Perfume Engineering

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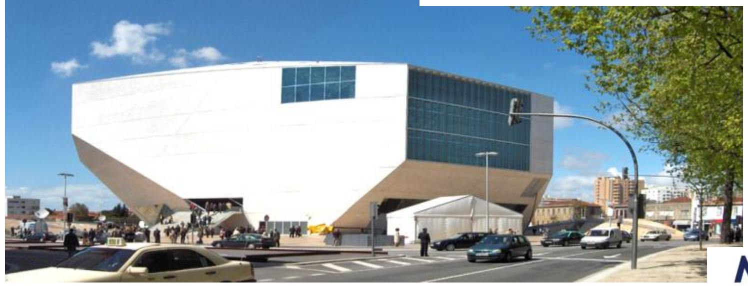
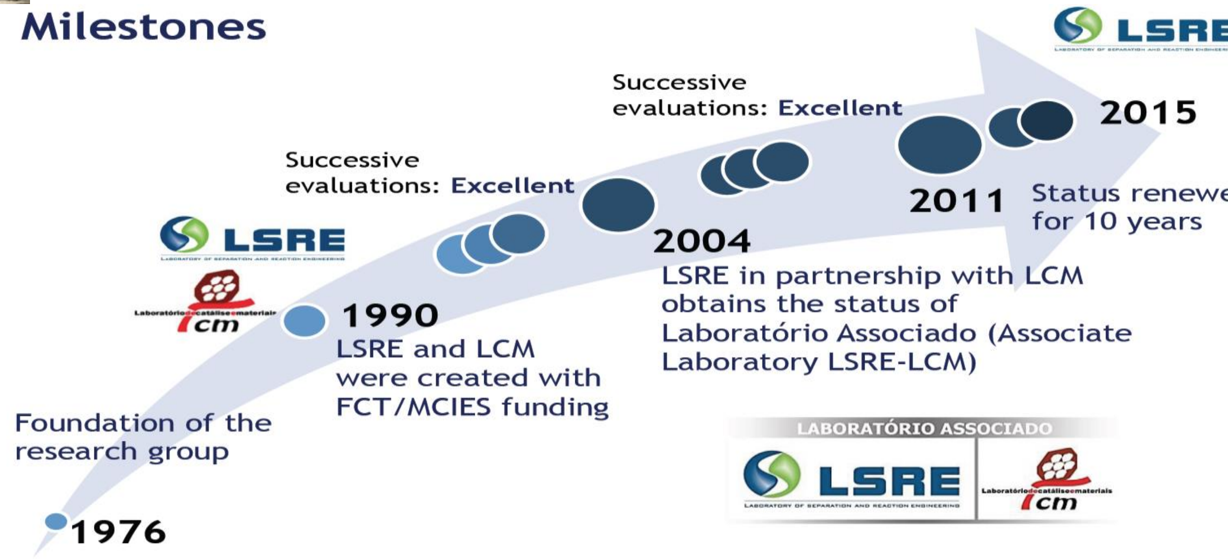
P O R T O

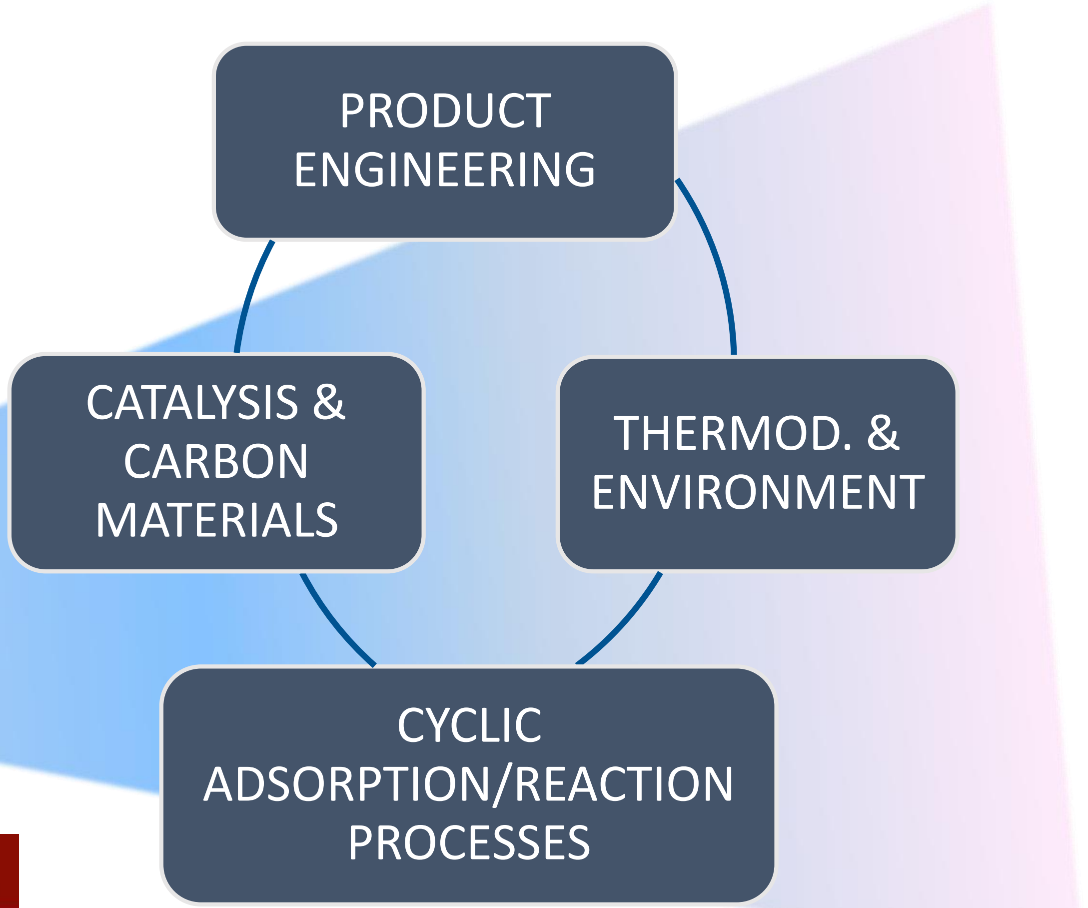


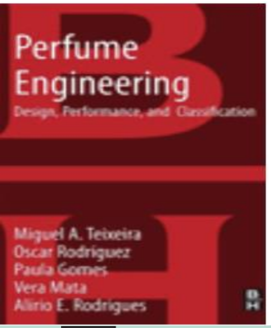

Milestones
LSRE
1976
Foundation of the research group
1990
LSRE and LCM were created with FCT/MCIES funding
Successive evaluations: Excellent
2004
LSRE in partnership with LCM obtains the status of Laboratório Associado (Associate Laboratory LSRE-LCM)
Successive evaluations: Excellent
2011
2015
Status renewe
for 10 years
LABORATÓRIO ASSOCIADO
LSRE
cm

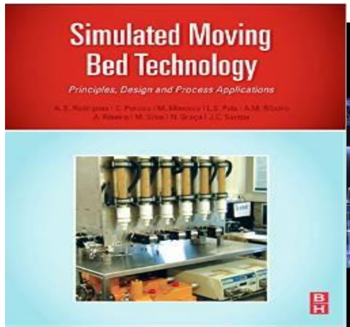
Research lines and Groups

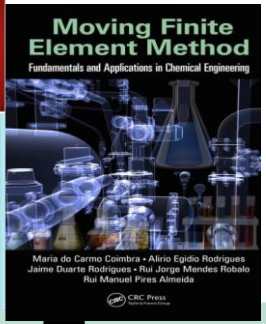
New technologies of cyclic separations/reactions

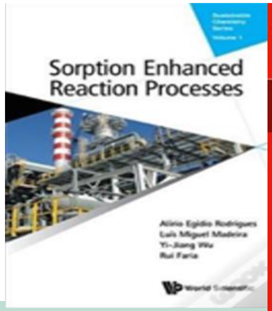
Synthesis and formulation of high-added value products

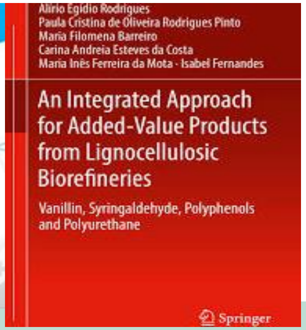












Ask the right question…

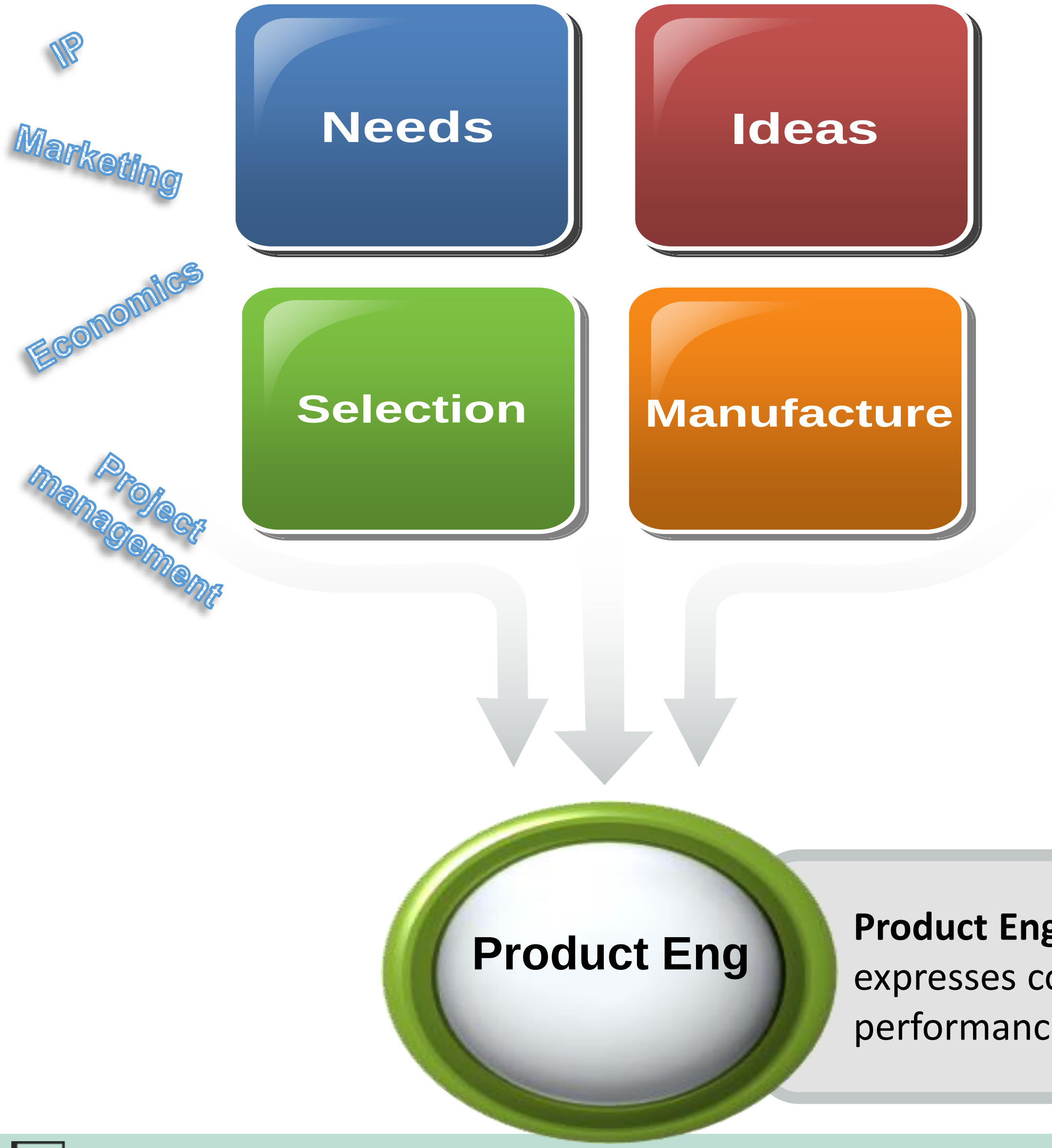
Given a liquid with composition x_i

What do we smell?

Outline

- Introduction to Product Engineering and odor perception
- Scientific Methodologies for Engineering Perfumes
  - Predicting the odor from the molecule
  - Perfumery Ternary Diagram (PTD®)Perfumery Quaternary-Quinary Diagram (PQ2D®)
  - Examples of applications. Effect of base notes.
  - Evaporation/release of fragrance mixtures
  - Propagation of odorants in air and odor performance analysis
  - Perfumery Radar
  - Sillage - The trail of perfumes
- Conclusions and Looking ahead

What is Product Engineering?



Product Classification

1. **Commodities-** Propylene, Vanillin, Acetals (SMBR)
2. **Specialty chemicals** - Chiral molecules
3. **Formulated products**

   Perfumes, Microcapsules
4. **Devices** - FlexSMB®, NetMix®)
5. **Virtual chemical products** - PTD®, PQ2D®, Perfumery Radar
6. **Bio-based products** - Lactobionic acid, Dextran
7. **Technology-based consumer goods-** Perfumed suits

Product Engineering
expresses consumer needs for a specific application or market into a new, high-performance and valuable product

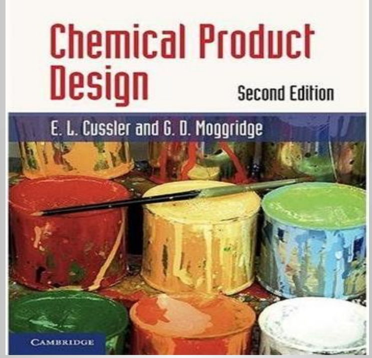
What is Product Engineering?

- How new products are conceived, designed, developed, manufactured and sold

(Wesselingh *et al.*, Design & development of biological, chemical, food and pharmaceutical products, 2007)

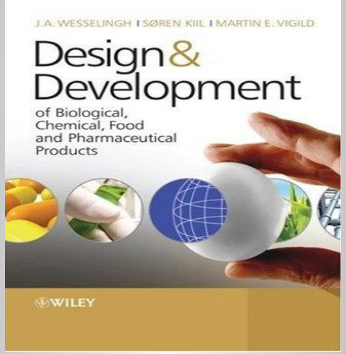
Ulrich & Eppinger 1995 - 2008

Cussler & Moggridge 2001 - 2011

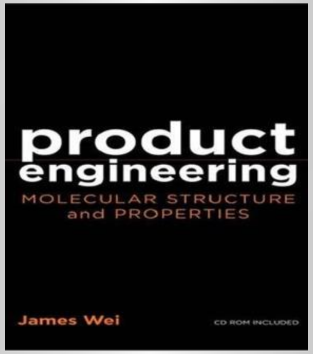


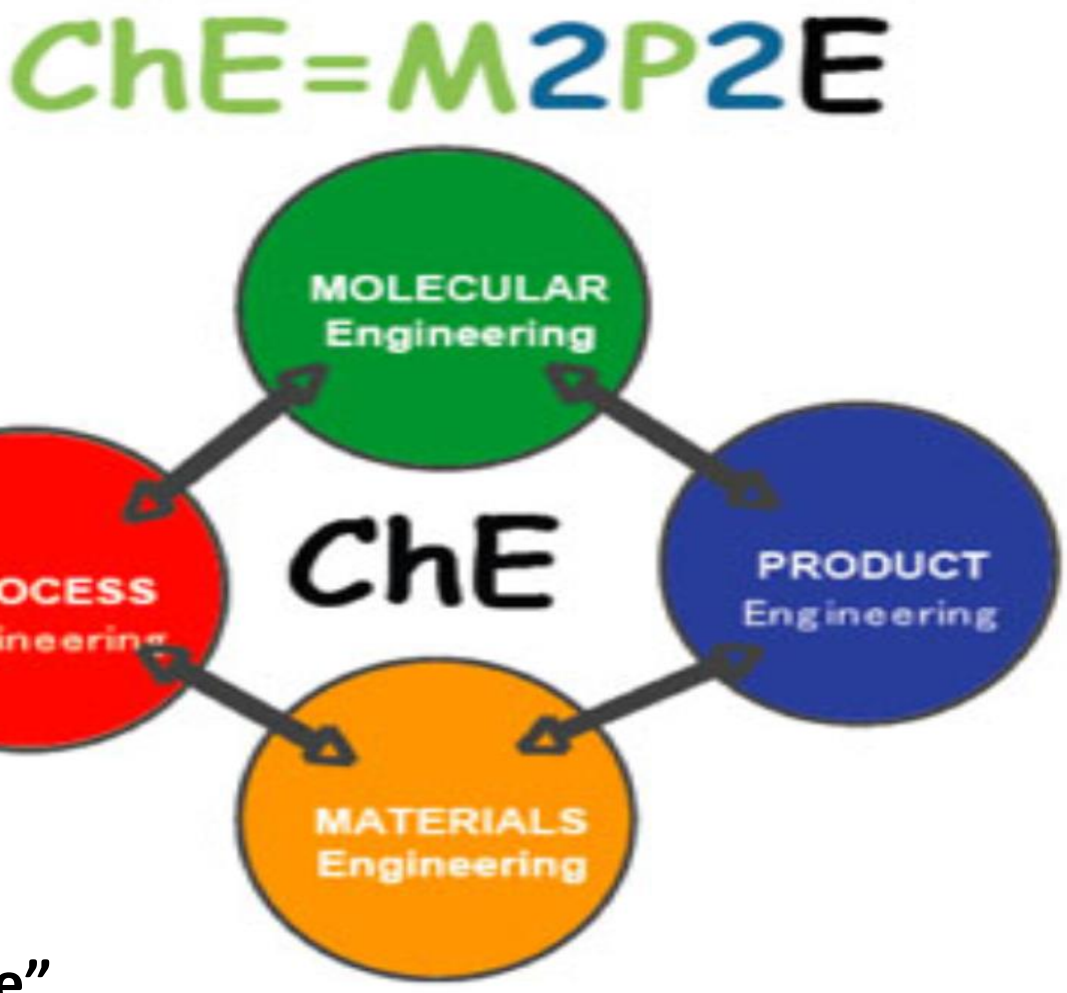
Ng *et al.* 2006

Wesselingh *et al.* 2007



J. Wei 2007





To "make", to "service", to "care"
Solke Bruin

My vision of ChE today

Rodrigues, A.E., et al., XXXIII Reunion Iberica de Adsorcion. Madrid, Spain, 13-14, 2008.

