U.S. EPA/OPPT and Sediments: Screening New and Existing Chemicals for Potential Environmental Effects

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Introduction

Since 1976, the Office of Pollution Prevention and Toxics (OPPT, formerly the Office of Toxic Substances, OTS) at the U.S. Environmental Protection Agency (U.S. EPA), has been the office that is responsible for assessing new and existing industrial chemicals. Prior to a reorganization within OPPT in 1997, the Environmental Effects Branch was the principal ecological group within that office. In the past, that group had been concerned primarily about the ecological effects of industrial chemicals in the water column (Zeeman and Gilford, 1993; Zeeman, 1995). However, in the last five to ten years, there has been more and more concern expressed about the possible effects of industrial chemicals upon organisms in the sediments (Clements et al., 1994; U.S. EPA, 1994; Nabholz et al., in press; Smrchek et al., 1995; Smrchek and Zeeman, 1997; Zeeman, 1993; Zeeman et al., 1995 and in press).

Following is a brief introduction to the U.S. EPA, the responsibilities of OPPT, especially the new and existing chemical programs, and the kind of assessments of these chemicals that are required under the Toxic Substances Control Act (TSCA, the law under which OTS [now OPPT] was formed in 1976). After this is a description of how OPPT went about requiring and getting sediment toxicity testing for a new industrial chemical. And finally, an example is presented on how OPPT developed a methodology that was used to screen thousands of existing chemicals to try to develop a list of higher priority chemicals for possible ecological testing concerns, including possible sediment testing.

Background

For those who think of the U.S. EPA as some sort of monolithic agency, it is not. It has about 17,000 to 18,000 employees in numerous programs and offices that were each set up at different times and for different purposes. The Agency's various programs and offices address responsibilities defined by several different environmental laws that were passed over decades by different legislative actions (Clean Air Act, Clean Water Act, TSCA, etc.). The Offices in the U.S. EPA were organized under broad legislative or environmental categories, such as Air and Radiation, Water, Pesticides and Toxic Substances, Solid Waste and Emergency Response (Superfund), and Research and Development. The figures on page 7-40 [U.S. EPA, OPPT] illustrate how the U.S. EPA is organized, with OPPT residing within the Office of Prevention, Pesticides, and Toxic Substances and the Environmental Effects Branch (EEB) residing within OPPT.

The ecological hazard and risk assessment functions of that Branch used to be in the Health and Environmental Review Division (HERD), and those functions now reside in the newly formed Risk Assessment Division (RAD, formed in 1997 from the combination of the staff and functions of both HERD and the Chemical Screening and Risk Assessment Division, CSRAD). The Economics, Exposure, and Technology Division (EETD) contains the staff responsible for performing the engineering and exposure assessment portions of the ecological risk assessments that are done in OPPT.

Why does/should OPPT care about bioaccumulation, bioconcentration, and sediments? Because there are industrial chemicals which adsorb strongly to sediments and which are quite likely to also bioaccumulate or bioconcentrate. When introduced into the food chain, they could be detrimental not only for those organisms in the sediment and water column environments, but also for humans. TSCA was passed in 1976 to regulate industrial chemicals, those chemicals used in commerce that were not regulated by other statutes, meaning that they are not pesticides, pharmaceuticals, food additives, or substances covered under other laws (see figure on page 7-41 [watering can]). For example, industrial

Back

chemicals are substances like solvents, plastics, dyes, adhesives, detergents, monomers, and polymers. They are chemicals that are widely used in commerce and are around us all of the time. An independent calculation of a partial sum of the 1989 production volumes of industrial chemicals in the United States was around 6 trillion pounds and it is undoubtedly even more now (Zeeman, 1997).

One of the first activities after TSCA was passed in 1976 was to develop an inventory of the industrial chemicals already in commerce in the U.S., the existing chemicals (see figure on page 7-42 [TSCA (Passed 1976)]). After more than two years, over 60,000 chemicals were identified as being in commerce and these became the TSCA Inventory of existing chemicals. These chemicals were basically grandfathered and the Agency was to look at them for environmental concerns on an ongoing basis.

By definition, anything that was not an existing chemical (i.e., on the Inventory) was a new industrial chemical, and if anyone wanted to make it or import it into the U.S., they would have to submit an application for its assessment to the U.S. EPA. This assessment program is not a registration program. Industry (the potential manufacturer or importer) submits a notice to OPPT called a Premanufacture Notification (PMN). OPPT receives a large number of these notices from industry each year (see figure on page 7-42). They need to submit only the data that they have or know about. They do not have to do any testing. OPPT then has 90 days to make a decision based on the available information or provide risk-based reasons for not allowing it to be made or imported.

The number of new chemicals that have gone through this process in OPPT and have become existing chemicals on the TSCA Inventory is currently around 15,000, which brings the Inventory total to about 75,000. OTS/OPPT has received around 30,000 new chemical notices from 1979 to 1996. From 1986 to the present, the average has been about 2,300 new chemical notices per year. That is almost 50 notices per week or 10 per work day that are received and must be assessed in a short time frame.

As mentioned earlier, OPPT does not receive a lot of information. What is required to be submitted with these PMNs? Manufacturers must furnish information such as the name of the chemical, the chemical structure, the amount to be produced, disposal and human exposure information, and any available test data since testing is not required (see figure on page 7-43 [Required Submission]). Nevertheless, OPPT staff must make these risk-based decisions in 90 days or the manufacturer will be able to make or import that chemical unless a risk-based case is made by OPPT that they should not.

