




An Inconvenient Fragrance

A photograph of a forest path with tall trees and sunlight filtering through the leaves. The text is overlaid on the image.

**There is no current
universally accepted
definition of a
Green Fragrance!**

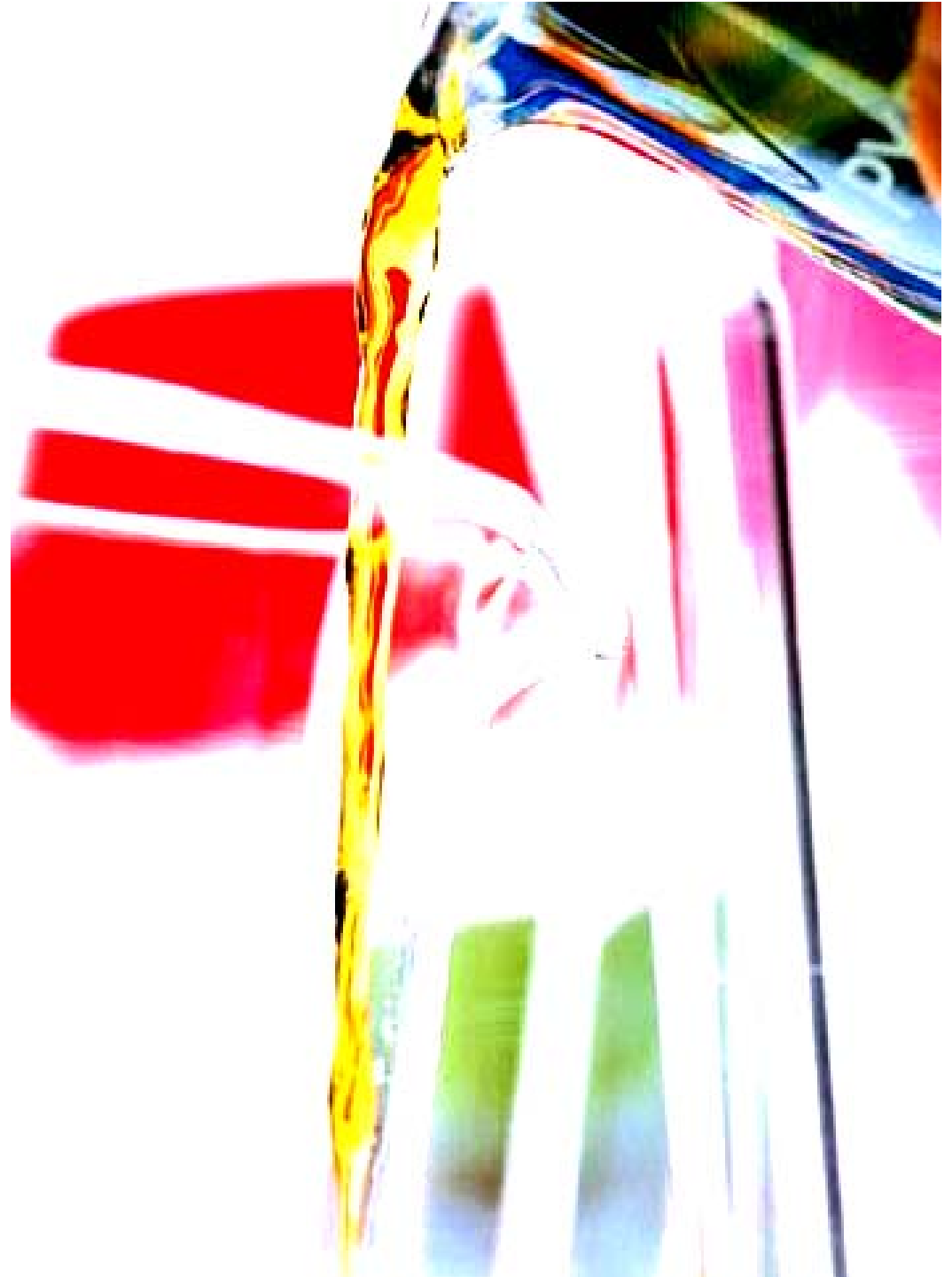


Concerns

Historically
skin safety,
now the
environmental footprint

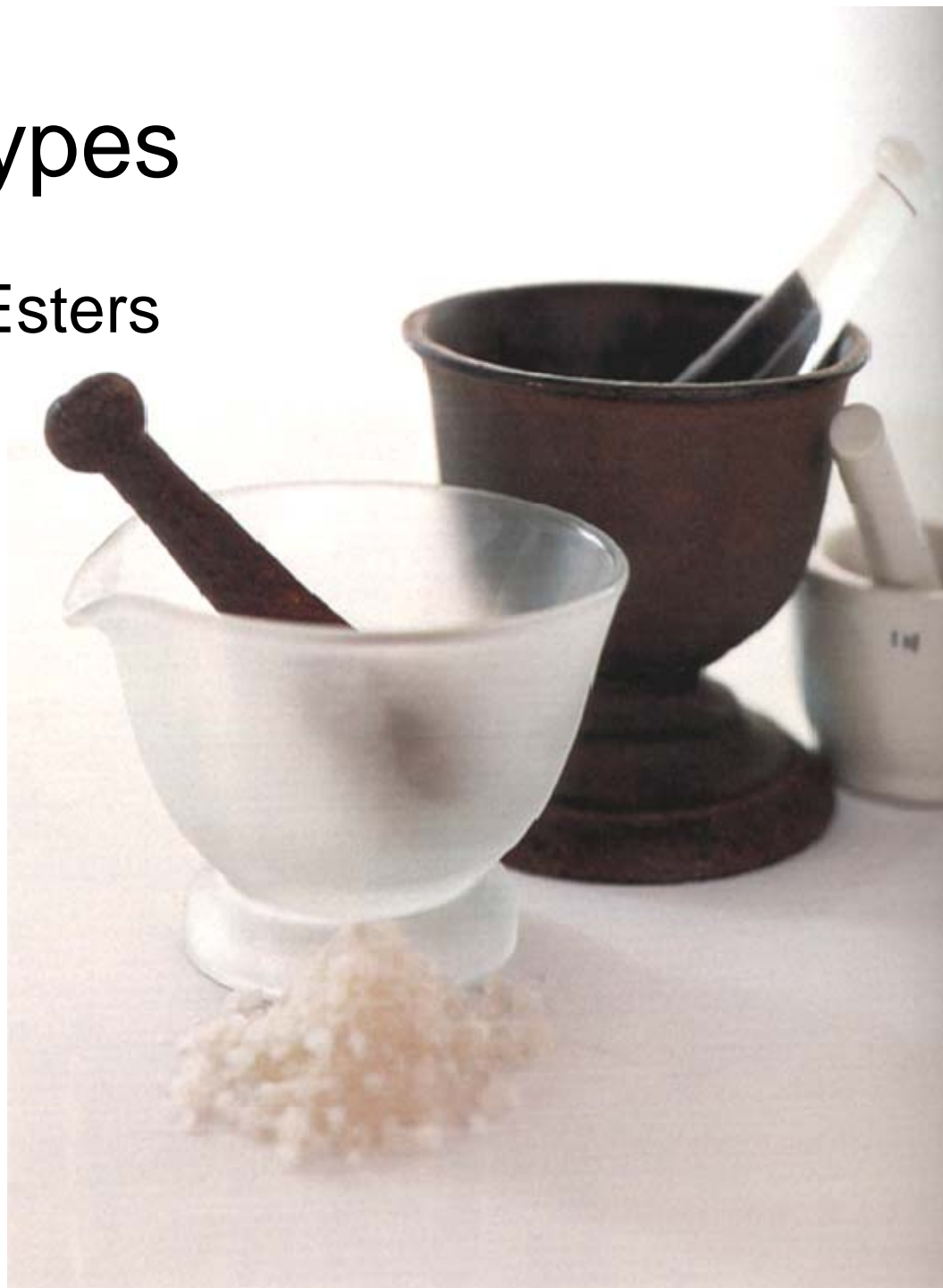
Fragrance Chemicals

- Low molecular wt
- Volatile