But...

Why apply Product Engineering to fragrances?

Perfumed products

- Fine Fragrance (Happy, Chanel No. 5…)
- Air Care (Candles, sent diffusers…)
- Fabric Care (Detergents, conditioners…)
- Personal Care (Shampoos, deodorants…)
- Personal Wash (Bar Soaps, liquid body or hand wash…)
- Home Care (Dish Wash, all purpose cleaners…)

¾ of the products we deal with every day contain a fragrance in it!

Application to Flavors & Fragrances: Relevance & Motivation

- Large *palette* of available essential oils and fragrances (~10^4)
- Formulation of perfumes is still an art…
- Mainly developed by perfumers…
- High number of test mixtures in the pre-formulation stage until achieving the final product
  - ***"Trial-and-error"***

Bois de Paradis (Parfums DelRae, 2005):
- > 2 years to be developed
- ~ 300 *trials* until reaching the final product

- **High production costs**
- **Long development time**

F&F Industry and Market

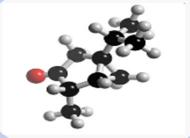
- Flavor & Fragrance business:

$9.6 bn → $12.9 bn → $16 bn → $22 bn

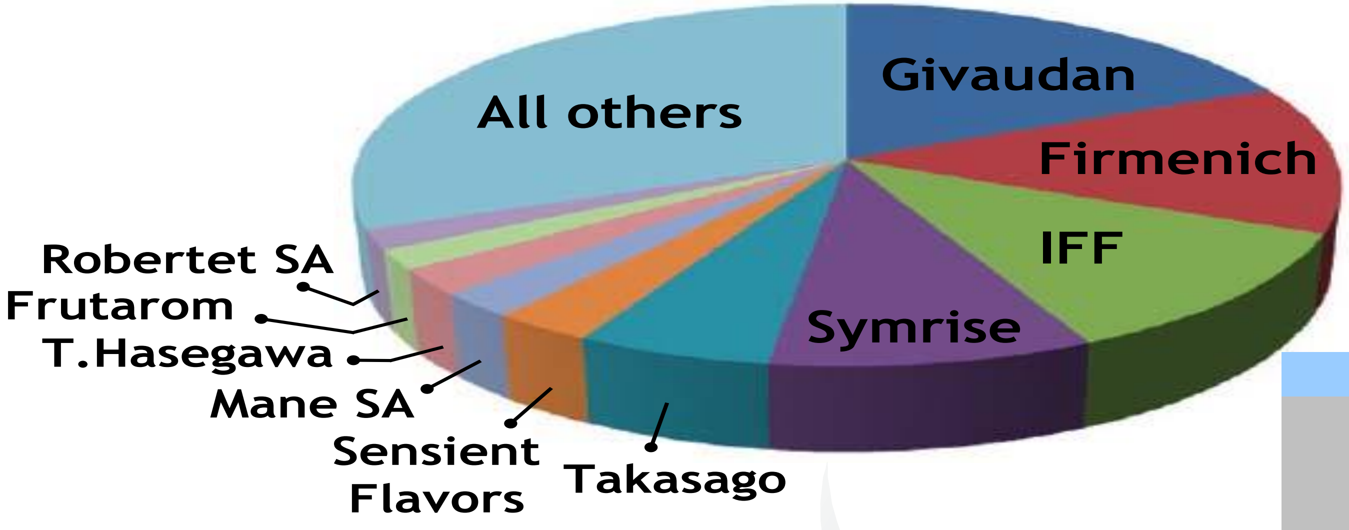
1995	2000	2005	2010
$9.6 bn	$12.9 bn	$16 bn	$22 bn

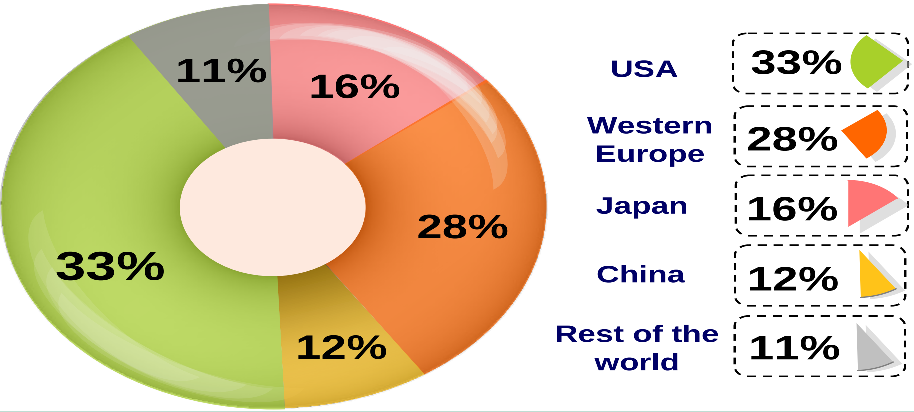
Increasing number of consumer products containing fragrances / aromas

Synthesis of new fragrance molecules (natural, *"natural-identical"* or synthetic)



F&F Industry and Market





- ✓ Multi-billion dollar market
- ✓ Top-5 companies control 63%

Rank	Company	US$	Market Share
1	Givaudan	4538	20.6%
2	Firmenich	3319	15.1%
3	IFF	2623	11.9%
4	Symrise	2107	9.6%
5	Takasago	1416	6.4%
6	Sensient Flavors	583	2.6%
7	Mane SA	643	2.9%
8	T. Hasegawa	557	2.5%
9	Robertet SA	485	2.2%
10	Frutarom	451	2.1%
Top 10	-	16722	76.0%
All others	-	5278	24.0%
Total Market	-	$21999	100.0%

Values in millions of $US in 2010.

In 2017 same top4; then Mané SA, Frutarom,Takasago, Sensient Tech,Robertet, Hasegawa Huabao Int…

Bridging Product Engineering to Fragrances

Definition of Needs

Trial-and-error

Fragrance development takes

1000-to-2000 tests

Long development times

Slow response to market

from 1 to 3 years

Lack of scientific tools

Low predictability

Short product diversity range

Lack of customized solutions

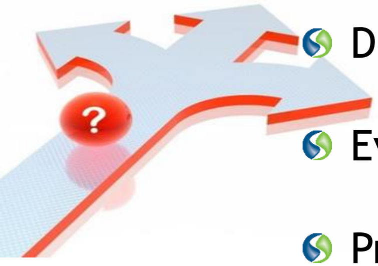
Waste of raw materials

Cost of natural raw materials may

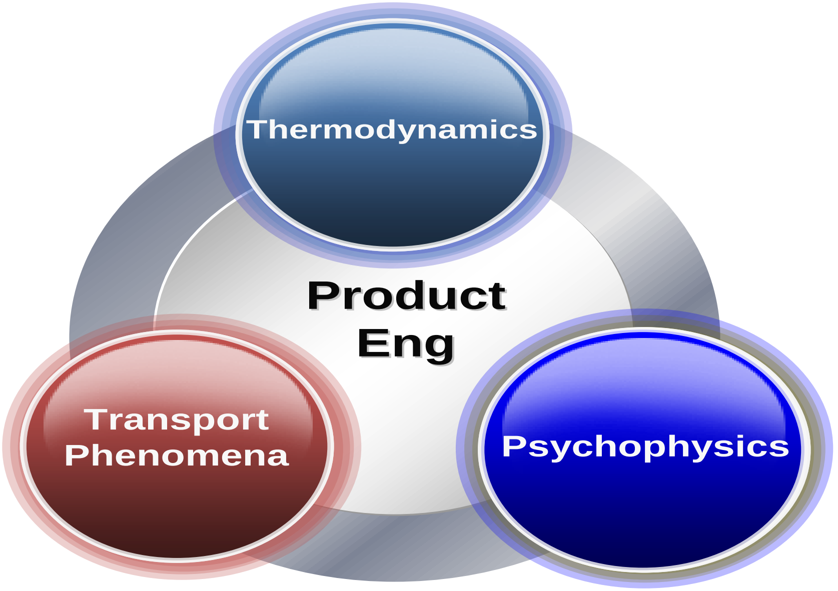
range from $10 to $50000 per kg

Bridging Product Engineering to Fragrances

- **Objectives:**
  - Prediction of the odor character of multi-component mixtures of fragrances
  - Describe the evaporation/release of fragrances
  - Evaluation of the diffusion and performance of perfumes
  - Prediction of odor detection thresholds
  - Classification of perfumes into olfactory families using scientific tools



Product Engineering applied to Flavors & Fragrances



Bridging Product Engineering to Fragrances

- **Objectives:**
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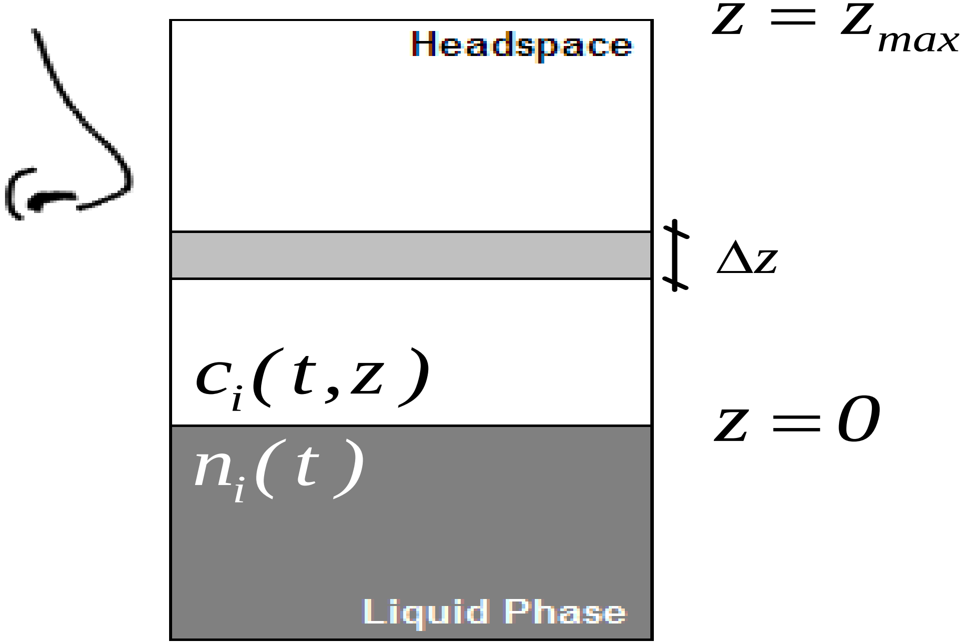
Product Engineering applied to Flavors & Fragrances

Perfume Engineering

Scientific methodologies for Perfume Engineering

- **Odor perception model**



Psychophysics

- **Odor Character:**
  - Strongest Component Model
- **Odor Intensity:**
  - Odor Value (OV), Stevens' Power Law, Weber-Fechner

Chemical Engineering

- **Perfume Diffusion:**
  - Fick's Law, Maxwell-Stefan
- **Perfume Evaporation:**
  - UNIFAC, ASOG, UNIFAC-D, A-UNIFAC methods

Teixeira, M.A.; Rodríguez, O.; Mata, V.G.; Rodrigues, A.E., Chemical Engineering Science 2009, 64, 2570-2589.

Odor Perception Model

Odor Character

Strongest Component Model

$$\psi_{mixture} = max\{\psi_i\}$$

Odor Intensity

Stevens' Power Law

$$\Psi_i = \left(\frac{C_i^g}{ODT_i}\right)^n$$

Ψ - *perceived odor intensity*
C^g - *odorant concentration in air*
ODT - odorant detection threshold
n - exponent power law

Diffusion

Fick's Law

$$\frac{\partial C_i}{\partial t} = D_{ij}\frac{\partial^2 C_i}{\partial x^2}$$

Maxwell-Stefan

$$d_i = \sum_{j=1}^{N}\frac{y_i y_j\left(u_i - u_j\right)}{D_{ij}}$$

Evaporation

Group contribution methods

UNIFAC, UNIFAC-D, UNIFAC-A, ASOG…

Other approaches:

COSMO-RS
Molecular Simulation

Odor Perception Model

- Odor intensity:

Odor Value

$$OV_i = \frac{C_i^g}{ODT_i}$$

$$\boxed{\mathbf{OV_i} = \gamma_i x_i \left(\frac{P_i^{sat} M_i}{ODT_i}\right)\left(\frac{1}{RT}\right)}$$

Stevens' Power Law

$$\Psi_i = \left(\frac{C_i^g}{ODT_i}\right)^n$$

$$\boxed{\Psi_i = \left[\gamma_i x_i \left(\frac{P_i^{sat} M_i}{ODT_i}\right)\left(\frac{1}{RT}\right)\right]^n}$$

- Odor character:

Strongest Component Model

$$OV_{mix} = max\{OV_i\}$$

Teixeira, M.A., Rodríguez, O., Mata, V.G., Rodrigues. A.E., AIChE Journal, 55(8), 2171-2185, 2009.