The consistent experience of OPPT is that we seldom receive the kind of data that is needed for ecological risk assessment. About 95 percent of the PMNs received by OPPT contain no ecotoxicity or environmental fate data (Zeeman and Gilford, 1993; Zeeman, 1995; Zeeman et al., 1995). The engineers and fate chemists in OPPT only get physical, chemical, or environmental fate data about 1 to 5 percent of the time (Zeeman et al., 1993 and 1995). They seldom get any bioaccumulation or bioconcentration data.

A retrospective was performed on the ecotoxicity data received for new chemicals and it was found that OPPT received ecotoxicity data less than five percent of the time, and the vast proportion of the data received was acute toxicity data (Zeeman, 1995). That means that 19 out of 20 times no ecotoxicity data are provided for new chemicals. Therefore, OPPT has been forced to rely heavily upon a modeling approach that uses structure-activity and quantitative structure-activity relationships (SAR/QSAR, or (Q)SAR) to estimate chemical properties, chemical fate, and the ecotoxicity of a chemical to organisms in the aquatic environment (Clements, 1988 and 1994; Nabholz et al., 1993; Zeeman et al., 1993 and 1995).

How does OPPT make decisions for ecological risk assessment in the new chemical program? A number of PMNs for new chemicals are received each week and they are generally assessed in groups. Within two or three weeks of receipt of a group of PMNs, OPPT holds what is called a FOCUS meeting (see figure on page 7-43 [Flow Chart]). That is the first level of risk assessment where a comparison is made of the hazard assessments, i.e., toxicity profile, and the exposure assessments for each chemical. What is important for ecotoxicity is whether the predicted environmental concentration (PEC, from the exposure assessment) exceeds what is called the concern concentration (CC, hazard assessment value(s) adjusted for uncertainty). In at least 90 percent of the cases, the PEC is not exceeded and a risk is not inferred. These chemicals are dropped from further evaluation. In the remaining five to ten percent of the cases, we proceed to standard review or a request for testing and perhaps through risk management, which can result in iterations to obtain additional data (Wagner et al., 1995).

Sediment Assessment of an OPPT New Chemical

Portions of the following specific new chemical sediment assessment example have been previously presented at a Society of Environmental Toxicology and Chemistry (SETAC) national meeting (Zeeman, 1993), and were also used as one case study of ecological risk assessment methods used by the Agency (U.S. EPA, 1994). Further elaborations of this sediment assessment will also be coming out soon as publications, in both a SETAC book on Uncertainty in Ecological Risk Assessment (Nabholz et al., in press), and in a White House OSTP publication on Ecological Risk Assessments in the Federal Government (Zeeman et al., in press).

The following describes the decision-making process for a specific new chemical where OPPT was able to get aquatic toxicity data, some generic and site-specific data (so predictions could be made on whether or not it would get into the sediments), and some sediment toxicity data. The figure on page 7-44 shows the physical and chemical properties of the chemical. This new chemical would be produced at the level of 100,000 kg per year, so it is not a trivial compound in terms of how much is going to be manufactured or imported. It is an alkylated diphenyl, and was classified into the SAR chemical class of neutral organic chemicals. OPPT is very comfortable in using its structure-activity relationship and quantitative structure-activity relationship [(Q)SAR] models for making predictions on neutral organic chemicals (Clements, 1988 and 1994; Nabholz et al., 1993; Zeeman et al., 1993).

Based upon the chemical structure, an estimate was made of the K_{ow} value (the octanol to water partition coefficient, often used to estimate both ecotoxicity and bioconcentration ability) and it was fairly high. An estimate of the K_{oc} value (the water to organic carbon partition coefficient, often used to estimate ability to partition to sediments) was also made, and it was relatively high. The water solubility was estimated to be fairly low. These are all strong indications that this chemical will be very likely to distribute selectively from the water column and into the sediments.

A hazard assessment (stressor-response) or toxicity profile for this chemical was prepared (see the figure on page 7-44). OPPT's structure-activity methods (Clements, 1988 and 1994; Nabholz et al., 1993) were used to predict the acute and chronic aquatic toxicity and to make a risk-based case that eventually resulted in test data. From this estimation information, OPPT inferred that this new chemical would be a highly toxic compound on a chronic exposure basis and that it would be very likely to be transported to sediments. A case was subsequently made through refined exposure assessment estimates that sediment toxicity testing was needed, and it was eventually provided (see below).

How well did the OPPT (Q)SAR estimates predict aquatic toxicity to fish and aquatic invertebrates? It was estimated that there would be no effects at saturation for acute toxicities, which was confirmed by the testing. Such short-term tests do not provide a long enough exposure time to observe any acute effects. It was also estimated that the longer term chronic toxicity values would be somewhere in the low parts per billion (ppb) range. The test data subsequently received confirmed that the OPPT (Q)SARs were very accurate with the actual chronic values of 13 ppb for fish and 7 ppb for daphnids being very close to the predicted ecotoxicity results.

