Environmental Impact Assessment for Biofuel Associated Chemicals

Chem 234
Chris Vulpe
Spring 2013
Environmental Impact Assessment

- Environmental Fate and Transport (EFT)
- Persistence (P)
- Bioaccumulation (B)
- Toxicity (T)

Additional Selected Impacts
- Water specific - Eutrophication potential
- Air specific - Ambient ozone formation
- Particulate formation

<table>
<thead>
<tr>
<th>Compound</th>
<th>Environmental Fate and Transport</th>
<th>Persistence</th>
<th>Bio-accumulation</th>
<th>Toxicity (acute)</th>
<th>Toxicity (chronic)</th>
</tr>
</thead>
<tbody>
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</table>
Environmental Fate and Transport (EFT)

• Rarely measured
• Use Environmental Fate models to estimate distribution to different media (air, soil, water)
• Use Transport models to estimate movement through each media
• Important for determination of appropriate endpoints (bad things we should worry about) for each chemical.
Environmental Fate and Transport Data

• Environmental Fate Data Base –

• eChem Portal property search
  – http://www.echemportal.org/
Environmental Fate Data Base (EFDB)

Substructure search all of EFDB, TSCATS and PHYSPROP using ChemS³.

Click on one of the buttons below to search the database online.
Click here for more information.

- **DATALOG** is a bibliographic file containing 18 types of environmental fate data.
- **BIOLOG**, or the Microbial Degradation/Toxicity File, provides sources of microbial toxicity and biodegradation data.
- **CHEMFATE** is a data value file containing 25 categories of environmental fate and physical/chemical property information on commercially important chemical compounds. CHEMFATE has not been updated since the mid 1980's. For up-to-date physical properties, please go to the PHYSPROP database.
- **BIODEG** contains experimental values relating to biodegradation subjects. Records in BIODEG and BIODEG SUMMARY have been updated at varying times from the mid 1980's to approximately 2004 depending upon funding from EPA. The actual time of update can be found by searching individual records in BIODEG or by searching BIODEG SUMMARY by all reliability codes.
- **BIODEG SUMMARY** provides summary evaluation and reliability codes for different test methods, as well as summaries for biodegradability under aerobic and anaerobic conditions.

Databases last updated on July 16, 2008

EFDB provided on our site through partial support from

EPA, Procter & Gamble, and DuPont
• Environmental Fate and Transport Data

eChem Portal property search
http://www.echemportal.org/
EFT Prediction and Models

• EPI suite
  – [http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm](http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm)
  – Have to download and run on windows

• OECD Pov and LRTP Screening Tool
A tool for estimating overall persistence (POV) and long-range transport potential (LRTP) of ORGANIC chemicals
Plots results in comparison to ten compounds with known LRTD and POV (high and low)
In Class Exercise

• Pick on chemical of interest to you
• Use the Environmental Fate and LRTP tools to determine or estimate EF and LRTP
• Suggest each team member use different tool
• 15 minutes – report to class on findings/problems
Persistence (P)

- Usually predicted based on physico-chemical properties using computational models
- Degradation and Metabolism databases exist to predict likely metabolites which may have different properties
- Laboratory bio-degradation assays can be used for each media – generally based on use of chemical as carbon source
- Can be measured *in situ* by targeted analytical tools
Persistence/Biodegradation data sources

• eChem Portal property search

• Environmental Fate Data Base –

• University of Minnesota Biocatalysis/Biodegradation Database
Persistence/Biodegradation data sources

- eChem Portal property search
  – http://www.chemportal.org/
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EFDB provided on our site through partial support from EPA, Procter & Gamble, and DuPont.
Persistence/Bio-degradation prediction tools

• PBT profiler
  – http://www.pbtprofiler.net/

Chemicals that Should Not be Profiled

- Chemicals with Experimental Data
- Inorganic Chemicals
- Reactive Chemicals
- Salts (Organic Salts)
- High Molecular Weight Compounds
- Chemicals with Unknown or Variable Composition
- Mixtures
- Surfactants
- Highly Fluorinated Compounds
PBT profiler

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. 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

Black-and-white version

NOTE: The estimation modules used by the PBT Profiler have been updated. Some chemicals may produce different profiles than in prior versions. For a full list of updates see the "What's new" section.