From vapors to the nose: the perception of odors

The Nobel Prize in Physiology or Medicine 2004
Richard Axel, Linda B. Buck

The Nobel Prize in Physiology or Medicine 2004

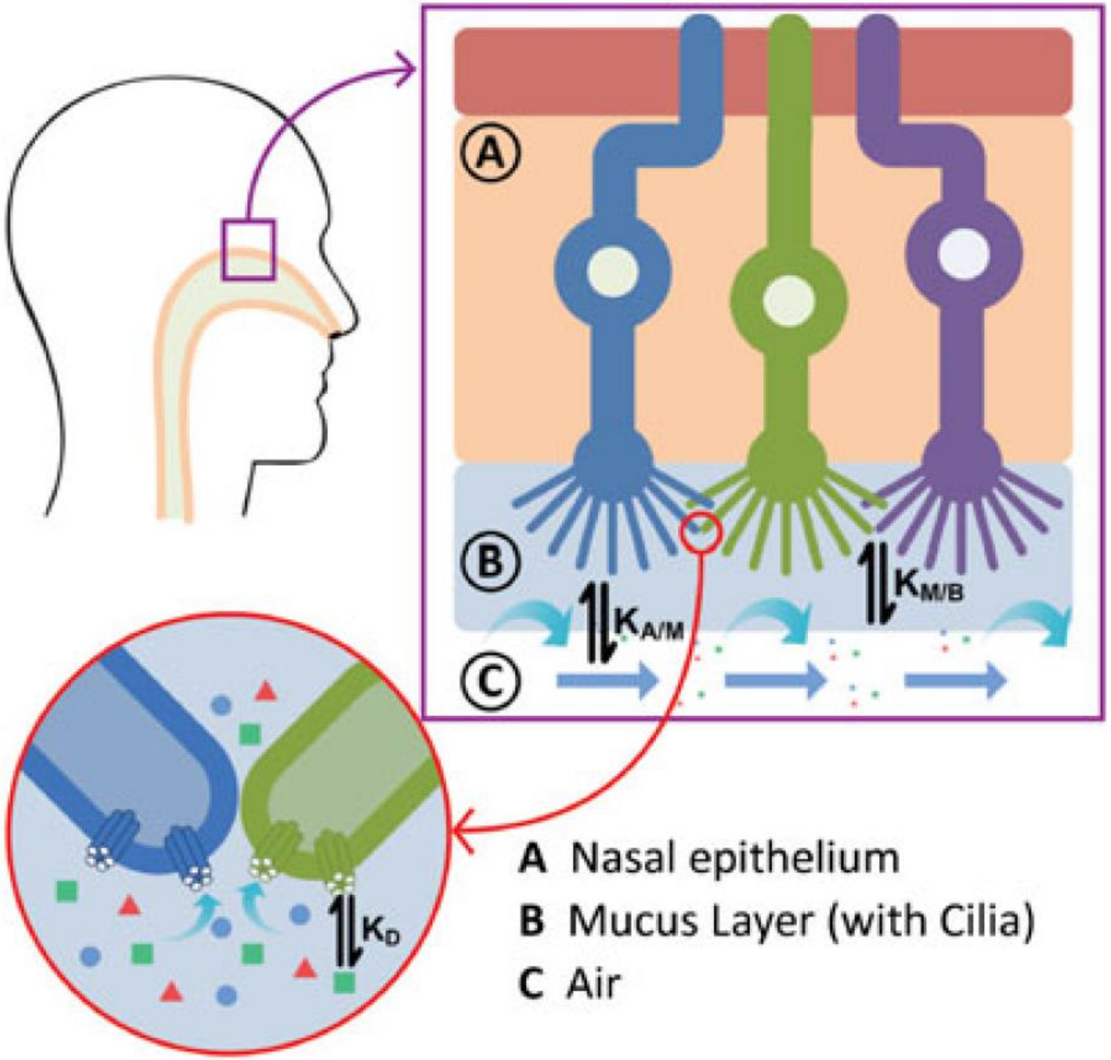
Richard Axel

Linda B. Buck

The Nobel Prize in Physiology or Medicine 2004 was awarded jointly to Richard Axel and Linda B. Buck *"for their discoveries of odorant receptor: and the organization of the olfactory system"*

$$C_i^{\text{air}} \xleftrightarrow{K_{\text{air/mucus}} = \frac{C_i^{\text{mucus}}}{C_i^{\text{air}}}} C_i^{\text{mucus}} \xleftrightarrow{K_{\text{mucus/biophase}} = \frac{C_i^{\text{biophase}}}{C_i^{\text{mucus}}}} C_i^{\text{biophase}}$$

$$\text{ODT}_i \propto \frac{K_{\text{AW}}}{K_{\text{OW}}} = \frac{P_i^{\text{s}}}{K_{\text{OW}} C_{i,\text{W}} RT}$$



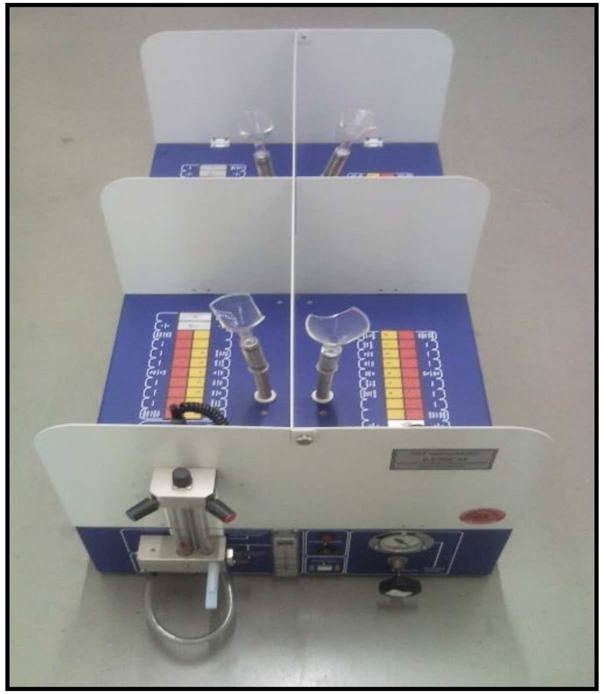
O. Rodriguez, M. Teixeira and AE Rodrigues, FFJ,2011,26, 421-428

Odor Thresholds

Odor detection threshold (ODT)
Minimum concentration of an odorant that can be detected by humans

Odor recognition threshold (ORT)
Lowest odorant concentration at which its recognition becomes possible

Olfactometer



ODT is the concentration of an odorous chemical at which the physiological effect elicits a response for 50% of the panelists.
ASTM (Method E 679-91)

Odor Thresholds

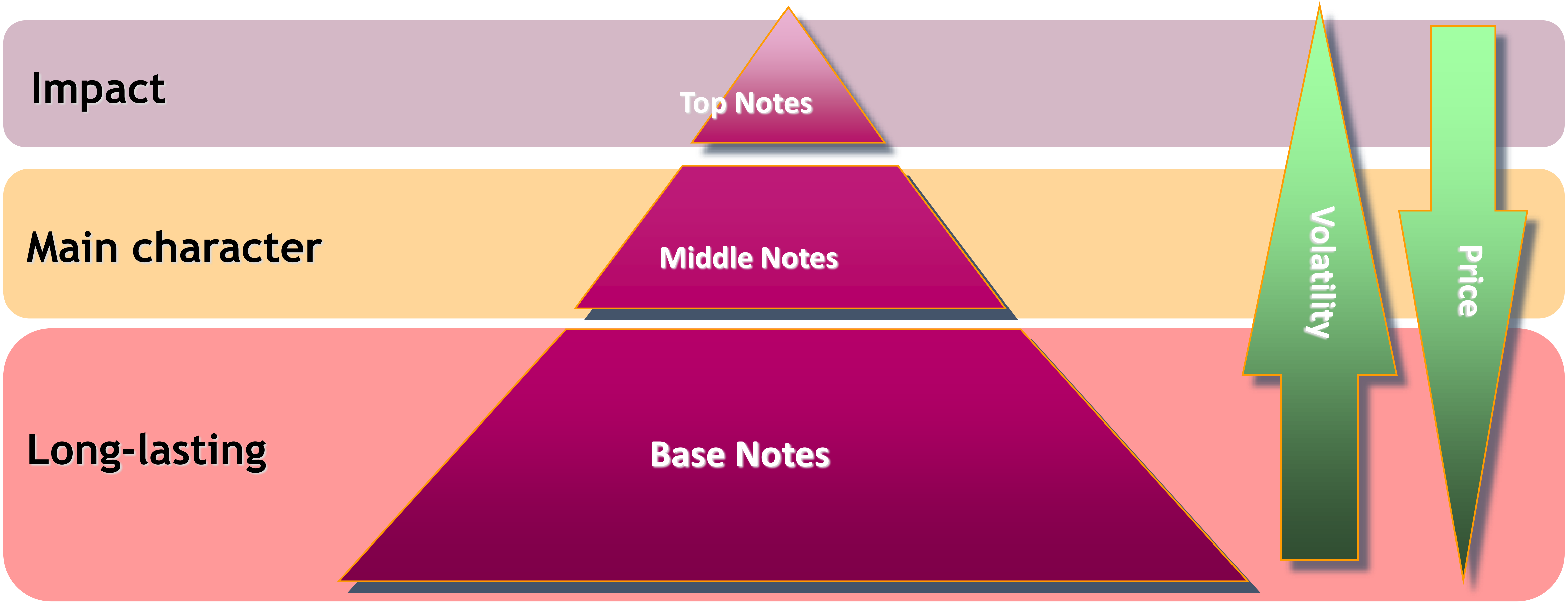
Table 15.1 *Human odor detection thresholds*

Compound	Odor Threshold in Air (parts per billion)
Methanol	141,000
Acetone	15,000
Formaldehyde	870
Menthol	40
T-butyl mercaptan	0.3

Source: From Devos et al. (1990).

Scientific methodologies for Perfume Engineering

Perfume structure

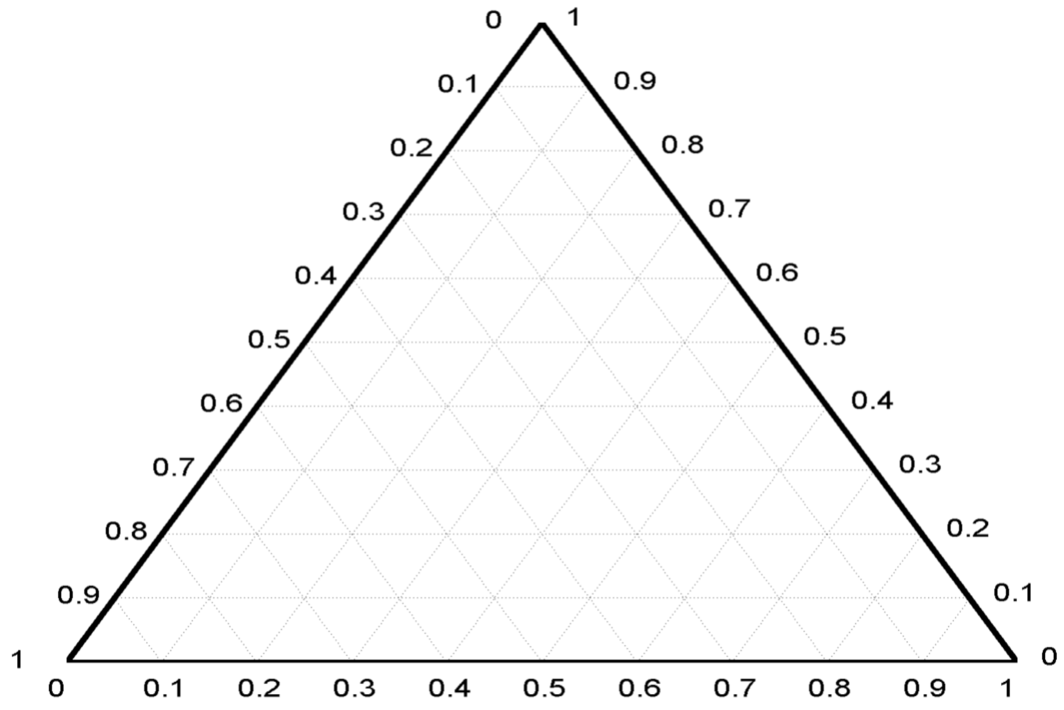


Carles, J., Soap Perfumery Cosmetics 35, 328-335, 1962; IFF, Kerschner, J., Bergen Academy, 2006.

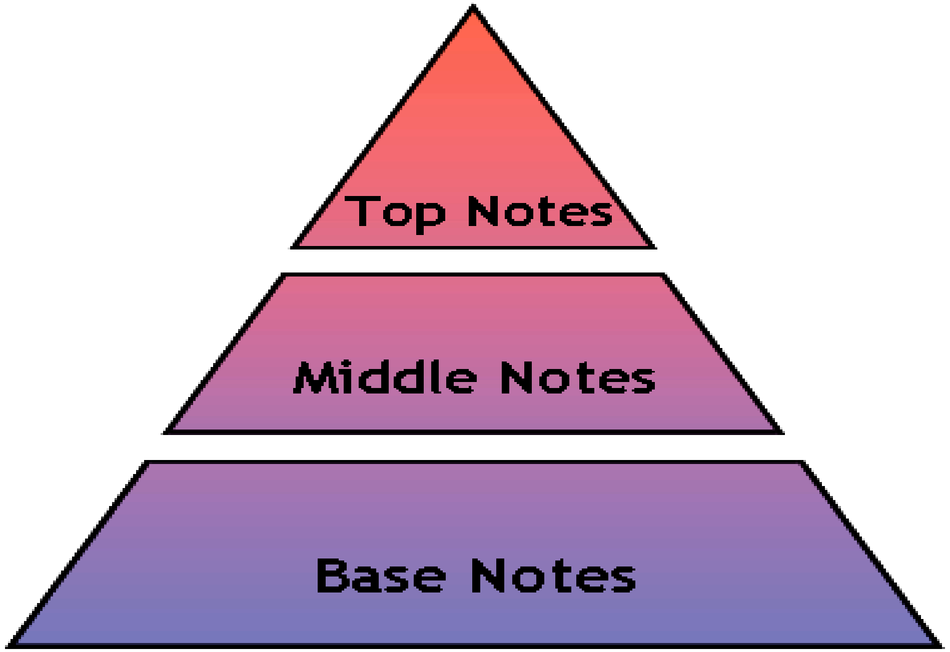
The Concept of the Perfumery Ternary Diagram (PTD®)

- Results from the combination of

- Engineering Ternary Diagrams



- Perfumery Pyramid Structure



Mata, V.G., Rodrigues, A.E., AIChE Journal, 52, 2938-2948, 2006.

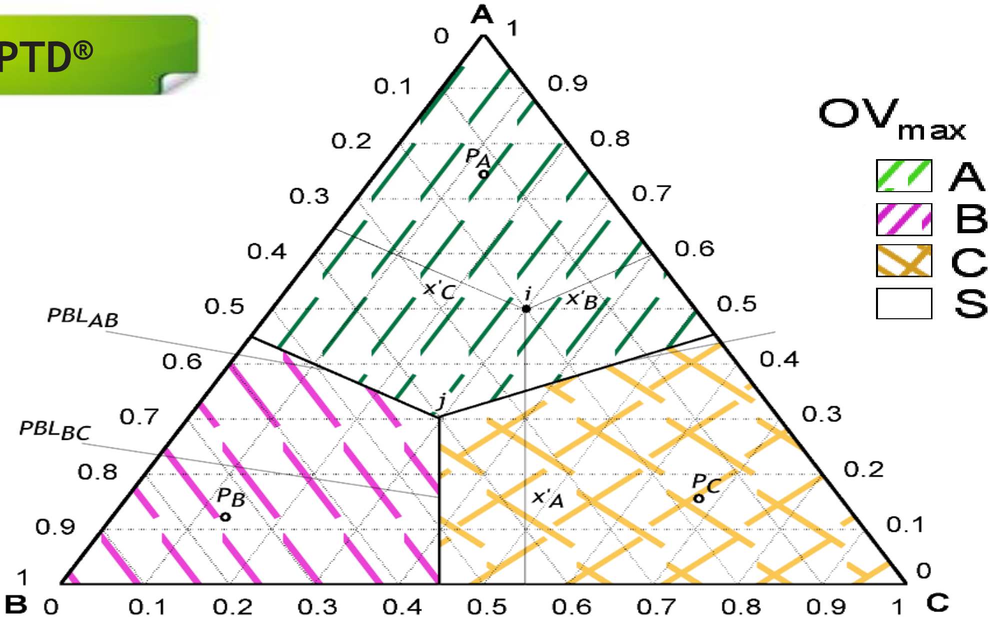
The Perfumery Ternary Diagram (PTD®)

- Mapping the OV vs compositions allows the definition of Odor Zones where one odorant intensity prevails (OV_{max})

- Notes represented in the PTD®:
  - A – Top Note
  - B – Middle Note
  - C – Base Note
  - S - Solvent

- Four component: solvent-free basis

PTD®



Combination of the Perfume Pyramid Structure with the ternary phase diagrams.

$$x'_A = \frac{x_A}{x_A + x_B + x_C} \qquad x'_B = \frac{x_B}{x_A + x_B + x_C} \qquad x'_C = \frac{x_C}{x_A + x_B + x_C}$$

Odor Character for any ternary mixture is represented

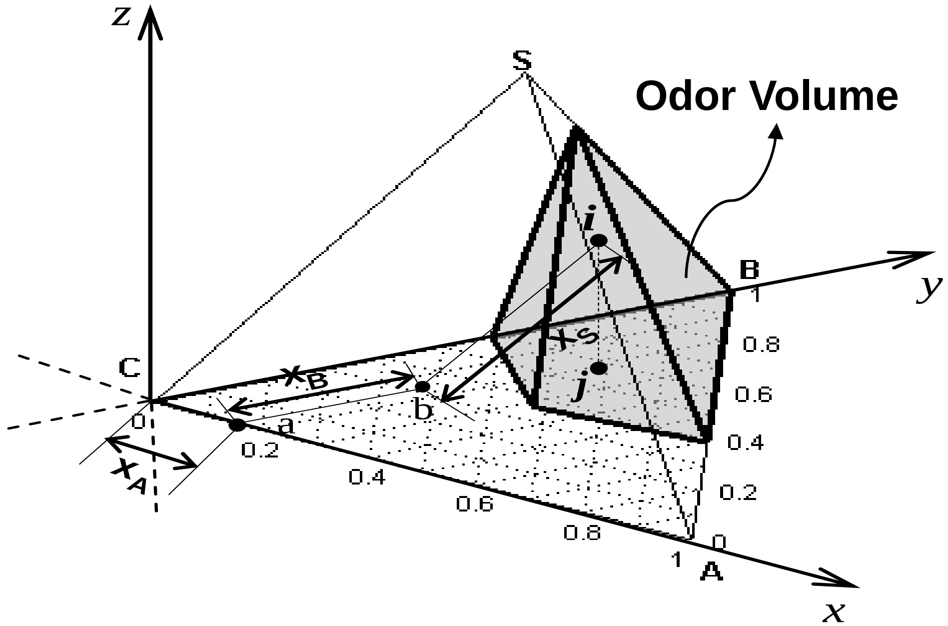
Teixeira, M.A., Rodríguez, O., Mata, V.G., Rodrigues. A.E., AIChE Journal, 55(8), 2171-2185, 2009.