OPPT went through a number of iterations to characterize the risk associated with this new chemical (see the figure on page 7-45 [Summary...]). Initially it was thought that fish would be the most sensitive species. This did not turn out to be the case. However, the concern concentration (CC, the level in the water below which OPPT would not take any regulatory action) turned out to be around 1 ppb using either the fish or the aquatic invertebrate toxicity data. A risk-based case was then made through our initial and subsequent iterations assessing exposures. Generic production data and some site-specific data were then obtained to improve the input for our exposure models. The resulting estimates of exposure were contrasted with estimates of benthic toxicity and the estimates of risk to organisms indicated that the manufacturer should consider chronic testing in sediments. The manufacturer did perform a 28-day sediment toxicity test with chironomids, which showed that there would be a moderate level of toxicity.

What risk management decision was made about this new chemical? It was decided that this new chemical could be used only at the three sites for which they provided specific information and that they should limit the water column concentrations of the chemical to 1 ppb or less. OPPT also warned the manufacturer that this chemical would, over the years, be likely to accumulate in sediments.

Existing Chemicals and Sediments

The TSCA Inventory of existing chemicals consists of about 75,000 chemicals that include polymers, mixtures and salts, organometallics, and discrete organic chemicals. A focus on discrete organics was used for an approach that was developed by OPPT for screening possible persistent bioaccumulative chemicals on the TSCA Inventory. Using this approach, thousands of discrete existing chemicals were screened to identify those that might have the chemical characteristics to be persistent and bioaccumulate, and therefore, have potential for concern for selectively partitioning into sediments (Zeeman et al., 1995).

In 1990, OPPT asked the EPA research laboratory in Duluth, MN to screen the TSCA Inventory for discrete organic chemicals which could have log K_{ow} values greater than 3.5. For this screening effort, the Duluth lab created a database and estimated the log K_{ow} (also known as log P). They started the screening process with about 20,000 chemicals and ended it with 6,668 chemicals with log K_{ow} values greater than 3.5 (see figure on page 7-45 [Screening for Persistent Bioaccumulators]). The log K_{ow} value of 3.5 was chosen as a lower limit because it represents a fish bioconcentration factor of about 250, which was derived using an equation from research performed at the Duluth lab (Veith and Kosian, 1982). That limit approximately defines the subset of chemicals that should be cause for moderate or greater concern for bioconcentration in aquatic organisms such as fish.

After this initial screening, OPPT continued with a series of steps to reduce the list of chemicals to a more manageable size. The first step was to do an intersection between the Duluth database and the OPPT Chemical Update System (CUS) database, which includes about 8,600 industrial chemicals that industry reports producing in quantities of more than 10,000 pounds per site per year (see figure on page 7-46). The intersection resulted in the identification of about 1,000 chemicals with this level of production and log K_{ow} values greater than 3.5. The next level of assessment was to consider chemicals with log K_{ow} values between 3.5 (initially 4.3 was used) and 8.0 to focus on those chemicals that had the highest probability of causing the most critical problems. Then persistence was evaluated using a degradation half-life of greater than 30 days as the threshold. This reduced the list to about 80 chemicals. Finally, we considered chemicals that were being produced in quantities greater than 1 million pounds per year. Applying this final criterion, a list of 34 chemicals resulted and these chemicals were examined further because they could be of concern for persistence, bioaccumulation, and partitioning into sediments (Zeeman et al., 1995).

What are the next steps? Obviously, one of the things that would be important is to obtain information on actual environmental loadings. It has been suggested that

OPPT list some of these chemicals on the Toxics Release Inventory (TRI) to find out if those chemicals that were proposed to be only chemical intermediates were actually being released into the environment. When this list of 34 chemicals was presented at a SETAC Workshop on the Environmental Risk Assessment of Organochlorine Chemicals (Clements et al., 1994), one of the chemicals was supposed to be a chemical intermediate that would not be released into the environment. A researcher from Canada came up after the presentation and said that they had been finding this chemical in gull eggs along the Great Lakes.

OPPT has also developed a sequence of tests that persistent bioaccumulative chemicals should be considered for (see figure on page 7-46 [Potential Testing ...]). First, we would like to determine whether or not these chemicals are likely to degrade in a sediment and water system. Chemicals that do not degrade should be evaluated further for bioconcentration in fish. Finally, for the chemicals whose results indicate that they can bioconcentrate, then these chemicals need to be considered for testing to estimate their chronic toxicity to aquatic and sediment dwelling organisms (e.g., see figure on page 7-47 [Preliminary Testing Scheme ...], adapted from Smrchek and Zeeman, 1997).

Discussion and Summary

Sediment issues for both new and existing industrial chemicals are becoming more and more important to OPPT (see figure on page 7-48 [OPPT Sediment Issues]). OPPT has asked for, received, and evaluated the results of sediment toxicity testing for both new and existing industrial chemicals (Smrchek et al., 1995; Smrchek and Zeeman, 1997). It has also been interested in the sediment toxicity test methods being developed nationally through the American Society for Testing and Materials (ASTM) and the U.S. EPA, and internationally through the Organization for Economic Cooperation and Development — the OECD (Ingersoll, 1995; OECD, 1997; Smrchek and Zeeman, 1997). OPPT also continues to have an interest in and support the ongoing refinements in true chronic toxicity testing of sediment organisms, i.e., longer duration chronic testing, such as the 65-day life-cycle test recently developed for *Chironomus tentans* (Benoit et al., 1997).