- Great diversity of chemical types

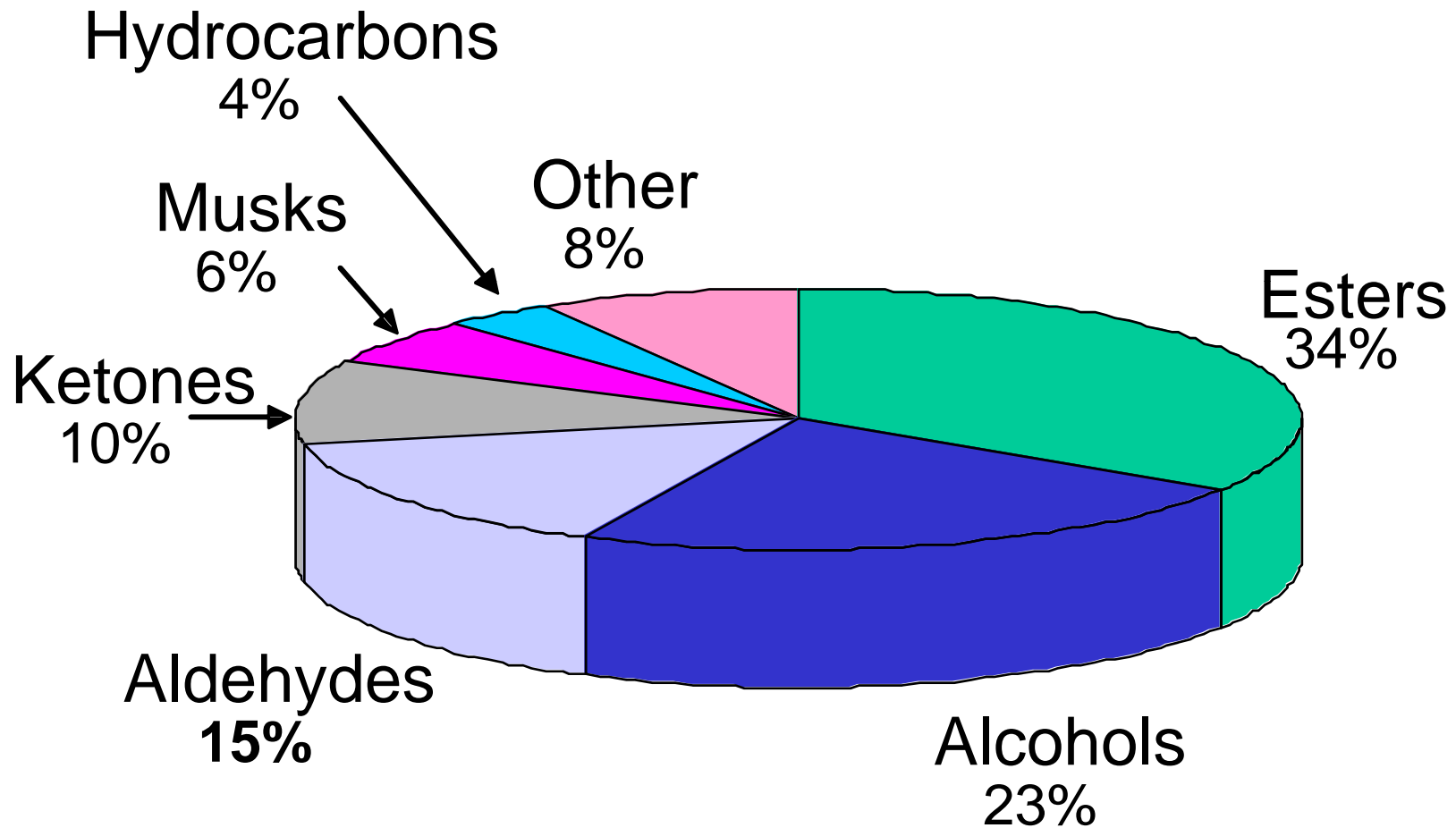


Chemical Types

- Aliphatic & Aromatic Esters
- Aldehydes & Ketones
- Alcohols
- Terpenes
- Phenols
- Nitriles
- Lactones
- Heterocyclics
- Acids
- Sulphur compounds



Commercial Fragrances



The Black Box

Without patent or copyright protection, the fragrance industry maintains confidentiality of formulae.





RIFM/IFRA

For thirty years, the fragrance industry has been essentially self-regulating

Physiological Considerations

- Skin irritation
- Phototoxicity
- Carcinogens



Hydroxycitronellal

Last Amendment April 28, 2000

First Issued March 01, 1987

CAS #	Recommendation	Skin Contact	Non-Skin Contact
107-75-5	Restricted	1%	10%

Hydroxycitronellal should not be used such that the level in consumer products exceeds 1%. This is equivalent to 5% in a fragrance compound used at 20% in the consumer product.

