A Framework for Conducting Environmental Risk Assessments on Fragrance Materials

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ABSTRACT

Over 2100 discrete organic chemicals are listed in the RIFM/FEMA Database as available for use in consumer products as fragrance materials. These materials represent a wide range of physical chemical properties and structural groups. Their use in consumer products results in their disposal down the drain to become components of domestic wastewater. A screening level risk assessment procedure using quantitative structure activity relationships (QSARs) to model removal during sewage treatment and toxicity to freshwater aquatic organisms was developed. These QSARs are based on a materials physical chemical properties and its reported volume of use. The resulting model outputs were used to calculate the ratio of Predicted Environmental Concentration (PEC) to Predicted No Effect Concentration (PNEC). Negligible environmental risk is defined by a resultant PEC to PNEC ratio below one. The framework incorporates procedures for using other available information as well as an optimized strategy for generating new data that are needed to refine and improve the risk assessments. Of the greater than 2100 materials screened through this framework, less than 8% remain requiring further review for risk assessment refinement. The predicted PECs and PNECs were compared with those based upon measured data. This validation confirmed the conservative nature of this framework. This framework is shown to be an effective and precautionary tool to quickly screen a large number of materials to predict their potential environmental risk.

Un modelo para estimar el riesgo ambiental de los materiales de fragancia

Más de 2.100 químicos orgánicos en el "RIFM/FEMA Database" pueden ser usados en productos personales como los materiales de fragancia. Hay mucha variación en la escala de las propiedades físico-químicas y de los grupos estructurales de éstas substancias químicas. Cuando éstas substancias químicas son usadas en productos personales, la ruta principal al medio ambiente es de aguas residuales. Para que comprendamos mejor si habrá un riesgo ambiental, hicimos un modelo que predice si la concentración en el medio acuático (La Concentración del Medio Ambiente Predicho o "PEC") es mas o menos de la concentración que nos dará problemas para los organismos acuáticos (La Concentración Sin Efecto Predicho o "PNEC"). Cuando éste cociente es menos de 1, nosotoros decimos que el riesgo ambiental será minimo. En nuestro modelo, la PEC y la PNEC son calculadas usando las relaciones cuantitativas de estructura-actividad ("QSAR"). Primero, éstas QSARs son calculadas usando el peso molécular, el coeficiente que reparte el octanol y el agua ("K_{ow}"), y el volumen regional en comercio. Para determinar la PNEC, usamos un factor conservador de incertidumbre. Después de ésta primera calculación, nosotros eliminamos las substancias químicas que tienen el cociente PEC/PNEC menos de 1. Nosotros hacemos una segunda calculación para las substancias químicas que tienen el cociente PEC/PNEC más de 1. En ésta calculación usamos una QSAR ecotoxicológico diferente que es más especifica que la QSAR en la primera calculación porque nos ayuda a reducir la incertidumbre del PNEC. Otra vez, después de ésta calculación nosotros eliminamos las substancias químicas que tienen el cociente PEC/PNEC menos de 1. Finalmente, para el grupo de las substancias que tienen un cociente PEC/PNEC más de 1, nosotros usamos datos experimentales del medio ambiente, como biodegradación si disponible, para calcular el final cociente PEC/PNEC. Usamos éste grupo final para manejar nuestro programa de análisis del medio ambiente. La primera vez que usamos éste modelo eliminamos más de 92 por ciento de las substancias químicas que tienen un cociente la PEC/PNEC menos de 1.

INTRODUCTION

- This is a first tier, screening-level approach to assessing risk to the aquatic environment from fragrance materials and other organic molecules
- Ability to rank large and structurally diverse sets of organic chemicals (i.e., ascribing relative risk or safety)
- Built upon generally accepted principles (PEC/PNEC concept—EU Technical Guidance Document)
- This Framework is developed with an ability to consider biodegradation in the estimation of treatment removal
- Initial results can be refined with laboratory and field data or alternate model predictions (e.g., ECOSAR)
- The Framework assists in the setting of research and testing priorities

USEPA's Paradigm for Ecological Risk Assessment

- Problem Formulation
- Analysis
  - Characterization of Exposure
  - Characterization of Ecological Effects
- Risk Characterization