In summary, sediment issues have been a concern for both OPPT's new and existing industrial chemicals for almost a decade. OPPT receives notices from industry for about 2,300 new chemicals per year. Most of the time there does not appear to be a problem related to sediments. But in those few cases where we are concerned that there could be such problems, OPPT has been able to either get results from sediment toxicity testing, or identify ways to mitigate the concerns for those chemicals. Sediment toxicity testing has also been requested and received for existing chemicals. However, the current focus with existing chemicals is likely to continue the use of screening methods to identify those high production volume chemicals that might have characteristics that result in concerns for partitioning into the sediments and having the potential to adversely affect organisms in the environment.

Disclaimer

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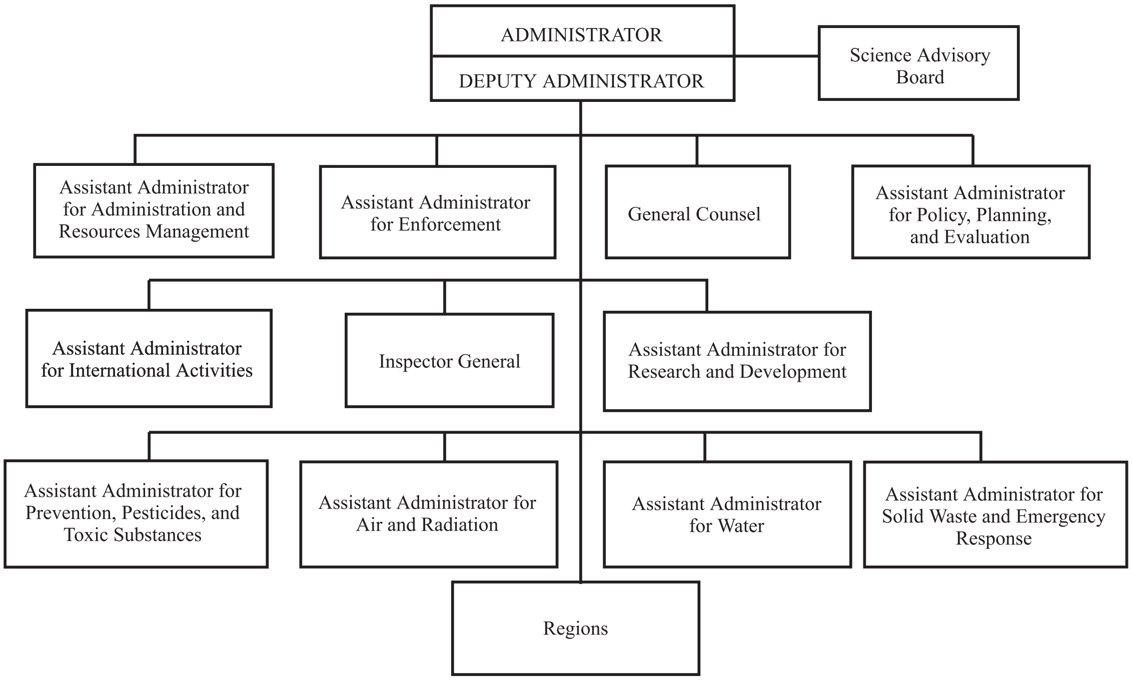
U.S. Environmental Protection Agency