Developed by the Environmental Health Analysis Center under contract to the Office of Chemical Safety and Pollution Prevention, U.S. Environmental Protection Agency

Computer Resources Donated by SRC, Inc.   Ver 2.000   Last Updated September 4, 2012
Bioaccumulation (B)

• Often linked with persistence/biodegradation
  – octanol-water partition coefficient ($K_{OW}$)
    • the ratio of the solubility of a compound in octanol (a non-polar solvent) to its solubility in water (a polar solvent).
  – bioconcentration factor (BCF)
    • ratio of the pollutant concentration in organism to that in water
  – bioaccumulation factor (BAF)
    • the ratio of contaminant concentration measured in biota in the field (or under multiple exposure conditions) to the concentration measured in the surrounding water.
  – biomagnification factor (BMF)
    • ratio of contaminant concentration in biota to that in the surrounding water when the biota was exposed via contaminated food
  – trophic magnification factor (TMF)
    • slope of a regression between the chemical concentration and trophic level of organisms in the food web.
Bioaccumulation Data sources

• ECOTOX
  – http://cfpub.epa.gov/ecotox/

• Ambit Database
  – http://ambit.sourceforge.net/euras/

Other sources – not too user friendly.
BSAF (Biota-Sediment Accumulation Factor)
http://www.epa.gov/med/Prods_Pubs/bsaf.htm
Welcome to ECOTOX Release 4.0. The ECOTOX (ECOTOXicology) database provides single chemical toxicity information for aquatic and terrestrial life.

For information on the latest data releases please see the Recent Additions.

View the Quick User Guide (PDF, 2 p. 244 KB) to help get you started.

You will need to turn off pop-up blockers for this site.

You should consult the original scientific paper to ensure an understanding of the context of the data retrieved from the ECOTOX database.
Quick Database Query

1. Select Query Parameters
   Scroll to or click on Chemical, Taxonomic, Effect, Publication Years

2. Select Report Format
   Scroll to or click on Report Format

3. Perform Query
   Click on Perform Query for Aquatic Data or Perform Query for Terrestrial Data buttons under Key Functions box.

Search Tip: Browse Species Index to find the best input format for your species information.

Kingdom:  
- Animals
- Plants

Effect Measurements

Search Tip: Browse the Effects Index to find the best input format for your effects.

- Endpoint Not Reported (NR)
- Statistics, No Endpoint
- Endpoint Reported

- Accumulation
- Behavior
- Biochemical
<table>
<thead>
<tr>
<th>Spec. Sci. Name</th>
<th>Exp. Type</th>
<th>Media Type</th>
<th>Resp. Site</th>
<th>Endpoint</th>
<th>Trend</th>
<th>Effect</th>
<th>Conc (ug/L)</th>
<th>Stat. Signif.</th>
<th>Ref#</th>
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<tr>
<td>Ulva rigida</td>
<td>S M</td>
<td>SW LAB</td>
<td>7</td>
<td>BCF</td>
<td></td>
<td></td>
<td>ACC RSDE</td>
<td>A 1000 ug/L</td>
<td>7588</td>
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Ambit Database
http://ambit.sourceforge.net/euras/