The Perfumery Quaternary-Quinary Diagram (PQ2D®)

- The PTD® methodology is a valuable tool for ternary mixtures but is ***limited*** when applied to quaternary systems

- ***Only*** with the ***Perfumery Quaternary-Quinary Diagram (PQ2D®)*** it is possible to show the complete odor distribution for quaternary mixtures in 3D graphs

PQ2D®

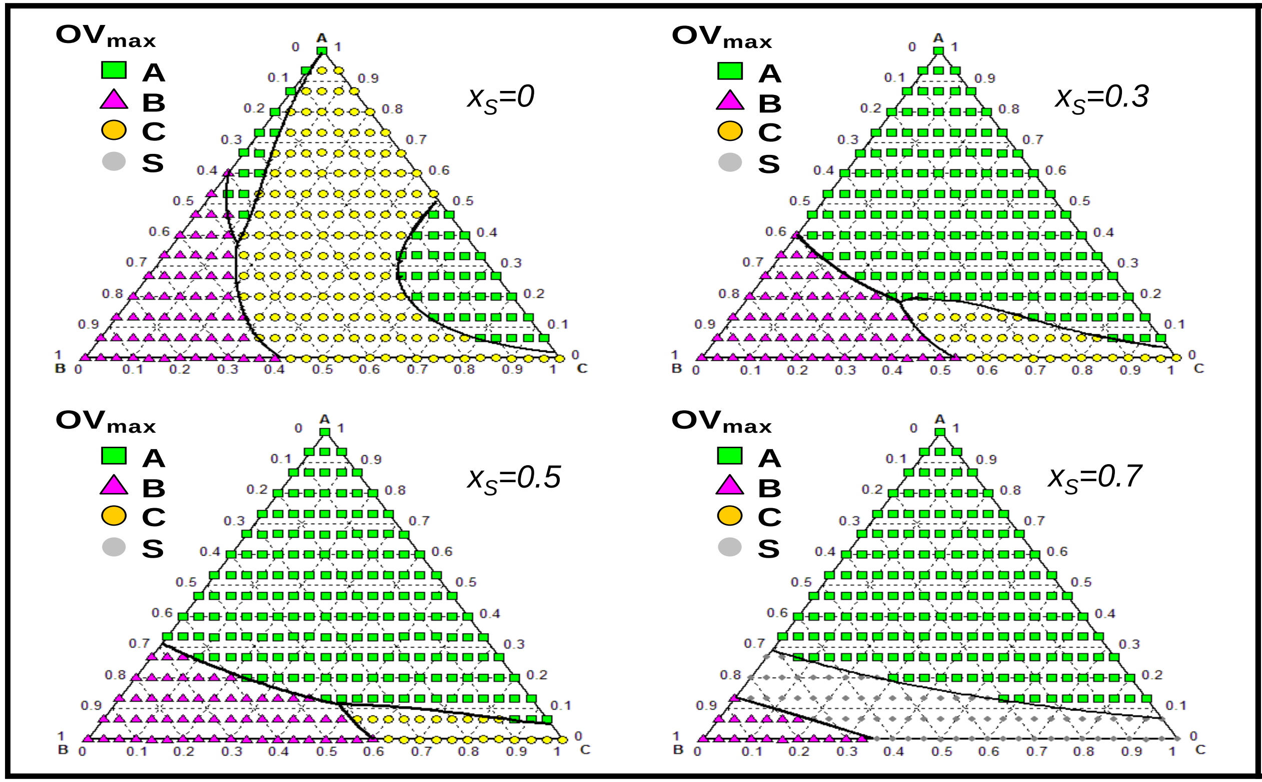


Relationship between the PQ2D® and the Engineering Quaternary Diagrams.

Teixeira, M.A., Rodríguez, O., Mata, V.G., Rodrigues. A.E., AIChE Journal, 55(8), 2171-2185, 2009.

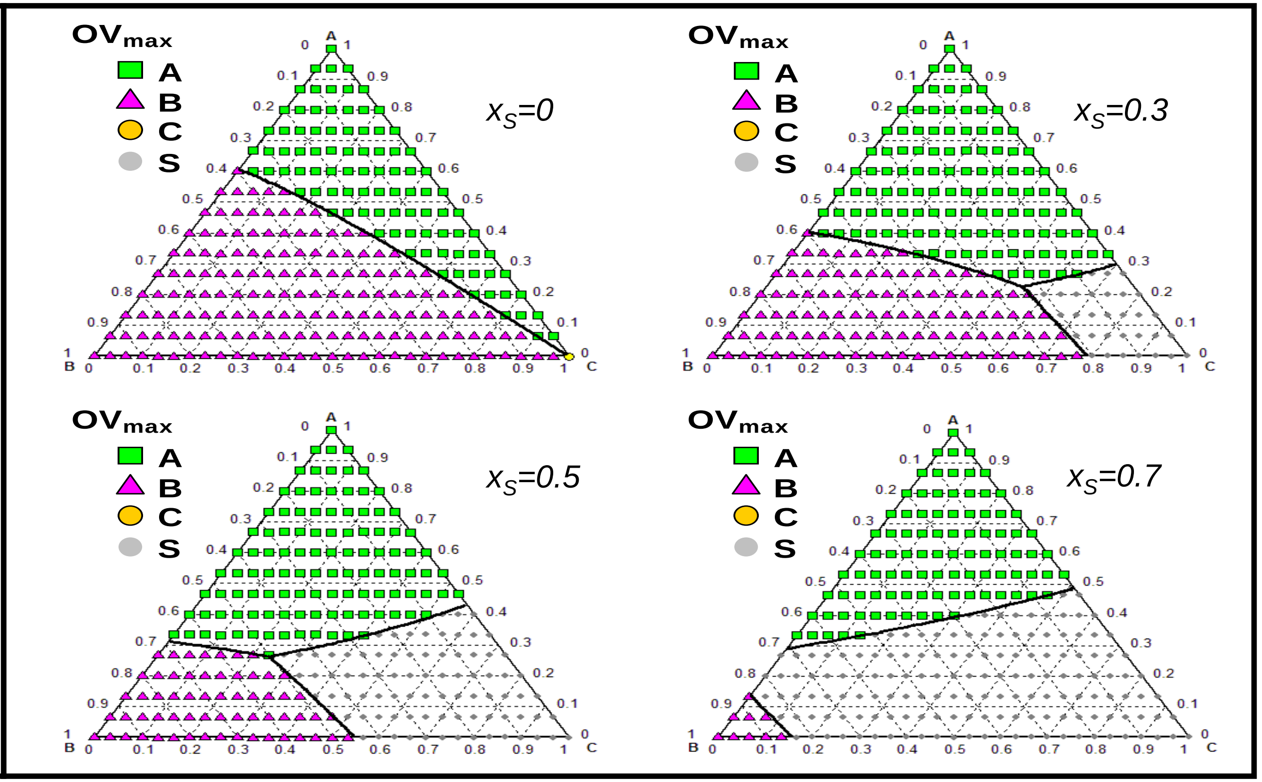
Examples of applications of the PTD® and PQ2D®

Effect of base notes and fixatives



A: limonene, B: geraniol,

C: vanillin, S: ethanol



A: limonene, B: geraniol,

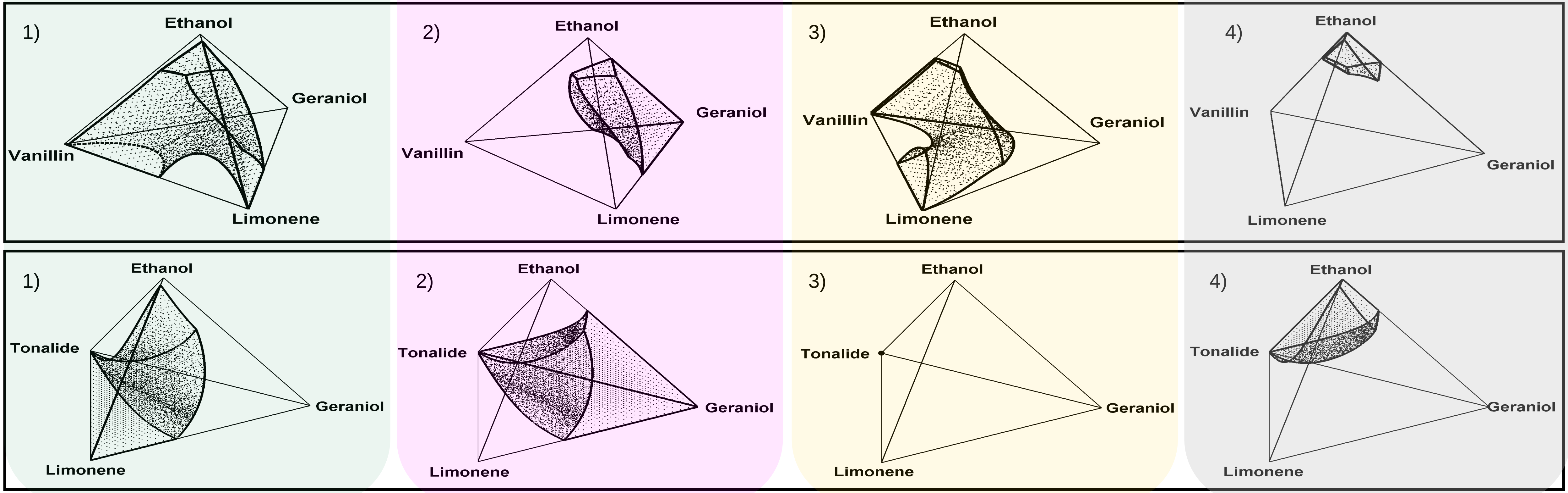
C: tonalide, S: ethanol

Teixeira, M.A., Rodríguez, O., Mata, V.G., Rodrigues. A.E., AIChE Journal, 55(8), 2171-2185, 2009.

The Perfumery Quaternary-Quinary Diagram (PQ2D®)

- Each Fragrance Volume can be seen separately in the PQ2D®

1.Limonene 2.Geraniol 3.Vanillin or Tonalide 4.Ethanol

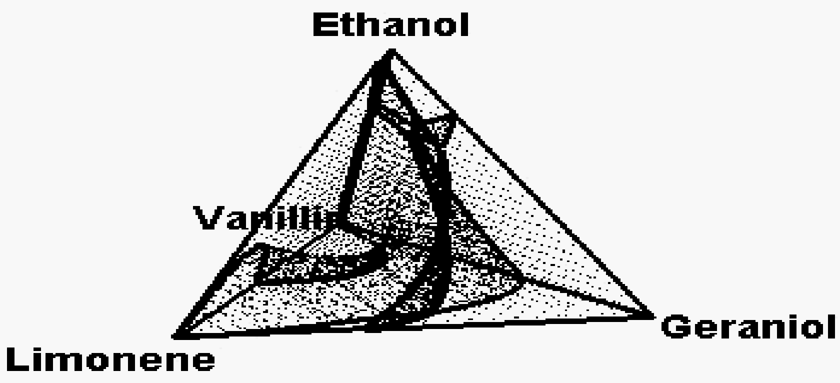


The Perfumery Quaternary-Quinary Diagram (PQ2D®)

- Each Fragrance Volume can be seen separately in the PQ2D®

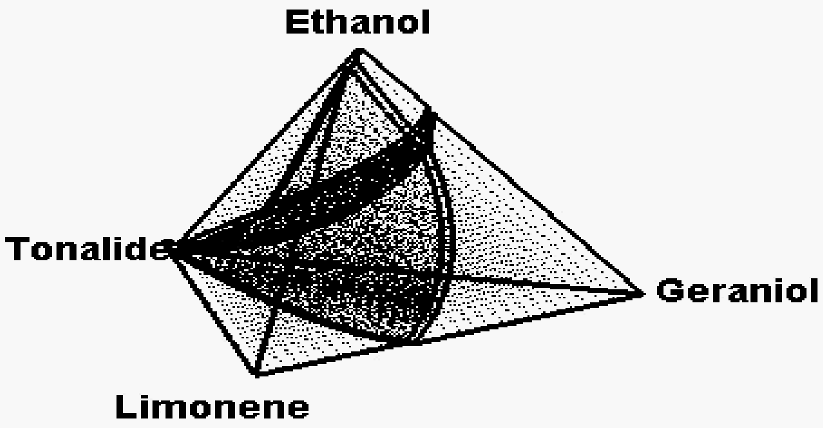
Perfumery fragrance volumes:

1. Limonene, 2. Geraniol, 3. <u>Vanillin</u>, 4. Ethanol.



Perfumery fragrance volumes:

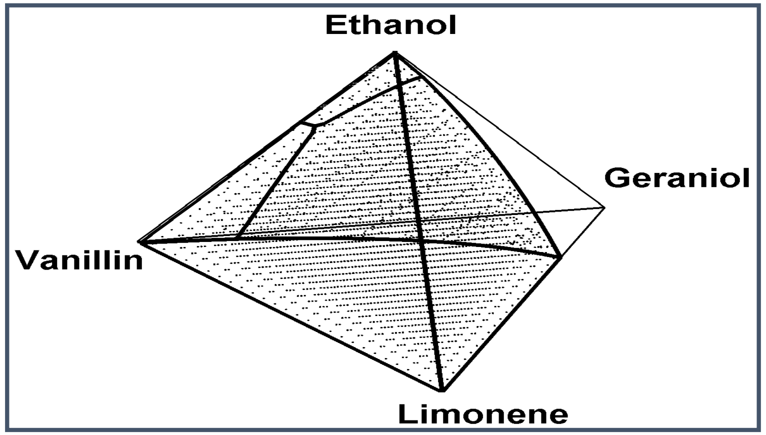
1. Limonene, 2. Geraniol, 3. <u>Tonalide</u>, 4. Ethanol.