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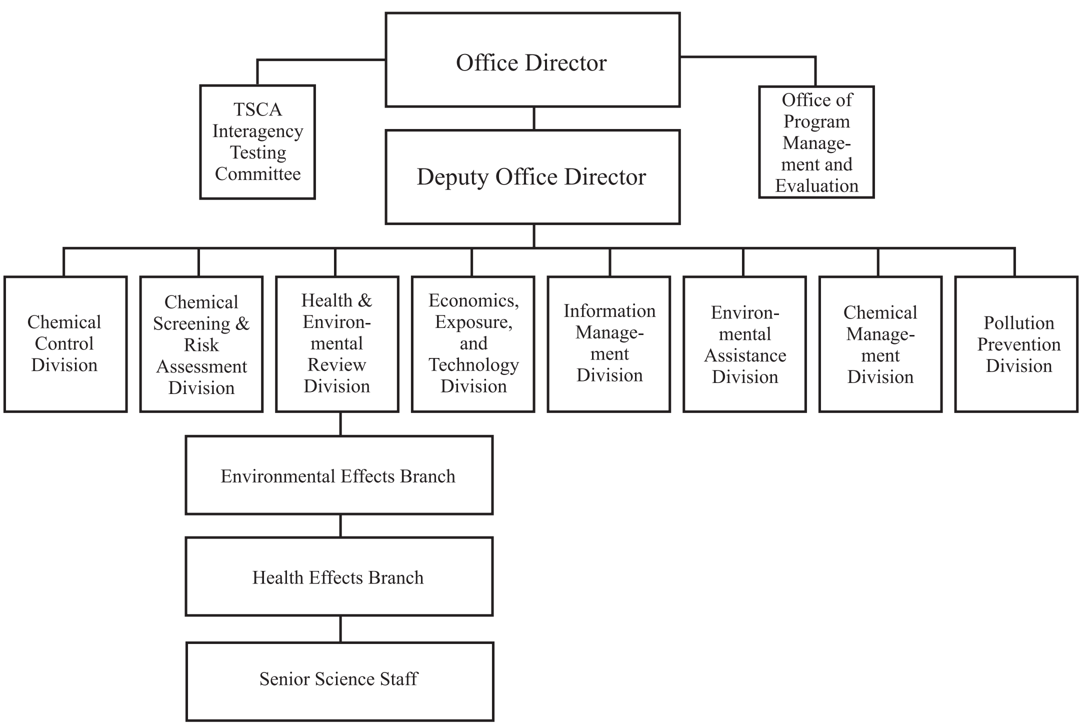
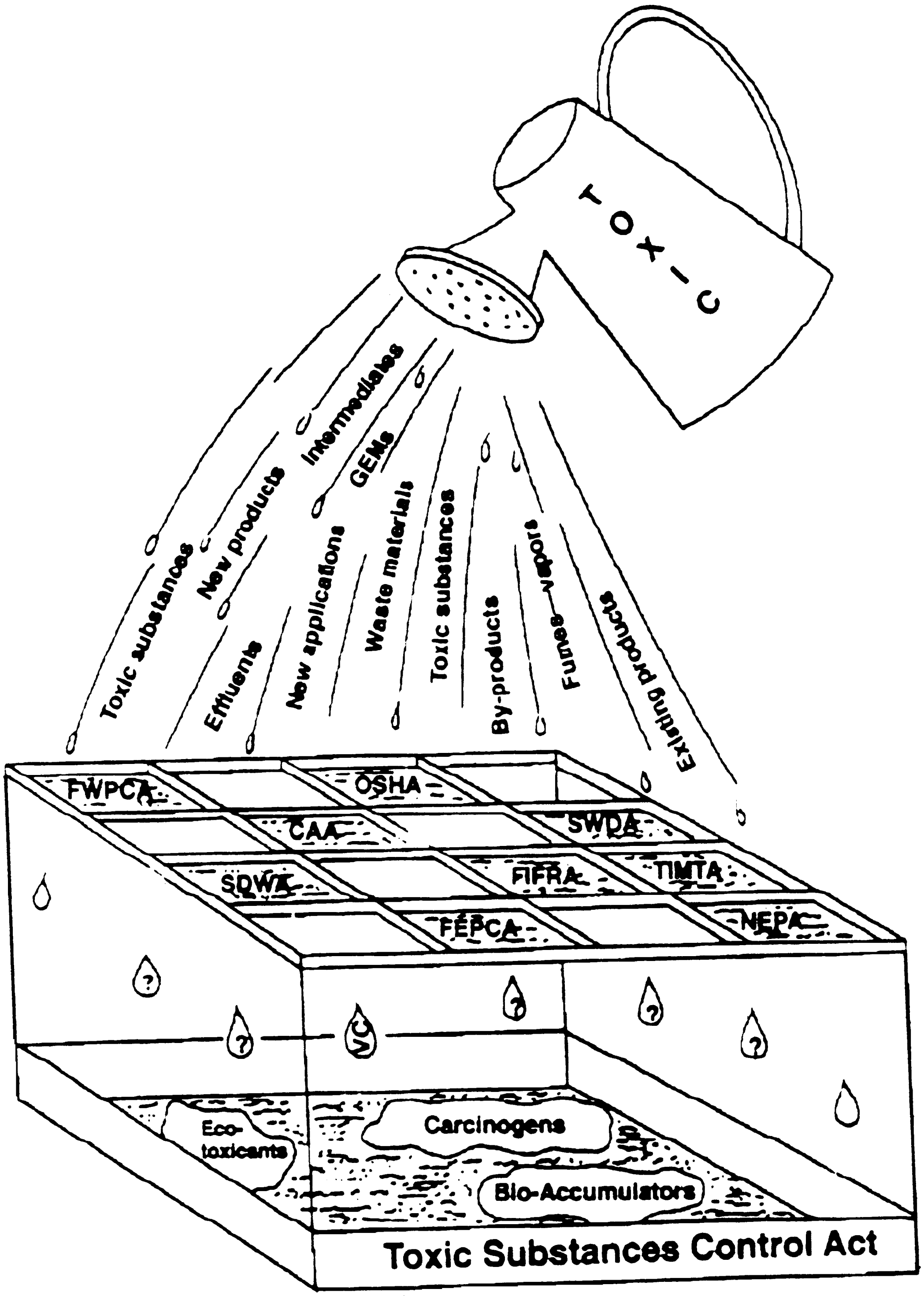