This recommendation is based on a no-effect level of 10% in diethyl phthalate and on a no-effect level of 2.5% in ethanol/diethyl phthalate in standard Human Repeated Insult Patch Tests (R.A. Ford and A.M. Api, Fd. Chem. Toxic. Vol. 26, p. 921-926, 1988). The RIFM Expert Panel reviewed these data in September 1999 and concluded that no further actions were required.

Category 1 Lip Products, Toys, Insect Repellents

Category 2 Deodorants/Antiperspirants

Category 3 Hydroalcoholic Products for Shaved Skin,
Eye Products Men's Facial Creams & Balms,
Tampons

Category 4 Hydroalcoholic Products for Unshaved Skin,
Hair Styling Aids & Sprays, Body Creams

Category 5 Women's Facial Cream/Facial Make-up, Hand Cream,
Facial Masks, Wipes/Refreshing Tissue for Hands,
Face, Neck, Body

Category 6 Mouthwash, Toothpaste

Category 7 Intimate Wipes, Baby Wipes

Category 8 Make-up remover, Hair Styling Aids Non-spray,
Nail Care

Category 9 Shampoo, Rinse-off Conditioners, Bar Soap,
Feminine Hygiene Pads and liners

Category 10 Detergents, hard Surface Cleaners, Diapers

Category 11 All Non-skin or Incidental skin contact products

Hydroxycitronellal

CAS N°: 107-75-5

Empirical formula: C₁₀H₂₀O₂
(CH₃)₂C(OH)-(CH₂)₃-CH(CH₃)-CH₂-CHO

Synonyms: Citronellalhydrate
3,7-Dimethyl-7-hydroxyoctanal
Octanal, 7-hydroxy-3,7-dimethyl-
Oxydihydrocitronellal
Laurinal, Laurine

History: Initial reviews: March 1987, September 2000, April 2005 (39th Amendment, new format only)
Current revision date: 2007
Last amendment number: 42
Last amendment date: May 16, 2007
Implementation date: For new submissions*: June 16, 2007
For existing fragrance compounds*: June 16, 2009
Next review date: 2012

* This date applies to the supply of fragrance compounds (formulas) only, not to the finished products in the marketplace.

Standard: RESTRICTED

RESTRICTIONS:

Limits in the finished product:			
For a description of the categories, refer to the QRA Informational Booklet.			
Category 1: See Note box (1)	0.1 %	Category 7:	0.4 %
Category 2:	0.2 %	Category 8:	2 %
Category 3:	0.8 %	Category 9:	5 %
Category 4:	2.3 %	Category 10:	2.5 %
Category 5:	1.2 %	Category 11: See Note box (2)	
Category 6: See Note box (1)	3.6 %		

Note box:
(1) IFRA would recommend that any material used to impart perfume or flavour in products intended for human ingestion should consist of ingredients that are in compliance with appropriate regulations for foods and food flavourings in the countries of planned distribution and, where these are lacking, with the recommendations laid down in the Code of Practice of IOFI (International Organisation of the Flavor Industry). Further information about IOFI can be found on its website (www.iofiorg.org).
(2) Category 11 includes all non-skin contact or incidental skin contact products. Due to the negligible skin contact from these types of products there is no justification for a restriction of the concentration of this fragrance ingredient in the finished product.

[List of Other Materials](#)

[QRA Information Booklet](#)

[QRA Technical Dossier](#)

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RIFM Summaries:

Hydroxycitronellal - Sensitization Potency Estimation Based on Weight of Evidence

LLNA weighted mean EC3 values (mg/cm ²) [no. studies]	Human Data			Potency Classification ²	WOE NESIL ³ (mg/cm ²)
	NOEL – HRIPT (induction) (mg/cm ²)	NOEL – MAX (induction) (mg/cm ²)	LOEL ¹ (induction) (mg/cm ²)		
5612 [9]	5000	NA	5906	Weak	5000

NOEL = No observed effect level; HRIPT = Human Repeat Insult Patch Test; MAX = Human Maximization Test;

LOEL = lowest observed effect level; NA = Not Available

¹Data derived from HRIPT or Human Max tests

²Gerberick *et al.*, 2001

³WoE NESIL limited to two significant figures

REXPAN Rationale / Conclusion:

The RIFM Expert Panel reviewed the critical effect data for hydroxycitronellal and, based on the weight of evidence, established the No Expected Sensitization Induction Level (NESIL) as 5000 µg/cm². They recommend the limits for the 11 different product categories, which are the acceptable use levels of hydroxycitronellal in the various product categories. These were derived from the application of the exposure-based quantitative risk assessment approach for fragrance ingredients, which is detailed in the QRA Expert Group Technical Dossier of June 22, 2006.