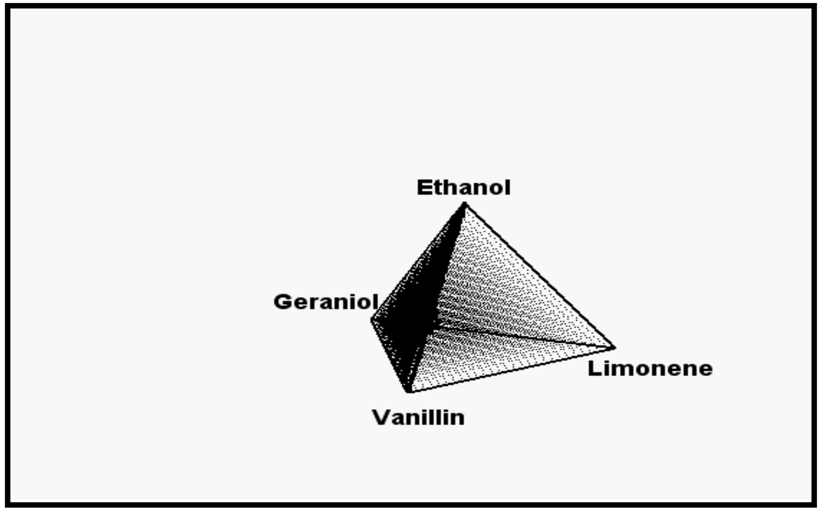


Quinary Mixtures

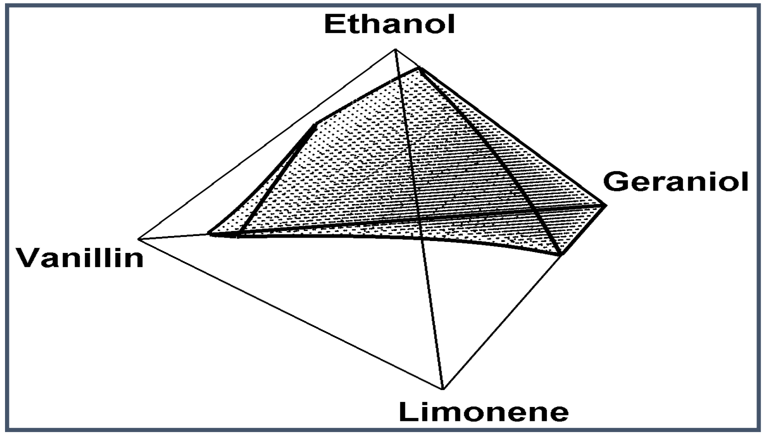
45% Water

Limonene

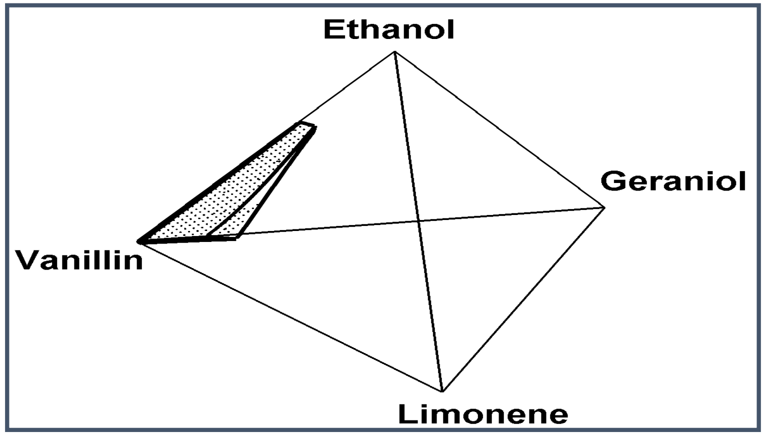




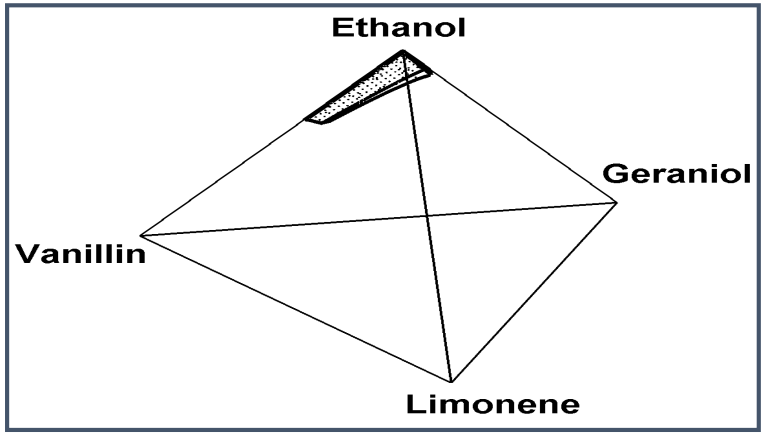
Geraniol



Vanillin



Ethanol

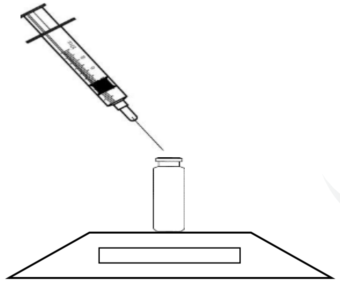


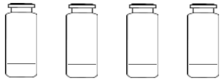
Teixeira, M. A.; Rodríguez, O.; Rodrigues, A. E., AIChE Journal 2010, 56, (4), 1090-1106.

- Evaporation/release of fragrance mixtures

Vapor-liquid equilibria of fragrance systems

- Vapor compositions were experimentally measured by headspace-gas chromatography

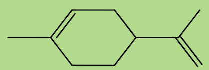


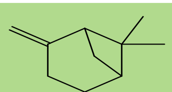


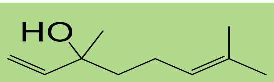
4 replicates of each mixture

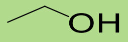
Allowed to equilibrate for 24h

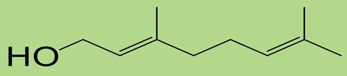
HS-GC analysis

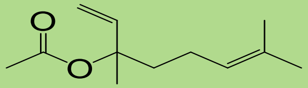

limonene

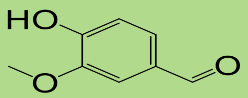

α-pinene


linalool


ethanol


geraniol


linalyl acetate


vanillin

- 65 data points
- Binary, ternary & quaternary mixtures

	Components						
FS1	α–pinene	+	Linalool				
FS2	Limonene	+	Linalool				
FS3	α–pinene	+	Limonene				
FS4	α–pinene	+	Limonene	+	Linalool		
FS5	α–pinene	+	Geraniol				
FS6	α–pinene	+	Limonene	+	Geraniol		
FS7	α–pinene	+	Linalool	+	Geraniol		
FS8	Linalool	+	Geraniol				
FS9	Limonene	+	Geraniol				
FS10	Limonene	+	Linalool	+	Geraniol		
FS11	α–pinene	+	Limonene	+	Linalool	+	Geraniol
FS12	α–pinene	+	Linalyl acetate				
FS13	Limonene	+	Linalyl acetate				
FS14	α–pinene	+	Limonene	+	Linalyl acetate		
FS15	Limonene	+	Linalool	+	Geraniol	+	Ethanol
FS16	Limonene	+	Geraniol	+	Vanillin	+	Ethanol

Vapor-liquid equilibria of fragrance systems

- Vapor compositions were also predicted using group-contribution methods which allow determining activity coefficients (γ_i)

$$\ln \gamma_i = \underbrace{\underbrace{\ln \gamma_i^C + \ln \gamma_i^R}_{\text{UNIFAC, ASOG, UNIFAC-D}} + \left(\ln \gamma_i^A\right)}_{\text{A-UNIFAC}}$$

- **ASOG** (1969) combines the Flory-Huggins theory with the Wilson equation
- **UNIFAC** (1975) is based on the UNIQUAC equation
- **UNIFAC-D** (1987)introduces changes in volume and interaction parameters
- **A-UNIFAC** (1999) uses the original UNIFAC with a new term for associative interactions

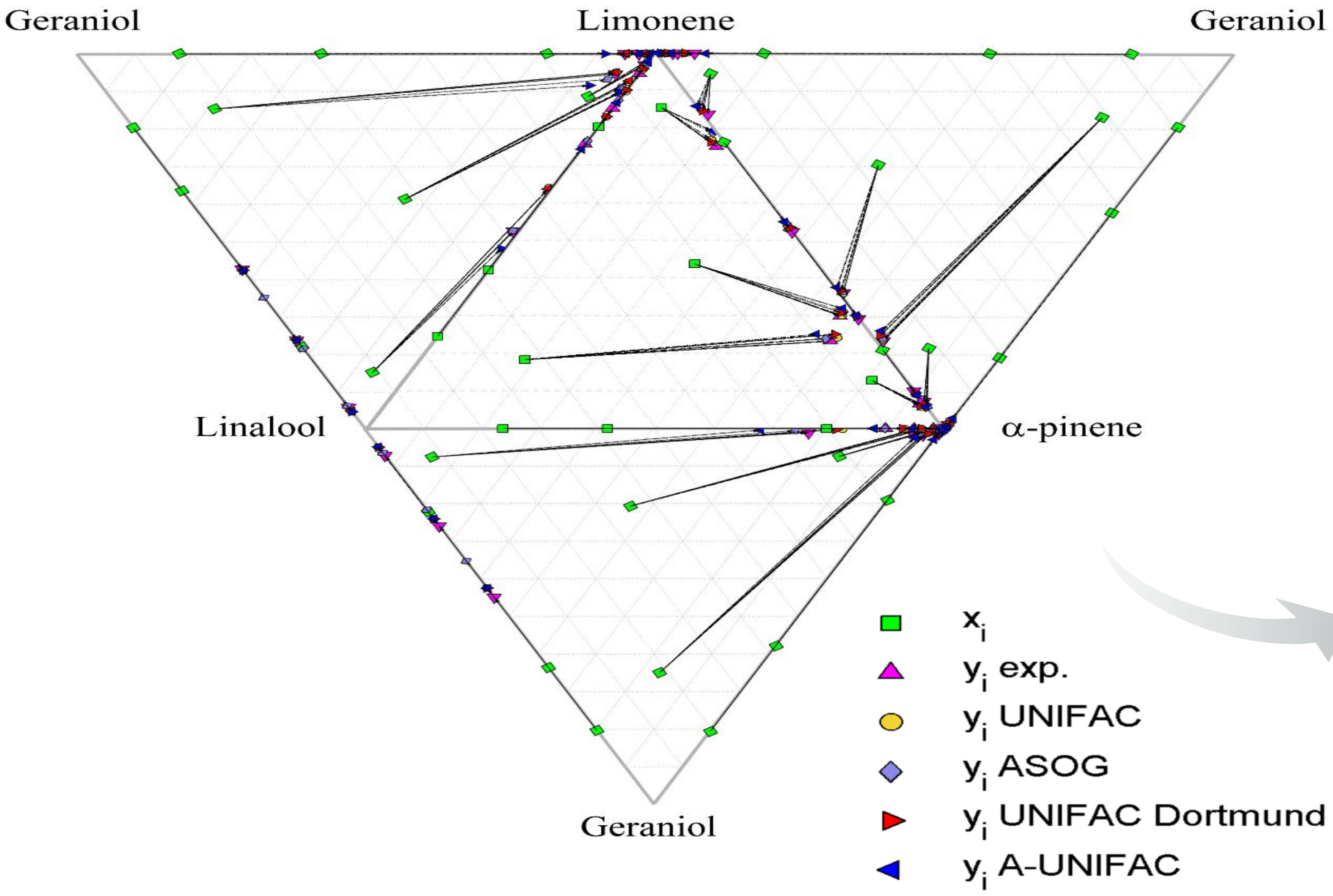
Liquid composition (x_i)

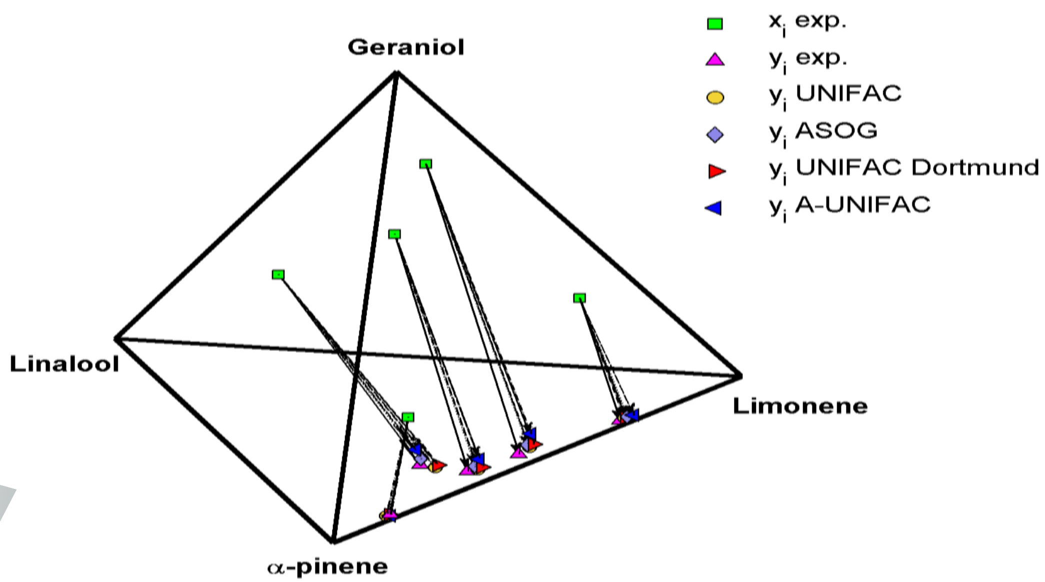
Molecules assigned to functional groups

$\longrightarrow$ Iterative procedure for calculation of activity coefficients and vapor-liquid compositions

Vapor-liquid equilibria of fragrance systems

- Comparison between the experimental and predicted vapor compositions





Teixeira, M.A.; Rodríguez, O.; Mota, F.L.; Macedo, E.A.; Rodrigues, A.E., Ind & Eng Chem Res 2011, 50, 9390-9402.

Comparison of predicted vs sensorial dominant odor

- However, from vapor compositions it is possible to calculate odor intensities

Predicted vapor compositions → Stevens' Power Law + Stronger component model

Experimental vapor compositions → Stevens' Power Law + Stronger component model

Method	Agreement with experimental dominant odor
UNIFAC	95.4%
ASOG	95.4%
UNIFAC-D	93.8%
A-UNIFAC	90.8%

- Non-trained panelists (~ consumers) also performed olfactory evaluations

Pure predictions agreed in 58% with panelists

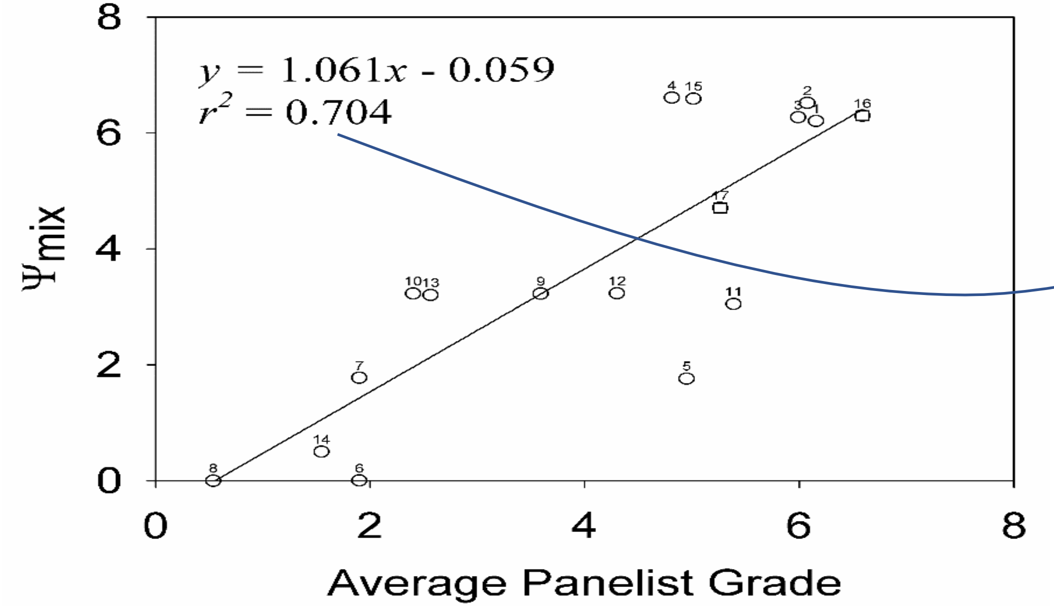
- The majority of the mismatches were observed for quaternary mixtures with ethanol

Teixeira, M.A.; Rodríguez, O.; Mota, F.L.; Macedo, E.A.; Rodrigues, A.E., Ind & Eng Chem Res 2011, 50, 9390-9402.