TSCA: The Gap Filling Law

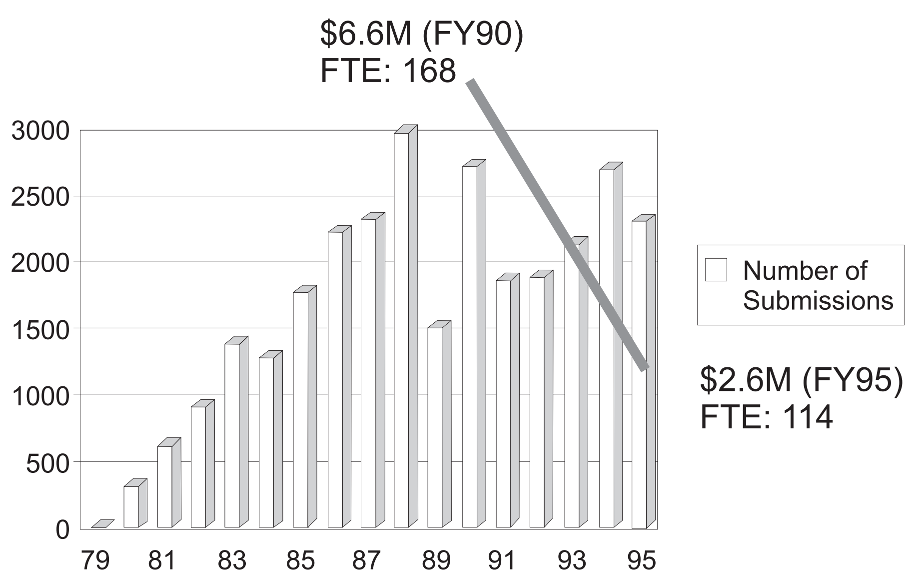


TSCA (Passed 1976)

- Existing Chemicals Inventory (1979) [§8, etc.]
  ~ 60,000 Chemicals (Grandfathered)
  ~ 10,000 Chemicals Added (by 1991)

- New Chemicals (PMN's) [§5]
  Chemical PMN's ~ 2,500/yr (currently)
  Genetically Engineered Microbe PMN's
  Submit Extant Data Only
  90-Day Clock (after submit PMN)

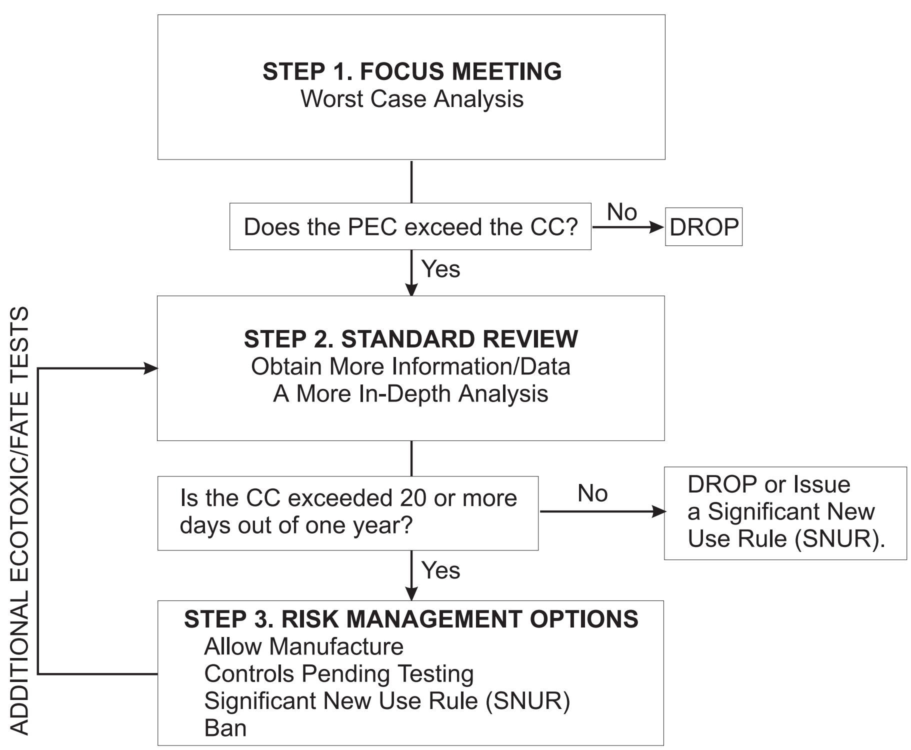
PMNs Received/Fiscal Year and FY90-FY95 Budget



Required Submission in New Chemical Notice

- Chemical Name
- Chemical Structure
- Production Volume
- Uses and Disposal Methods
- Human Exposure Estimates
- Any Extant Test Data
  (Testing *Not* Required)

Flow Chart and Decision Criteria for the Ecological Risk Assessment of a PMN Substance



PHYSICAL/CHEMICAL PROPERTIES OF PMN SUBSTANCE

Chemical Class: Neutral Organic

Chemical Name & Structure: CBI

Physical State: Liquid

Molecular Weight: 232

Log K_{OW}: 6.7 [Via CLOGP program (Leo and Weininger, 1985)]

Log K_{OC}: 6.56 [Via regression equation (Karickhoff et al., 1979)]

Water Solubility: 0.30 mg/L [Measured]

Vapor Pressure: < 0.001 Torr @ 20^{o} C.

PMN SUBSTANCE STRESSOR-RESPONSE PROFILE

QSAR ESTIMATED TOXICITY

(Clements, 1988)

Fish 96 hr. LC_{50}: No effects at saturation

Daphnid 48 hr. LC_{50}: No effects at saturation

Green Algae 96 hr. EC_{50}: No effects at saturation

Fish Chronic Value: 0.002 mg/L

Daphnid Chronic Value: 0.004 mg/L

Algal NOEC: No effects at saturation

ACTUAL MEASURED TOXICITY

Fish Acute Test (FHM; 96 hr): No effects at saturation

Fish Early Life Stage Test (FHM; 31-day):