VOCs

Any compound containing at least one carbon atom, with a vapor pressure greater than 0.1 mm Hg at 20° C



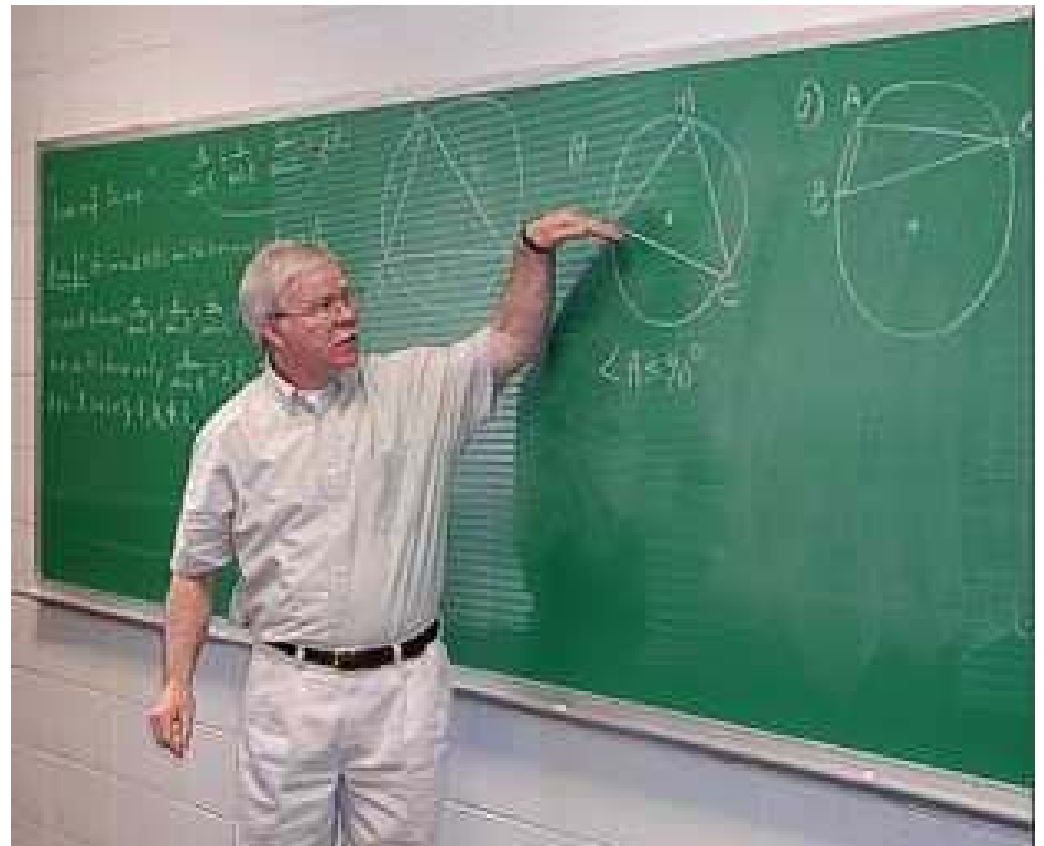
The vapor pressure of a mixture is the sum of the vapor pressure contributions of all the ingredients

VOC Formula

Vapor pressure contribution=

Vapor pressure X concentration X correction factor

- 1 MW 120 or greater
- 1.33 MW 100-120
- 1.66 MW 80-120
- 2 MW 60-80
- 3 MW less than 60



EU Allergens

- Amylcinnamyl alcohol
- Amyl cinnamal
- Benzyl alcohol
- Benzyl salicylate
- Cinnamyl alcohol
- Cinnamal
- Citral
- Coumarin
- Eugenol
- Geraniol
- Hydroxycitronellal
- Hydroxymethylpentyl
cyclohexenecarboxaldehyde
- Isoeugenol
- Anisyl alcohol
- Benzyl benzoate
- Benzyl cinnamate
- Citronellol
- Farnesol
- Hexylcinnamaldehyde
- Lilial
- D-Limonene
- Linalool
- Methyl heptine carbonate
- g-Methylionone
- Oak Moss
- Tree Moss