RIFM Framework: Problem Formulation

- The RIFM/FEMA Database of Materials consists of over 2100 discrete organic compounds
- Testing all 2100 materials is neither practical, cost effective, nor necessary
- A screening tool is needed to assess potential environmental risk, if any, from these materials and to effectively allocate resources on higher priority materials

Exposure Characterization– Predicted Environmental Concentration (PEC)

Model assumptions:

- All the fragrance usage volume is discharged down the drain
- No volatilization occurs
- Both primary and secondary treatment occurs
- Loss of material removal during treatment is only the result of sorption (no biodegradation or biotransformation)
- Minimal dilution (a factor of 3) occurs within the mixing zone

Ecological Effects Characterization– Predicted No Effects Concentration (PNEC)

- Assumption: All the fragrance material is considered bioavailable
- Screening QSAR Equation:
  LC_{50} (mg/L) = 0.1(0.87 x log K_{ow} + 1.13) x Mol. Wt. x 10^6
  where Mol. Wt. = molecular weight

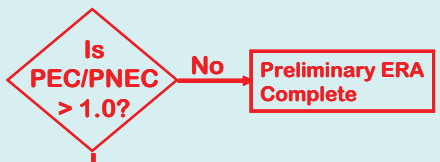
PNEC – Assessment Factors (AF)

- Used to add a margin of safety to a toxicological endpoint and provide for uncertainty in establishing an environmental concentration below which no impact to the aquatic biota is expected
- The AF for the RIFM QSAR was determined based upon principles described in the Technical Guidance Document of the European Commission
- The AF for the RIFM Framework is 10^6

Risk Characterization

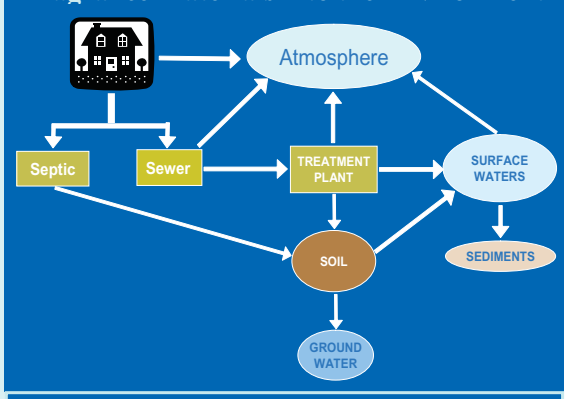
- Determination of materials whose PEC/PNEC ratio is >1.0
- Relative ranking of multiple materials to prioritize testing or other additional review (e.g., review available data for structurally similar compounds)
- Apply refinements to Framework; re-establish rankings

PEC/PNEC Refinement

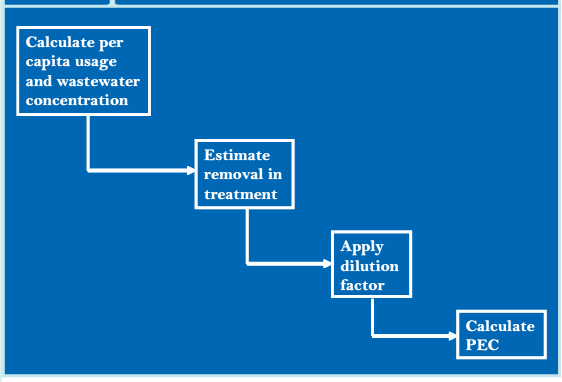


- If material is readily biodegradable, apply a first order rate constant to the calculation of estimated treatment removal
- If available, use measured environmental concentrations to validate the calculated PEC
- Use an alternate QSAR (e.g., ECOSAR) with reduced AFs
- Use laboratory ecotox results, also with reduced AFs

Primary Pathways for the Entrance of Fragrance Materials into the Environment



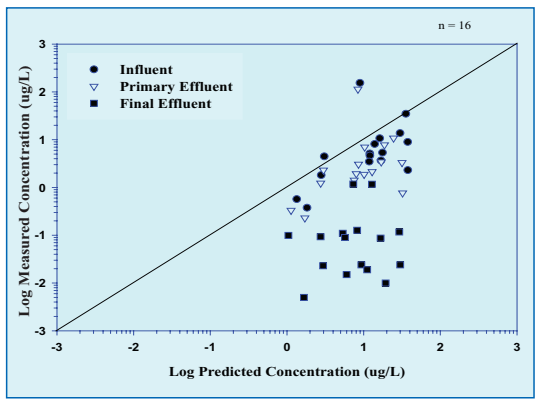
Exposure Characterization



Assessment Factors

Type of Data	Framework	EU TGD
Tier 1 QSAR	1,000,000	NA
Tier 2 QSAR	10,000	NA
Single Acute	5,000	NA
Three Acutes	1,000	1,000
One Chronic	100	100
Two Chronics	50	50
Three Chronic	10	10