Chronic Value (growth, mean wet weight): 0.013 mg/L

Chronic Value (survival, growth (length)): 0.061 mg/L

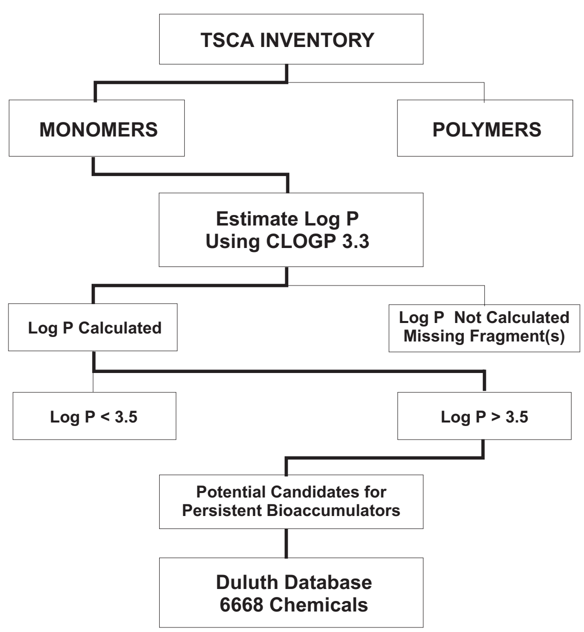
Daphnid Reproduction Test (D. magna; 21-day):

Chronic Value (survival, growth, reprod.): 0.007 mg/L

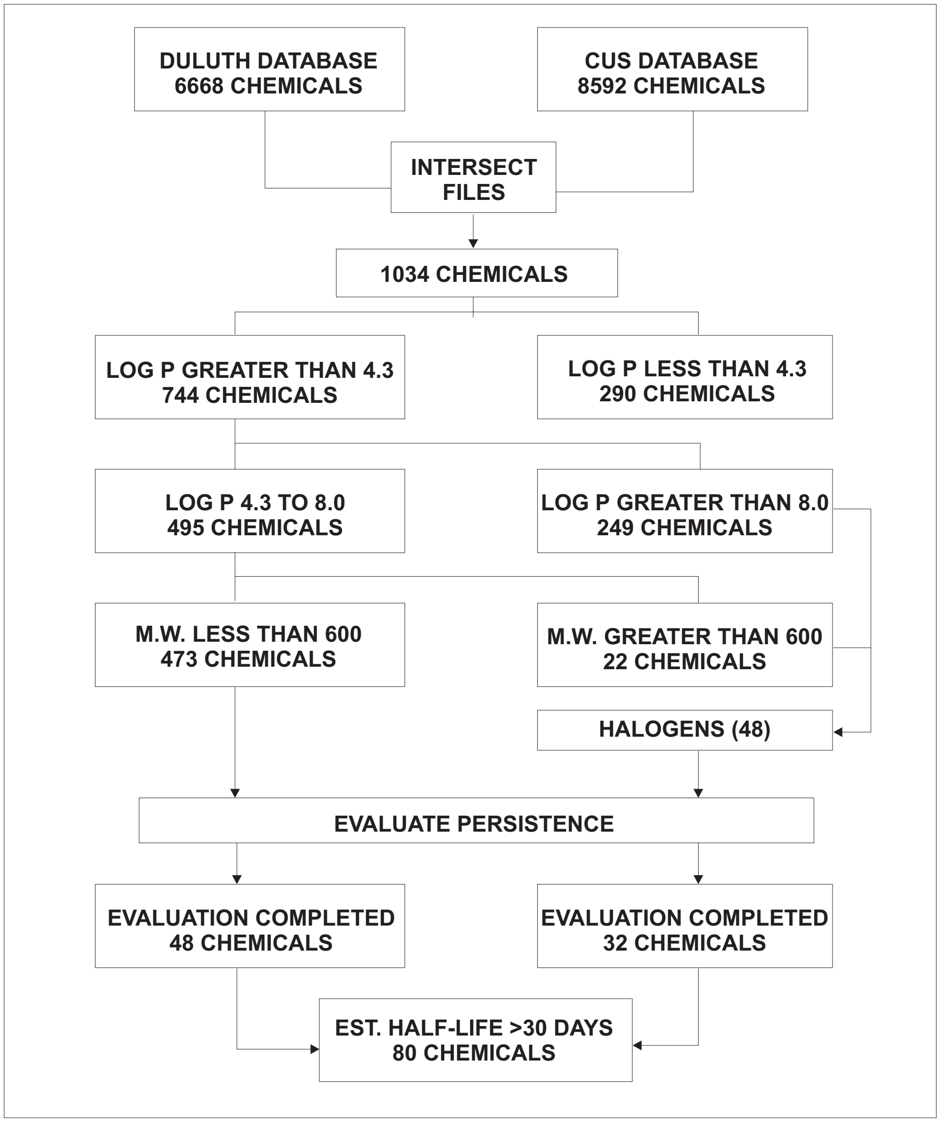
Summary of Five Risk Characterization Iterations

ITERATION	ESTIMATES / ASSUMPTIONS	UNCERTAINTY
1	Fish are the most sensitive species. CC = 1 ug/L. PMN substance mixes instantaneously in water. No losses.	Worst case. Actual test data not available.
2	Actual test data for Daphnids still yield a CC of 1 ug/L. Determine how often this concentration is exceeded using PDM3.	Worst case. Other species may be more sensitive.
3	Estimate risk to benthic organisms using Daphnid chronic value and mitigation by organic matter. EXAMS II used to estimate concentrations.	Generic production sites. Actual data for benthic invertebrates not available.
4	Site specific data obtained on use and disposal. EXAMS II rerun with new data.	Estimated toxicity for benthic invertebrates.
5	Actual test data for benthic organisms obtained.	Best estimates for identified sites. May not hold for other sites or uses.