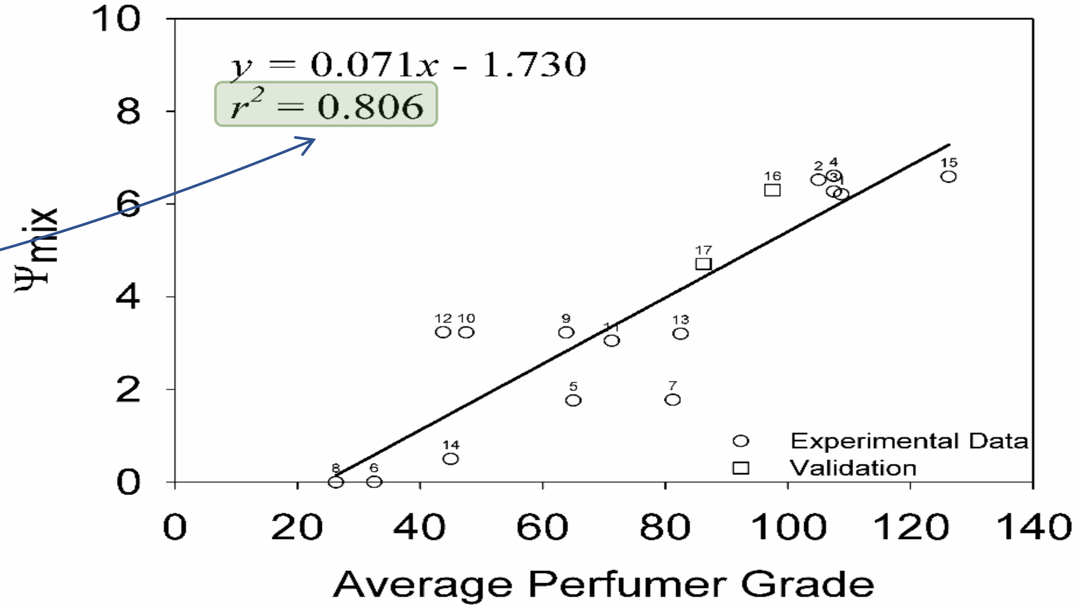
Comparison between models and panelists

- Good correlation between sensory panels and predictive models

Non-trained Panelists



Perfumers



In collaboration with P&G

Teixeira, M.A.; Rodríguez, O.; Rodrigues, A.E.; Selway, R.; Riveroll, M.; Chieffi, A., Ind & Eng Chem Res 2013, 52, 963-971

Propagation of odorants in air and performance

Pierre Le Goff, ENSIC

L'enseignement par la recherche

a) conservation equations (mass, energy, momentum, electric charge)
b) equilibrium laws at the interface(s)
c) constitutive laws
d) kinetic laws of heat/mass transfer and reaction
e) initial and boundary conditions
f) optimization criterion

"Le Génie Chimique c'est pas de la plomberie"

Daniel Tondeur, co-supervisor

Jacques Villermaux, Professor of CRE

Diffusion & Performance of Fragrances

- For diffusion of single components the **steady state solution** can be used:

From Fick's first law as a function of the molar flux relative to stationary coordinates:

$$N_{A_z} = -c_T D_{AB} \frac{\partial y_A}{\partial z} + y_A \left(N_{A_z} + N_{B_z} \right) \longrightarrow$$

The concentration profile of A in steady state can be calculated by:

$$\left(\frac{1-y_A}{1-y_{A_1}} \right) = \left(\frac{1-y_{A_2}}{1-y_{A_1}} \right)^{\frac{z-z_1}{z_2-z_1}}$$

- For diffusion of multi-component mixtures the **unsteady state** gives:
  - Gas Phase

$$\frac{\partial y_A}{\partial t} = \frac{D_{AB}\left[\left(\frac{\partial y_A}{\partial z} \right)\left(\frac{\partial y_A}{\partial z} \right) + (1-y_A)\frac{\partial^2 y_A}{\partial z^2} \right]}{(1-y_A)^2}$$

  - Liquid Phase

$$\frac{dn_A}{dt} = D_{AB} A_{gl} c_T \left. \frac{\partial x_A}{\partial z} \right|_{z=0}$$

- Boundary Conditions (BC)

$$t > 0$$

$$z = 0 \qquad y_A = y_{A_{eq}} = \frac{\gamma_i P_i^{sat}}{P} x_i$$

$$z = z_{max} \qquad y_A = 0$$

- Initial Conditions (IC)

$$Gas\ Phase:\ t = 0 \qquad y_A = y_{A_0} = 0$$

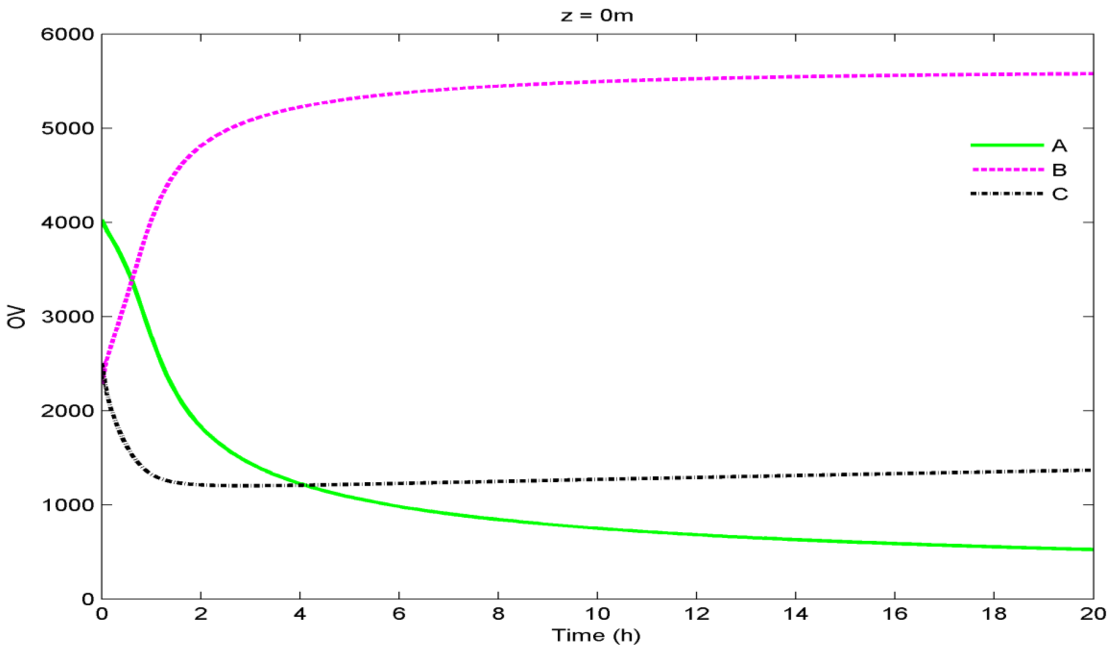
$$Liquid\ Phase:\ t = 0 \qquad n_A = n_{A_0}\ or\ x_A = x_{A_0}$$

Bird, R., Stewart, W., Lighfoot, E., Transport Phenomena, John Wiley & Sons, 1960

Perfume Diffusion Model

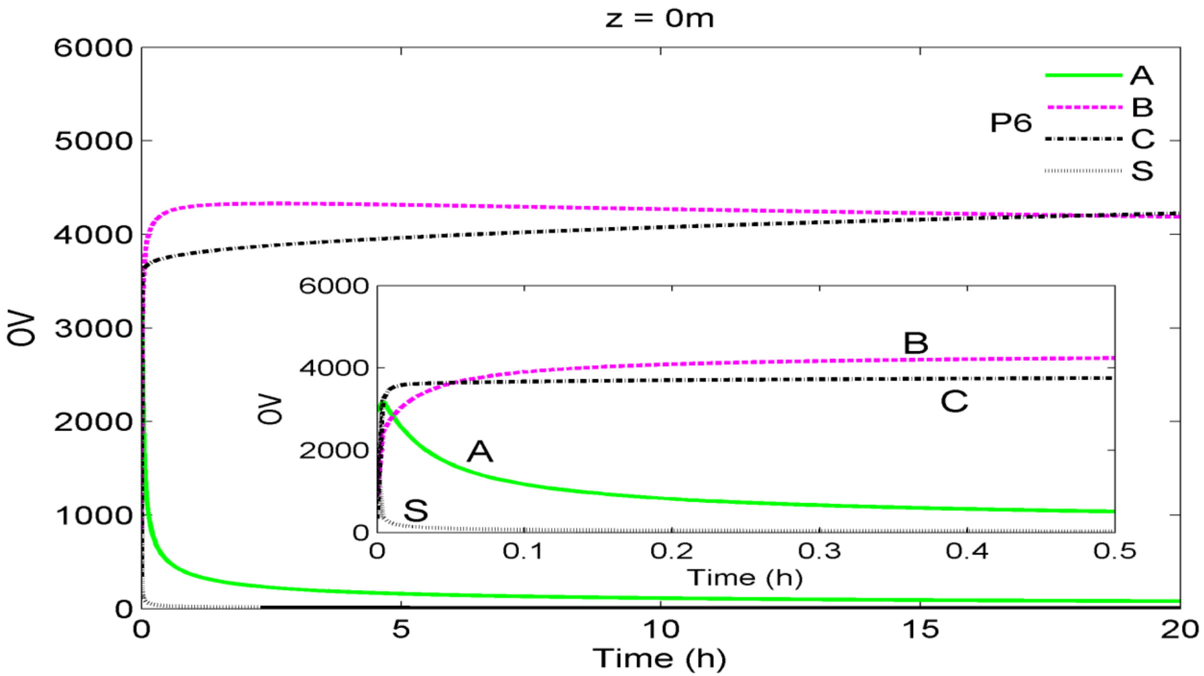
- **Odor Profiles**

  - **Ternary Mixtures**



Limonene (A) + Geraniol (B) + Vanillin (C)

  - **Quaternary Mixtures**



Limonene (A) + Geraniol (B) + Vanillin (C) + Ethanol (S)

Perfume Performance

Distance

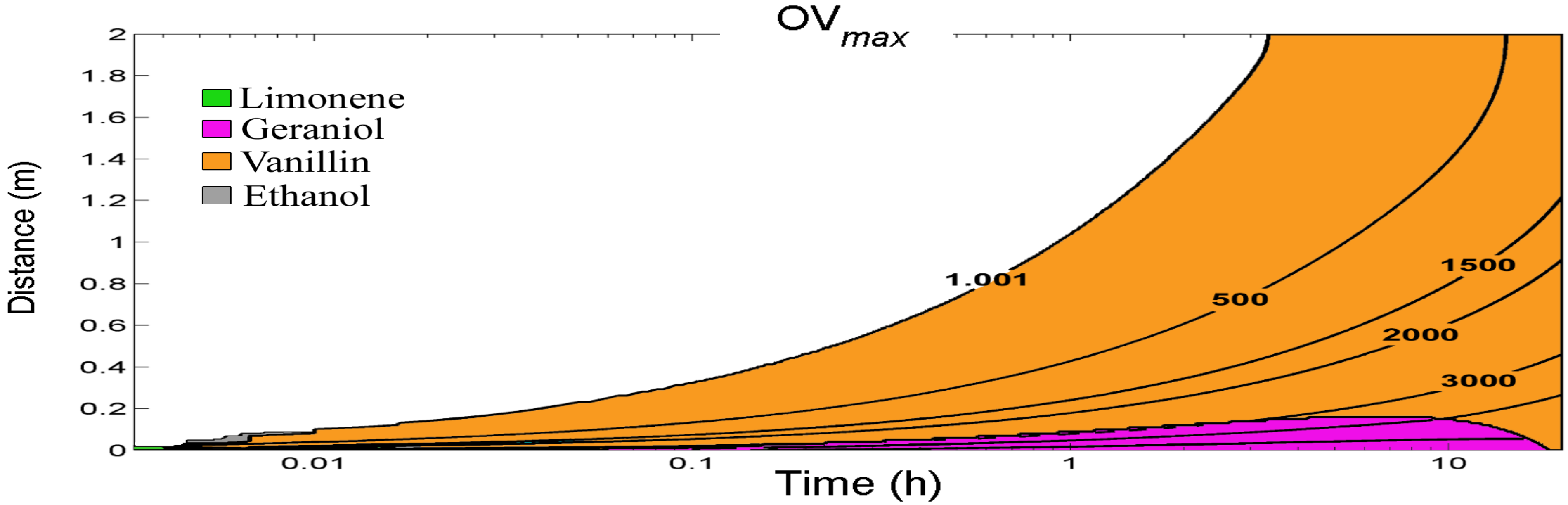
Diffusion:
efficacy of a perfume at some distance from the source at short times.

Volume:
effectiveness of a perfume over time and distance.

Impact:
immediate olfactory sensation.

Tenacity:
persistence of a fragrance after some time near the source.

Time



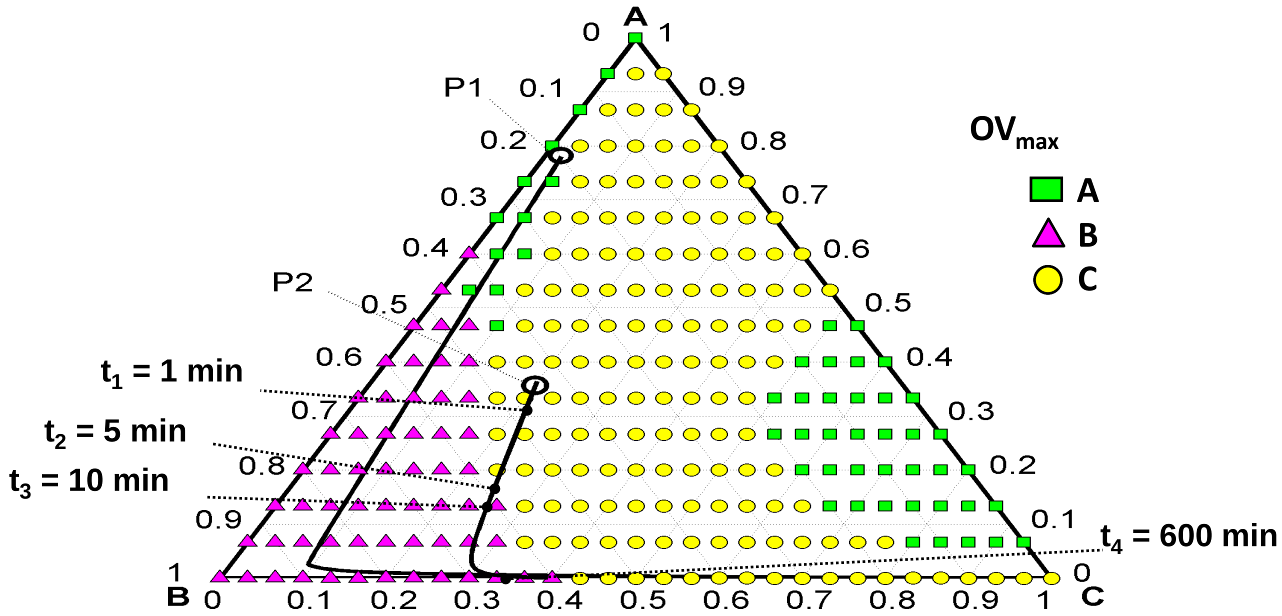
Odor character distribution over time and distance.

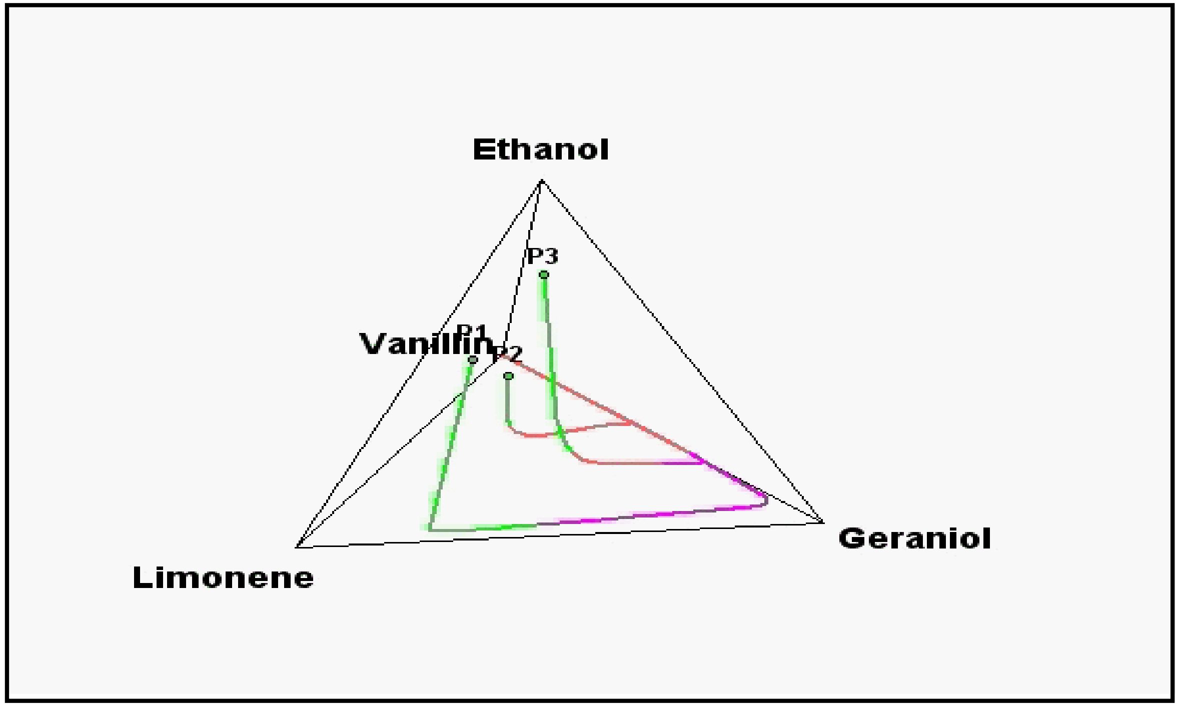
Teixeira, M.A., Rodríguez, O., Mata, V.G., Rodrigues, A.E., Chemical Engineering Science, 64, 2570–2589, 2009.