RIFM Today

- Risk Assessment
- Environmental
- QRA
- Respiratory

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Fragrance Materials

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for the Safe Use of Fragrance Materials

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IFRA

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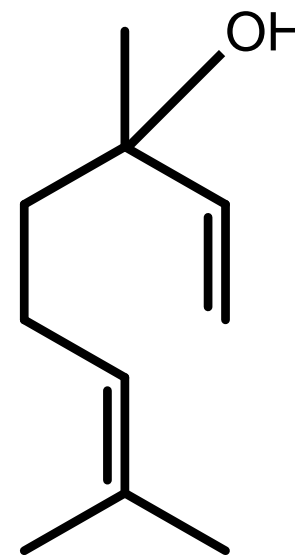
The Research Institute for Fragrance Materials, Inc. (RIFM) generates, evaluates and distributes scientific data on the safety assessment of fragrance raw materials found in perfumes, cosmetics, shampoos, creams, detergents, air fresheners, candles and other personal and household products.

The RIFM Database is the most comprehensive source worldwide of physical-chemical, toxicological and eco-toxicological data, literature and information on safety evaluation associated with known fragrance and flavor materials.

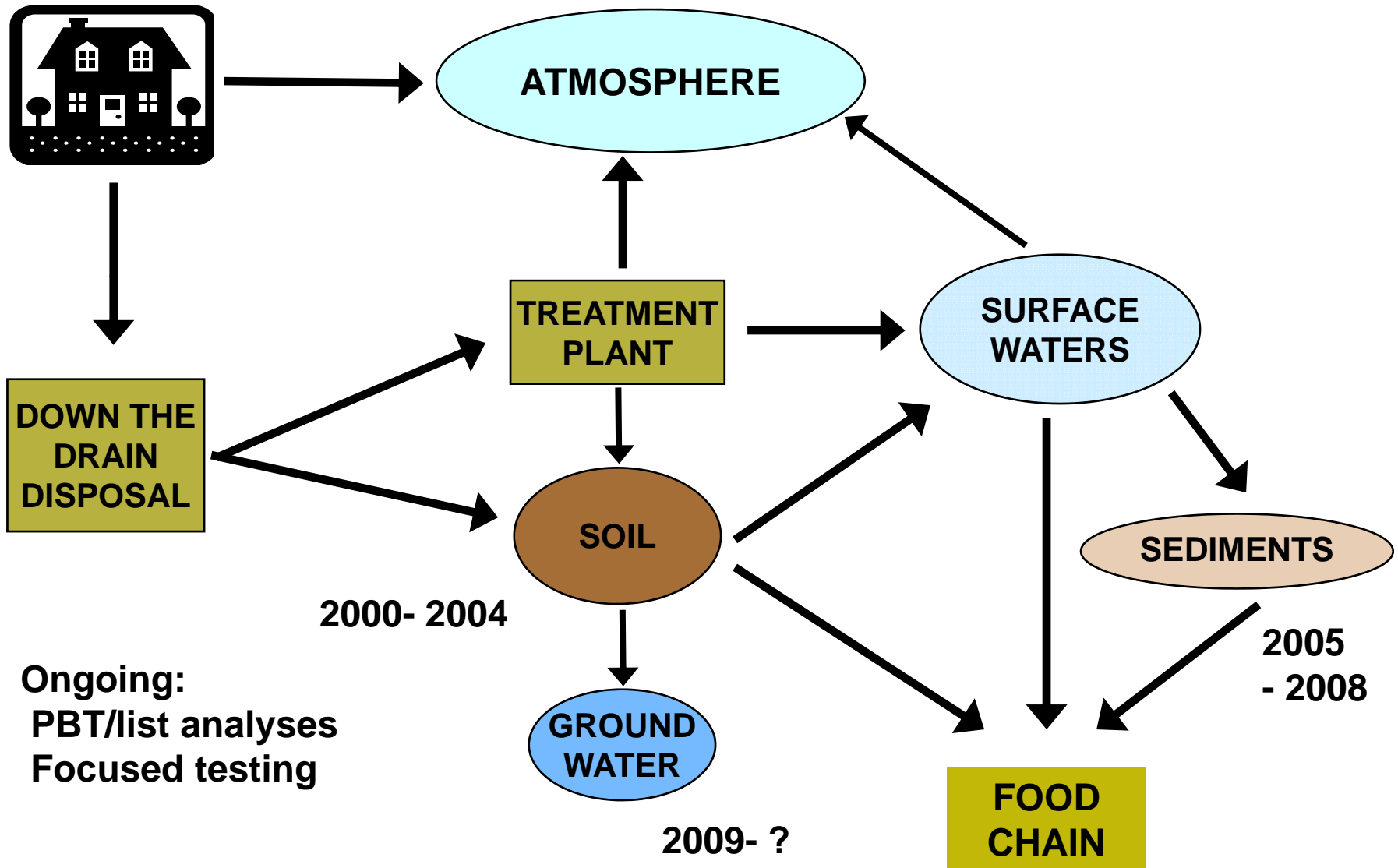
High Priority Material

- Structural Alerts
- Volume of use >1000 metric tons
- Maximum Dermal use level 4.3%
(fine fragrances)
- Total Score 34

Linalool



Environmental Pathways



Aquatic Risk



Environmental Toxicology and Chemistry, Vol. 21, No. 6, pp. 1301–1308, 2002

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Hazard/Risk Assessment

A FRAMEWORK FOR PRIORITIZING FRAGRANCE MATERIALS FOR AQUATIC RISK ASSESSMENT

