and Lathanide
- ✓ **Organo Metallic Compounds**
- ✓ **Highly Reactive Compounds**
- ✓ **High MW Compounds,** polymers, chems w MW >1,000
- ✓ **Mixtures** – Each substance in mixture can be evaluated
- ✓ **Chemicals with Unknown or Variable Composition**

29

Mixed Xylenes (CAS 1330-20-7)

Example of Flag for Mixtures

Start a New Profile

Note: The CAS Registry Number, 1330-20-7 [Xylene mixed], corresponds to a mixture of one or more substances. The PBT Profiler selected a representative structure for this mixture. This representative structure may, or may not, correspond to the mixture you are profiling. Therefore, the Persistence, Bioaccumulation, and Toxicity of this mixture may not be accurately represented by the PBT Profiler

As with all mixtures, the results of the PBT Profiler should be carefully scrutinized and used with caution. More information on the use of mixtures in the PBT Profiler is available on the Chemicals that Should Not be Profiled page.

[Add this Representative Structure to the Profile]
[Cancel]

30

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CAS 7439-97-6

Start a New Profile

This Chemical Can Not be Profiled.

The chemical, MERCURY, is either an inorganic compound or it contains a metallic element that the estimation methods used in the PBT Profiler were not designed for. More information on chemicals that can not be profiled using the PBT Profiler is available on this web site.

OK

31

PBT Profiler Security and Anonymity

- ✓ **All connections to the PBT Profiler are completely anonymous**
- ✓ **No user-entered or chemical information is purposefully or systematically written to a disk drive or other permanent storage device**
- ✓ **The only data collected are the number of PBT Profiles run**

32

PBT Profiler User Quotes

"The PBT profiler is an excellent tool to add to my risk assessment of existing and new chemicals"

"I will encourage my chemists to use it in their research projects in addition to the regulatory/tox assessment that I am responsible for."

"We think this is a useful tool... for new raw's we will surely check it."

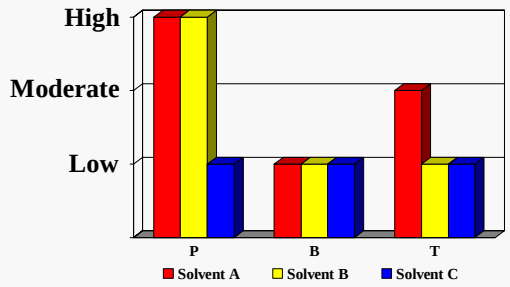
"This fits in well with our internal policy on lifecycle analysis and product stewardship."

"The PBT Profiler is an excellent instrument for a first screening of the potential impacts of substances"

33

P2 & PBT screening in the absence of data

PBT Comparison of Solvent A and Potential new Alternatives (B,C) **All solvents have no data**



34

The key to managing PBTs is Pollution Prevention

- ✓ **The EPA PBT Profiler is an excellent tool for Chemical Choosers and Chemical Formulators**

35

PBT Profiler: Next Steps

- ✓ **UNH Provides technology transfer and technical assistance in PBT Profiler**
- ✓ **Identify industry partners interested in using the PBT Profiler in case studies/success stories.**
- ✓ **Identify Small Business partners interested in using the PBT profiler in the decision making process.**

36

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PBT Profiler Contacts

Ihab Farag, UNH
ihab.farag@unh.edu
ph: 603-862-2313
fax: 603-862-3747

Dwight Peavey, EPA R1
peavey.dwight@epa.gov
ph: 617-918-1829
fax: 617-918-1810

Bill Waugh, USEPA
waugh.bill@epa.gov
ph: 202-564-7657
fax: 202-564-9063

Maggie Wilson, USEPA
wilson.maggie@epa.gov
ph: 202-564-8924
fax: 202-564-9063

37

Acknowledgment

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Bill Waugh 202-564-7657
Maggie Wilson 202-564-9063
Dwight Peavey 617-918-1829

38

39