Perfume Evaporation Paths

- **Evaporation lines in the PTD® and PQ2D®**

z = 0m

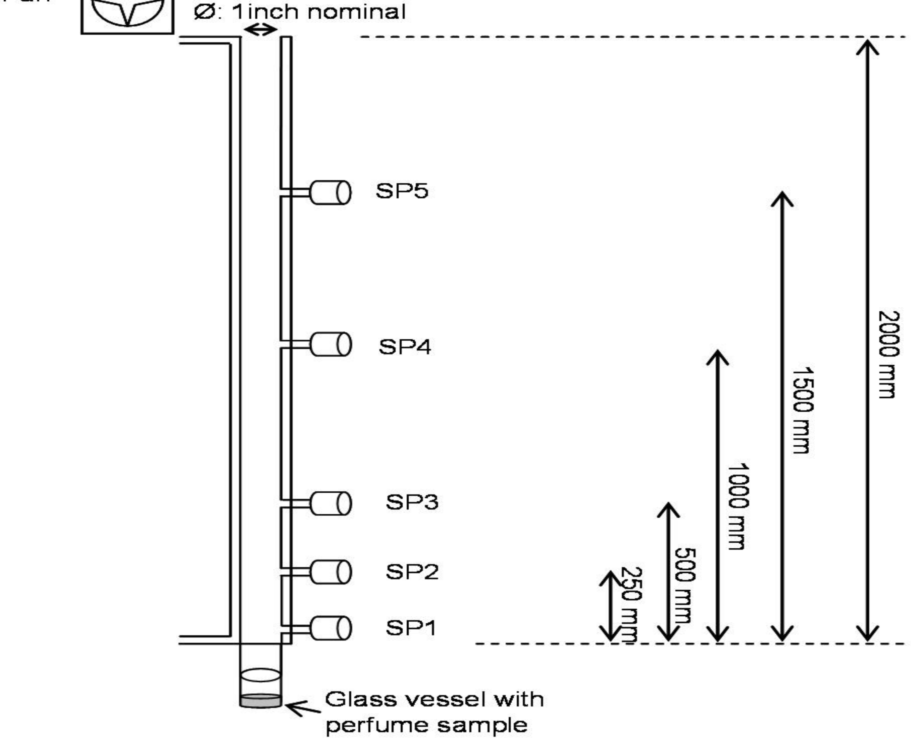




[Limonene (A) + Geraniol (B) + Vanillin (C) + Ethanol (S)]

Diffusion & Performance of Fragrances

- Proof of concept: experimental data
  - A diffusion tube was used to measure vapor concentrations over distance and time

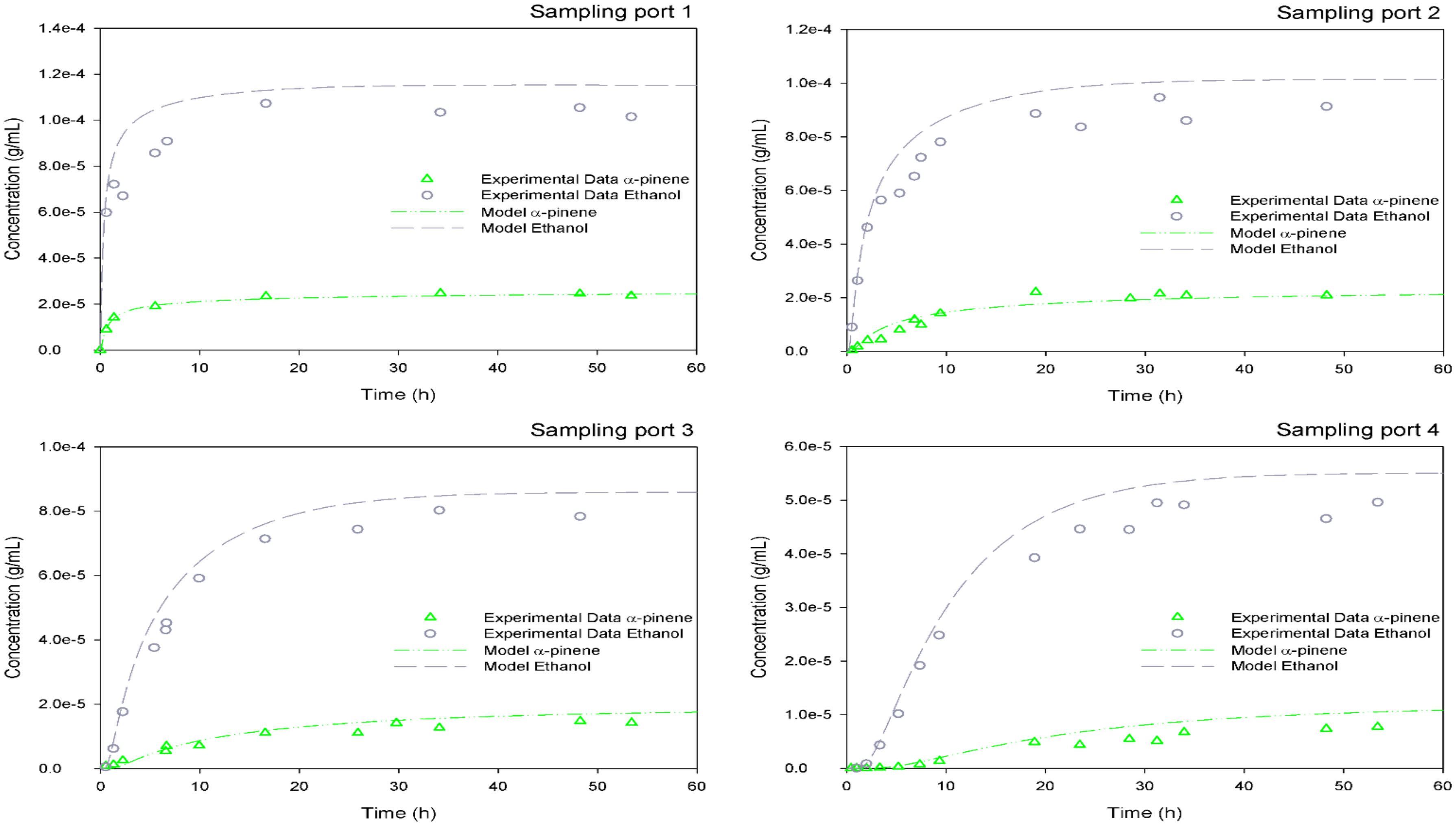


- 2 m stainless steel jacketed vertical tube
- 5 sampling ports
- Constant nominal pipe size (NPS)

- Sampling with gas-tight syringes
- Headspace calibration curves
- Analysis by GC-FID

Diffusion & Performance of Fragrances

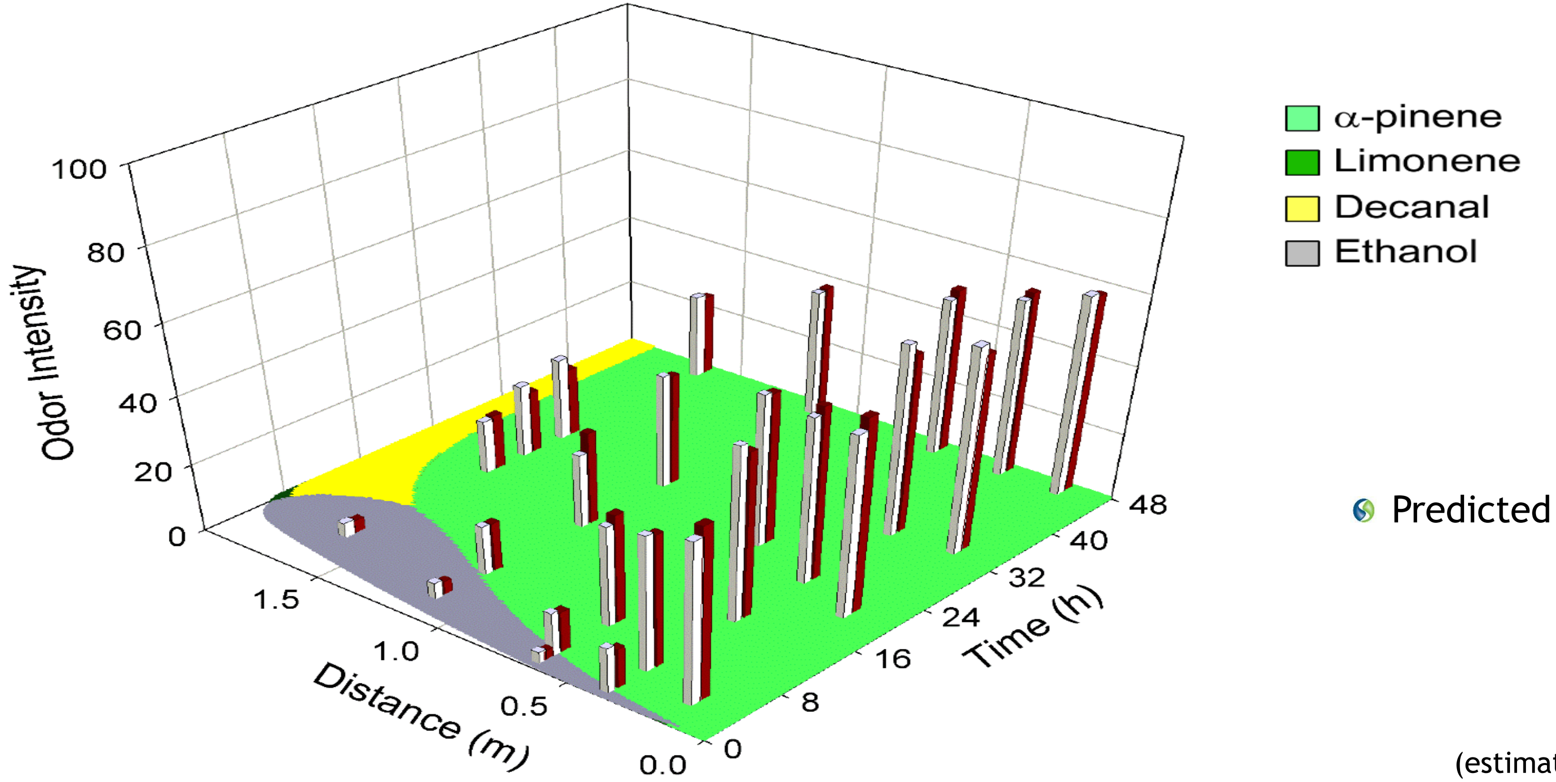
- Concentration profiles for binary mixture α-pinene + ethanol



Teixeira, M. A.; Rodríguez, O.; Rodrigues, A. E., AIChE Journal 2013, 59, (10), 3943-3957.

Diffusion & Performance of Fragrances

- Multi-component fragrance mixture



Comparison between predicted (red bars) and experimental (white bars) odor intensities for specific data points over time and distance.

- Predicted odor intensities are extremely close to experimental data

Overall ARD = <u>6.3%</u>

(estimation of vapor pressures have an error ~5%)

Teixeira, M. A.; Rodríguez, O.; Rodrigues, A. E., AIChE Journal 2013, 59, (10), 3943-3957.

Perfumery Radar

Perfumery Radar (PR) methodology

- A methodology for the classification of Perfumes into families

Validation:

- GC-MS analysis of perfumes
- Family odor intensity model
- Comparison with headspace and perfumers classifications

Step 1

- Classification of pure fragrances in olfactory families

citrus
fruity
floral
green
herbaceous
musk
oriental
woody

Step 2

- Prediction of the odor intensity for each fragrance

Odor Perception Model

Intensity & Character

Step 3

- Determination of the OV for each family and plot on PR

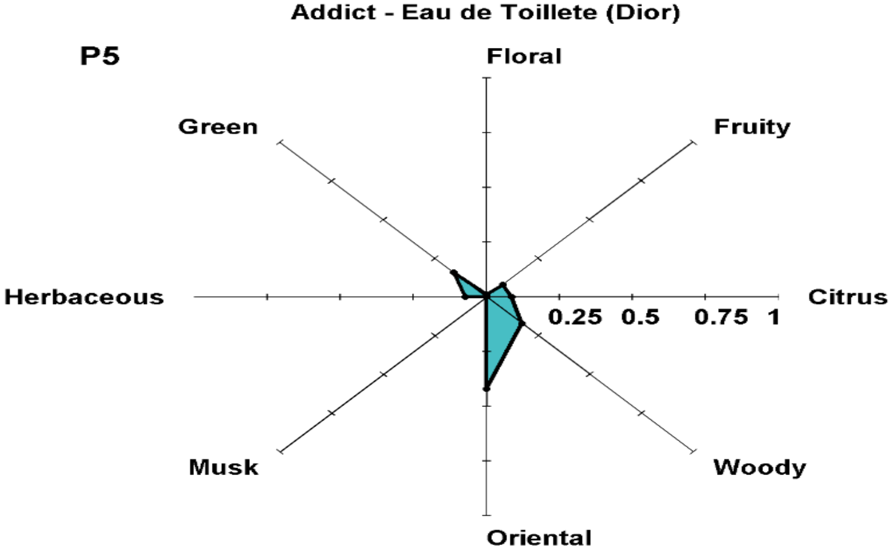
$$OV_j = \sum_{i=1}^{N} w_i^j \times OV_i$$

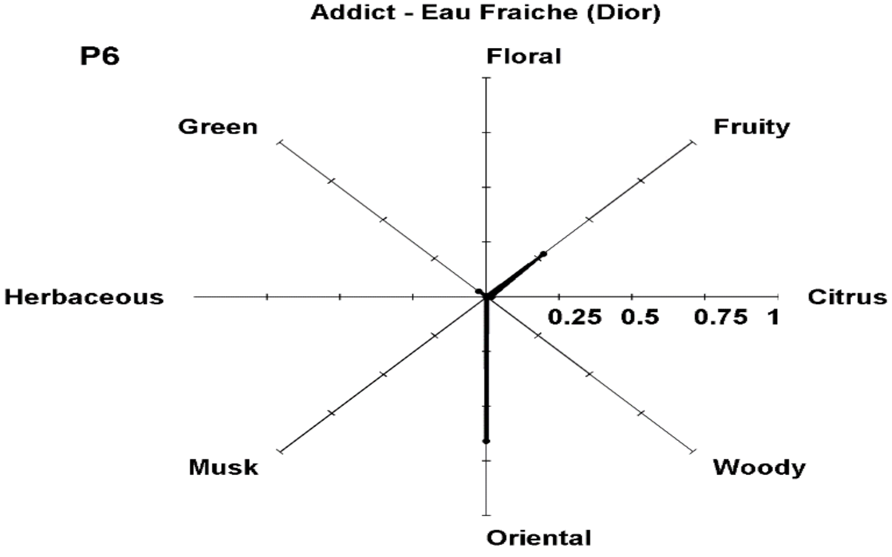
$$OV_j' = \frac{OV_j}{\sum_{j=1}^{L} OV_j}$$

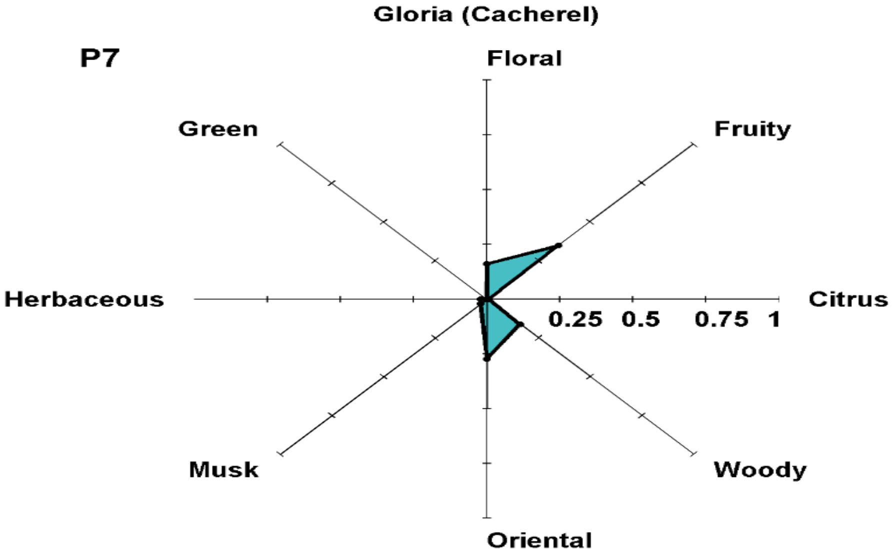
Plot of the Perfumery Radar

Teixeira, M.A., Rodríguez, O., Rodrigues, A.E., Ind. & Eng. Chem. Res., 49,11764-77, 2011.