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(Received 8 June 2001; Accepted 6 November 2001)

Negligible Risk

2100 fragrance materials
categorized for aquatic risk,
92.3 % have negligible risk
at current volume of use.

$$\frac{PEC}{PNEC} < 1$$

PEC = Predicted Environmental Concentration

PNEC = Predicted No-effect Concentration

QRA

- Determination of benchmarks (no expected sensitization induction level, or NESIL);
- Application of sensitization assessment factors (SAF)
- Calculation of consumer exposure (CEL) through product use.

Exposure

$$\text{Acceptable Exposure Level (AEL)} = \frac{\text{WoE NESIL}}{\text{SAF}}$$

NESIL = No-Expected-Sensitization Induction Level

WoE = Weight of Evidence

SAF = Sensitization Assessment Factor

Respiratory Safety

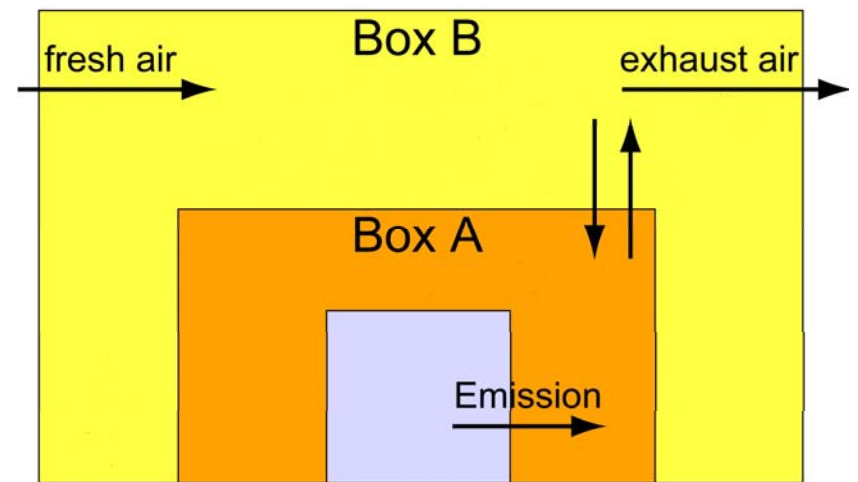
- Selected fragrance ingredients
 - Benzyl acetate
 - Eugenol
 - α -Hexyl cinnamic aldehyde (HCA)
 - HHCB
 - Hydroxycitronellal
 - β -ionone
 - d-limonene
 - Linalool
 - Methyl dihydrojasmonate



Respiratory

- Exhaled nitric oxide
- Forced expiratory volume
- Cell counts from induced sputum and nasal lavage
- Subjective symptoms

Allergens stimulate IgE, T_H1 , T_H2



Respiratory

Evaluated respiratory effects of fragrance on non asthmatics, mild asthmatics, and moderate asthmatics, no negative effect from Fragrance.