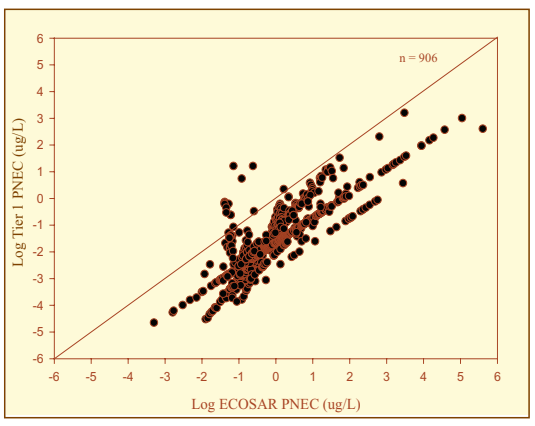
PEC Validation: Comparison of predicted influent, primary effluent, and final effluent wastewater concentrations with values measured by Simonich *et al*. for 16 fragrance materials.



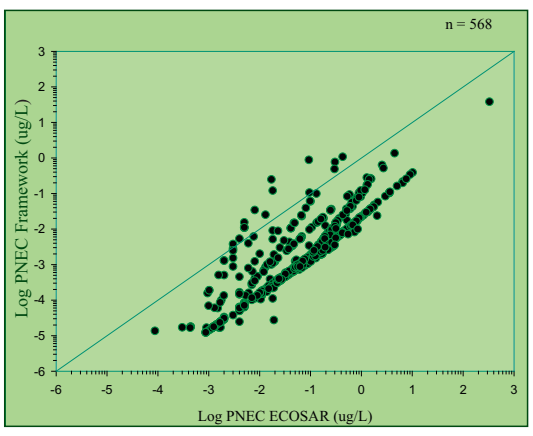
PNEC Validation

- Intermodel comparisons
- Comparisons between predicted and measured PNECs

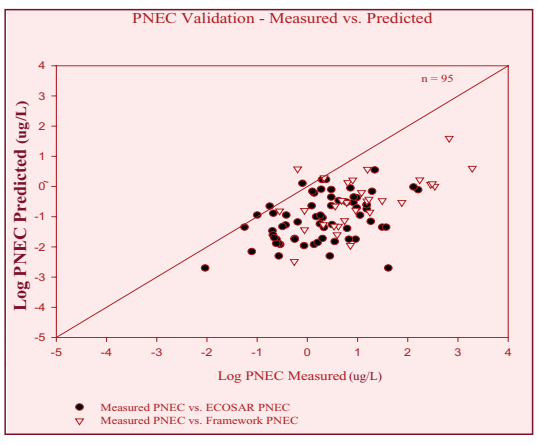
Comparison of tier 1 Predicted No Effect Concentrations (PNEC) with tier 2 PNECs for 906 fragrances (materials with estimated PEC/PNECs <1 after tier 1).



Comparison of tier 1 Predicted No Effect Concentrations (PNEC) with tier 2 PNECs for 568 fragrances (materials with estimated PEC/PNECs >1 after tier 1).



Comparison of Framework PNECs with PNECs based on measured ecotoxicity data, for 95 fragrance materials.



CONCLUSION

- It is based on established and accepted environmental principles (PEC/PNEC)
- Through its use, the Framework allows its predictions to be refined and validated
- The RIFM Framework is useful for performing a screening level risk assessment of large sets of organic chemicals; thereby establishing research and testing priorities
- *Assessing 2141 materials using the RIFM Framework resulted in 92.3% with PEC/PNEC <1*

Reference Salvito DT, Senna RJ, and Federle TW. 2002. A Framework for Prioritizing Fragrance Materials for Aquatic Risk Assessment. *Environ Toxicol Chem* 21 (6), 1301-1308.