<table>
<thead>
<tr>
<th>#</th>
<th>CAS</th>
<th>Substance common name</th>
<th>Reliability score</th>
<th>Species</th>
<th>Species sex,M/F/MF/nd</th>
<th>Fish weight,g</th>
<th>Fish length,cm</th>
<th>Fish age</th>
<th>Temperature,°C</th>
<th>Job</th>
<th>Tissue analyzed</th>
<th>BCFss</th>
<th>BCFs</th>
<th>BCFss lipid,Cf</th>
<th>Lipid,%</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>91-20-3</td>
<td>naphthalene</td>
<td>1</td>
<td>Cyprinodon variegatus (sheepshead minnow)</td>
<td>MF</td>
<td>2.47</td>
<td>4.7</td>
<td>adult 25</td>
<td>1</td>
<td>whole body</td>
<td>714</td>
<td>7360.824742 999</td>
<td>10307</td>
<td>9.7</td>
<td></td>
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| EURAS bioconcentration factor (BCF) Gold Standard Database
| CAS Registry number | Enter CAS registry number (hyphenated) or click on the CAS field in the result list
| Chemical name | Searches for names that sound like user specified name (e.g. naftalen' will hit 'naphthalene')
| Reliability score | Enter one of 1,2,3 or MITI or click on the 'Reliability score' field in the result list
| Species | Enter species latin name (e.g. Pimephales promelas) or click on the species field in the result list

All criteria are combined with 'logical AND'. If no criteria is specified, entire database is retrieved.
Bioaccumulation Prediction

• PBT Profiler - uses the atomic structure to estimate properties of a substance, but focuses on properties relating to persistence, bio-accumulation, and toxicity.

• ToxPredict – Open tox module
  – [http://www.opentox.org/toxicity-prediction](http://www.opentox.org/toxicity-prediction)

• Vega QSAR
  – Need to register and download Java program
  – Need smiles file - get from Chemspider
ToxPredict

Estimate toxicological hazard of a chemical structure

Please select the structure(s) for which you would like to apply some OpenTox models.

- Draw

Search

Query: benzene

Search mode

- Auto detect
- Exact structure
- Substructure search
- Similarity search

Search

Predictions

- [CADASTER FP7] UI: logKow (TAZ & BTAZ) Calculate
- [CADASTER FP7] logKow_MLRA_[EState], 20560 Calculate
- [CADASTER FP7] UI: BCF tutorial Calculate

Datasets

Environmental fate parameters >> Persistence: Biodegradation

START biodegradation and persistence plug-in Calculate
In Class Exercise

• Use same chemical as in previous example
• Use the Persistence and Bioaccumulation tools to determine/estimate persistence and bioaccumulation
• Suggest each team member use different tool
• 15 minutes – report to class on findings/problems
Toxicity (T)

• Most difficult to predict – very rarely measured *in vivo*.
• Empirical data in eco-indicator species used if available
• Important to consider organisms in different trophic levels
• Generally identify the most sensitive species as indicator of potential ecosystem toxicity
Toxicity Data Sources

Authoritative Body Lists and Lists of Lists
• Pharos project
  – http://www.pharosproject.net

Toxicity Databases
• EPA ecotox Database
  – http://cfpub.epa.gov/ecotox

• Toxnet – 14 databases

• eChem Portal – OECD 17 databases
  – http://www.echemportal.org/

• ESIS : European chemical Substances Information System -aggregates data from a number of other European databases
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Eco-Toxicity Prediction

• ECOSAR - Ecological Structure-Activity Relationship estimator, attempts to estimate the toxicity potential of a substance based on its atomic structure
  – [http://www.epa.gov/oppt/newchems/tools/21ecosar.htm]
  – Need to download and run on windows

• AIM, or Analog Identification Methodology – estimates toxicity hazard by comparing an unknown chemical to analogs which have been tested
  – [http://www.epa.gov/oppt/sf/tools/aim.htm]
  – Need to download and run on windows

• PBT Profiler - uses the atomic structure to estimate properties of a substance, but focuses on properties relating to persistence, bio-accumulation, and toxicity.
  – [http://www.pbtprofiler.net/]

• ToxPredict – Open tox module
  – [http://www.opentox.org/toxicity-prediction]
  – [http://apps.ideaconsult.net:8080/ToxPredict]
In Class Exercise

• Use same chemical as in previous example
• Use the toxicity tools to determine/estimate toxicity of chemical
• Suggest each team member use different tool
• 15 minutes – report to class on findings/problems
Finish Hazard Trait tables

• Use the tools outlined for EFT and PBT to complete the Hazard Trait tables for your chemicals of interest