Screening for Persistent Bioaccumulators



Initial screening process performed by ERL, Duluth to identify potential bioconcentrators.



Application of criteria to screen the Duluth database for potential bioaccumulators

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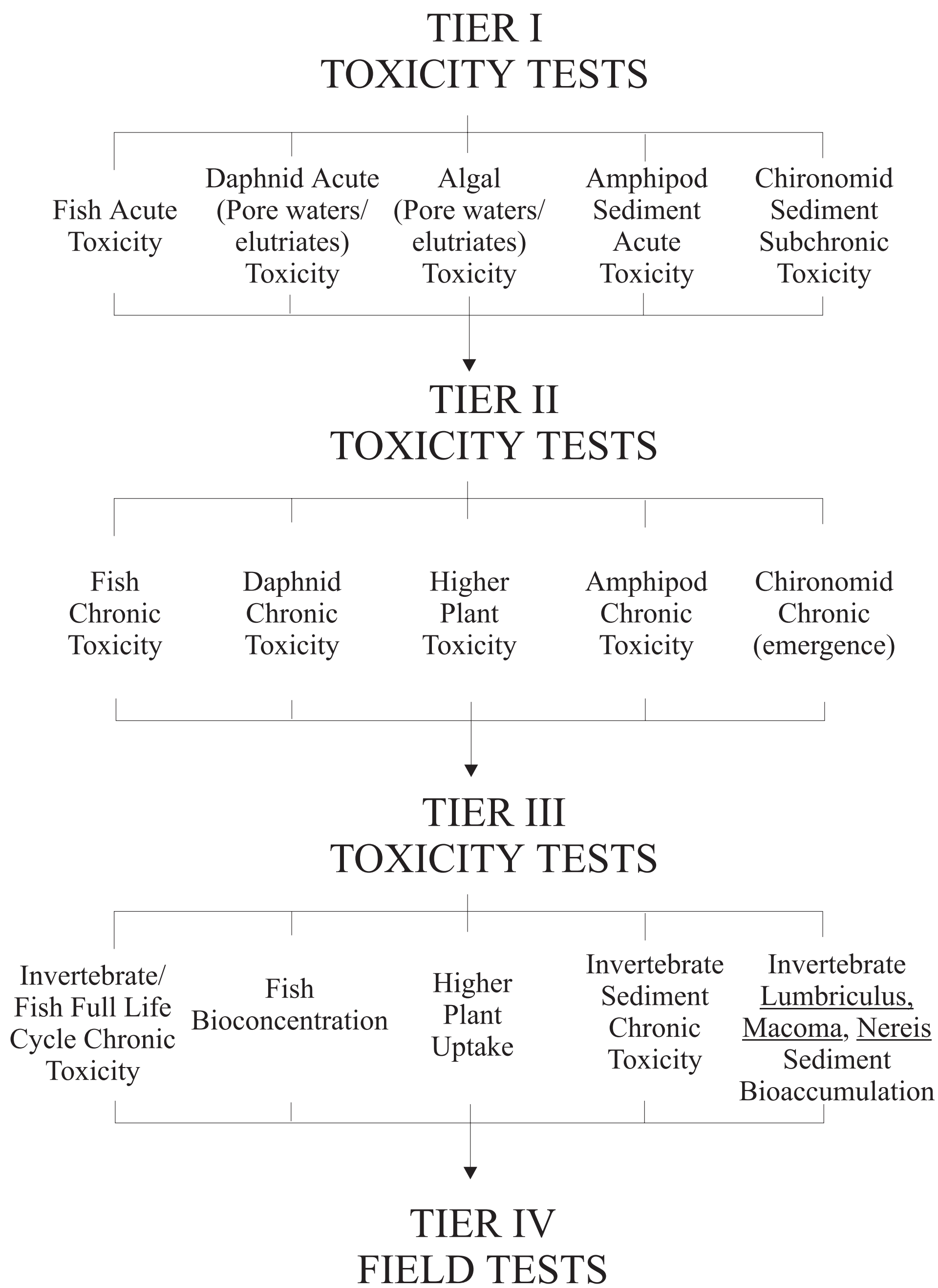
POTENTIAL TESTING OF PERSISTENT BIOACCUMULATORS

- Sediment/Water Biodegradation
  - Fish Bioconcentration
    - Chronic Aquatic Toxicity
      - Chronic Sediment Toxicity

Preliminary Testing Scheme For Determining Sediment Effects



(Adapted from Smrchek & Zeeman, 1997)

OPPT SEDIMENT ISSUES

NEW CHEMICALS

- 90 % Minimum Risks
- 5-10 % Further Review
- PMN Case Study — Sediments [EPA/630/R-94/003]

EXISTING CHEMICALS

- ITC Recommendations [e.g. OMCTS]
- Screening Methods [e.g., PB's see SAR/QSAR Env. Res. 3:179-201;1995]

"The work will teach you how to do it."

(Estonian Proverb)

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