Perfumery Radar (PR)





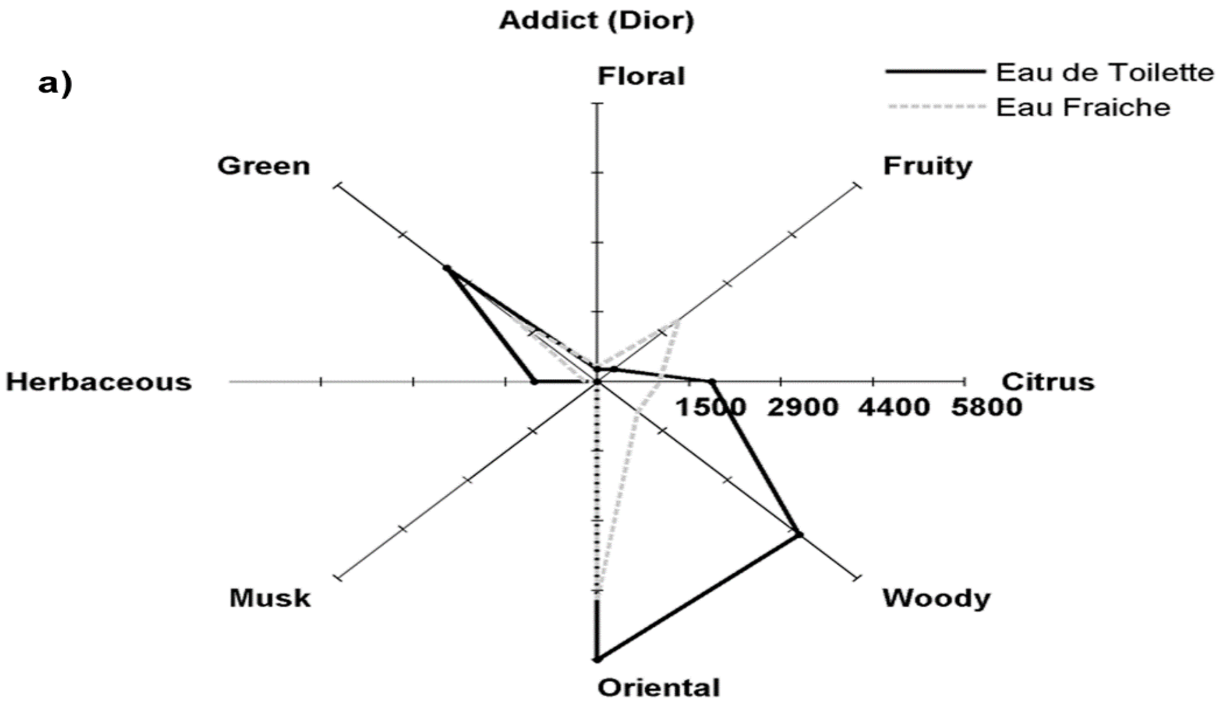


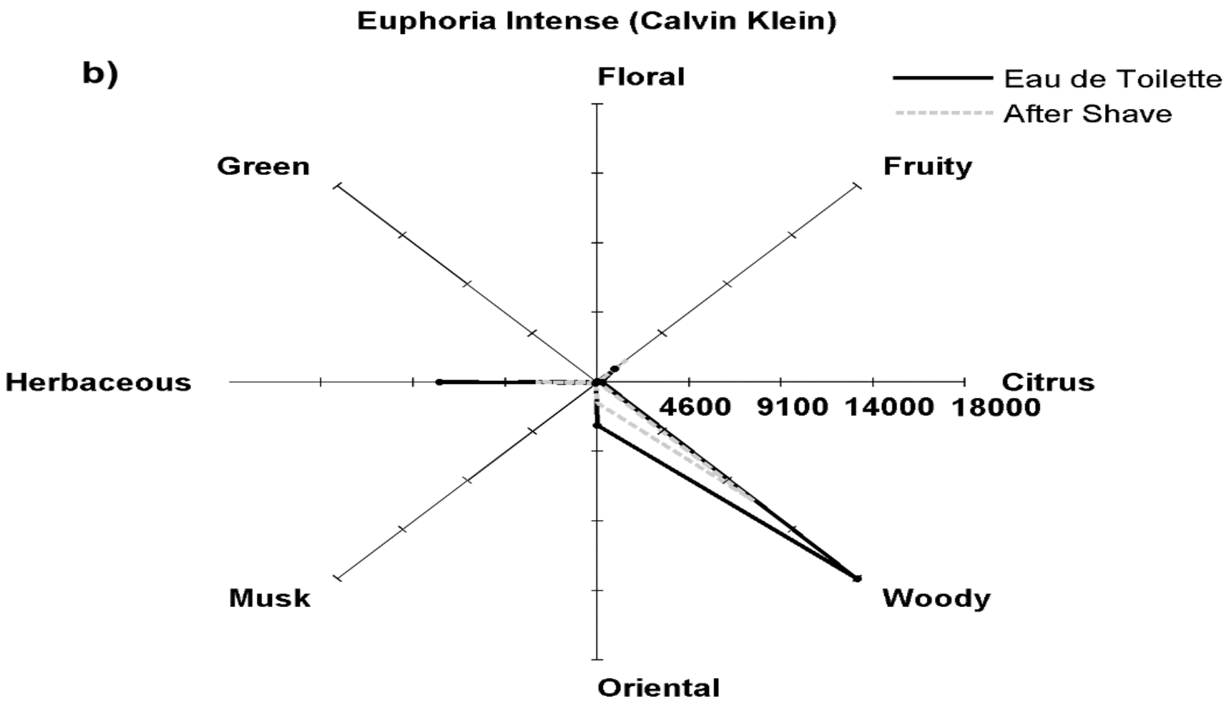
Teixeira, M.A., Rodríguez, O., Rodrigues, A.E., Ind. & Eng. Chem. Res., 49,11764–77, 2011.

Applications of the PR methodology

- Evaluation of odor intensities of similar perfumes

Eau de toilette vs Eau fraiche vs After shave



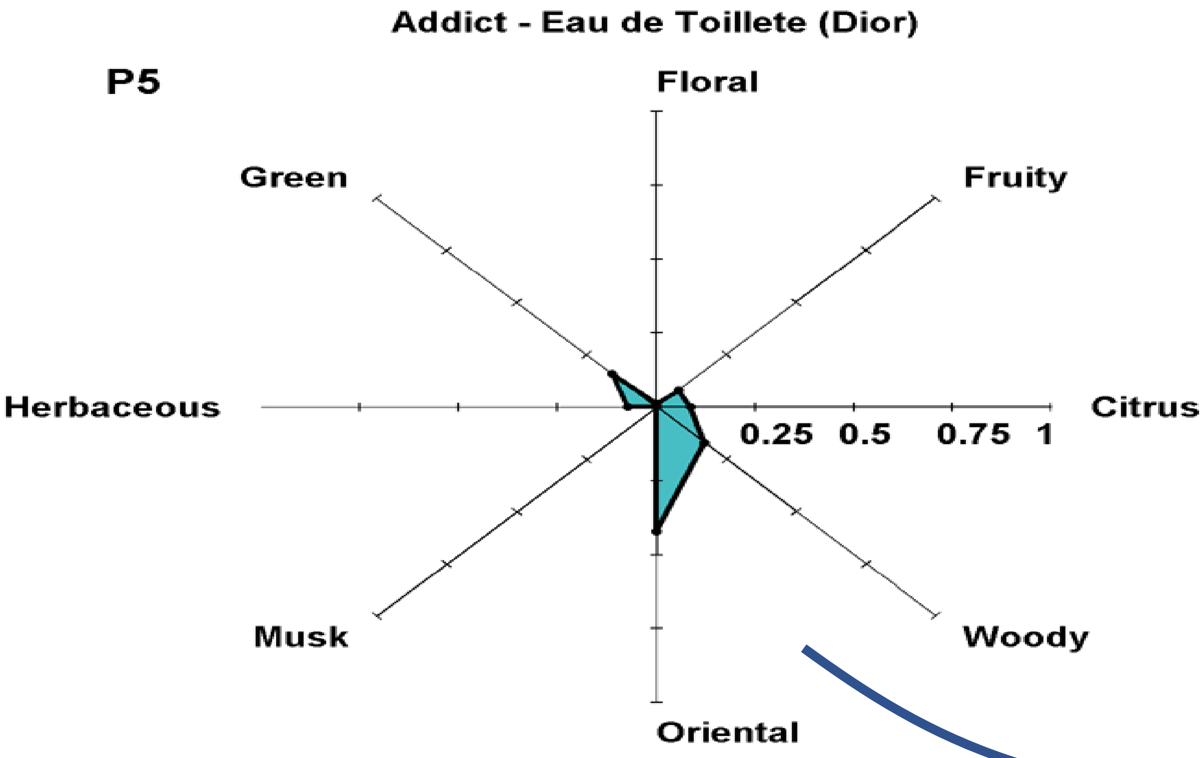


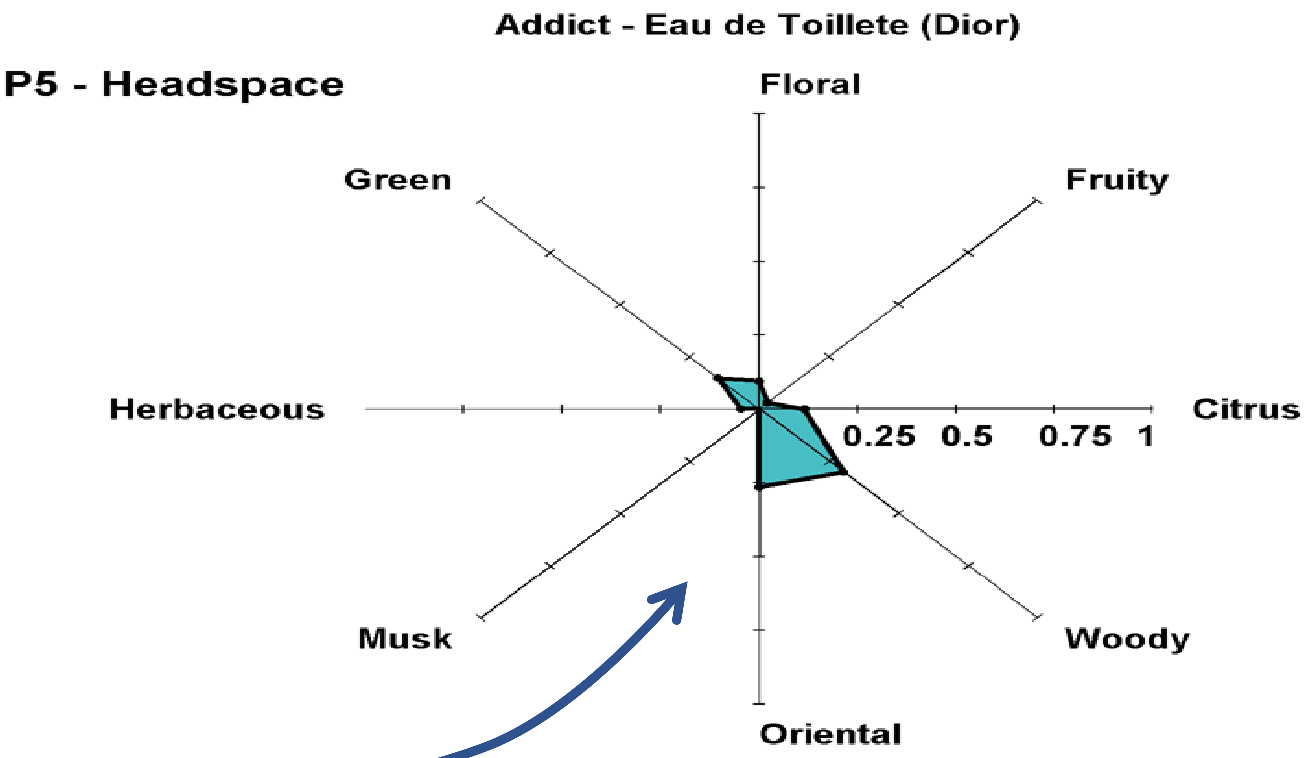
We observe that despite the ratio (water-ethanol):fragrance is different, the odor space is still similar

Perfumery Radar (PR) methodology

Experimental validation by Headspace

- **Predicted PR**
- **Experimental PR**



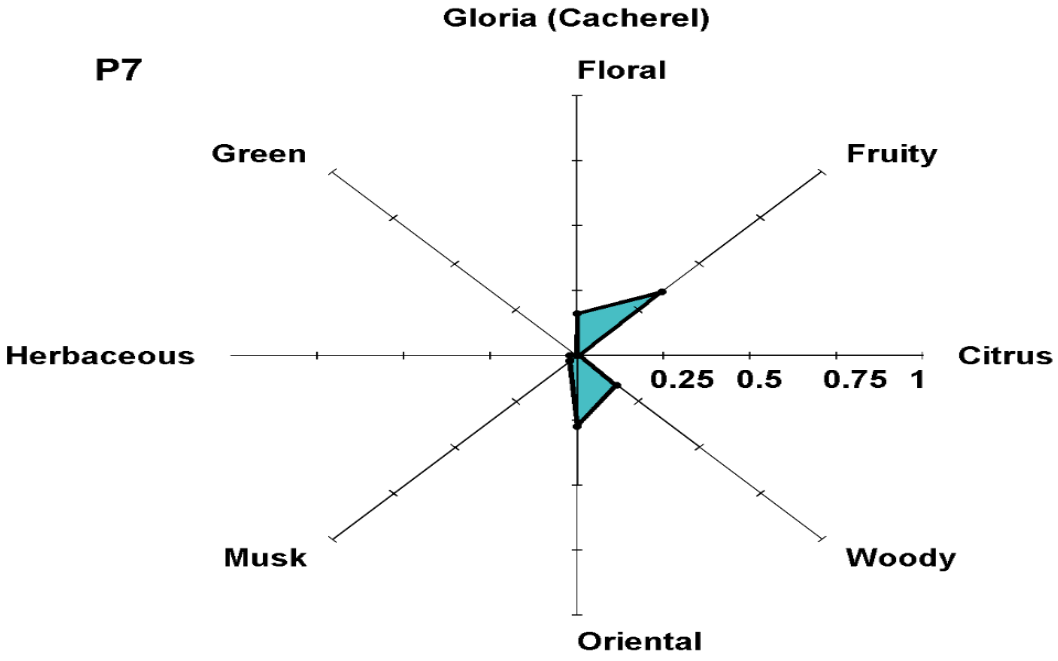


Despite minor differences, both experimental and predicted radars have the same relevant olfactory families

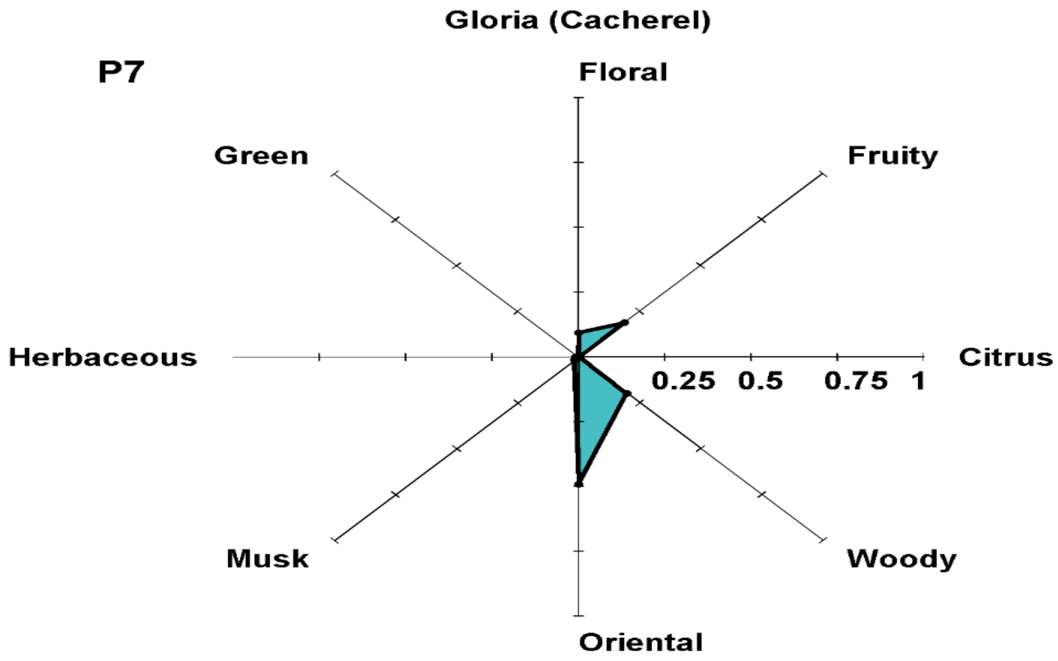
Application of the perfume diffusion model

- Combining the PR with a diffusion model:

• Initial



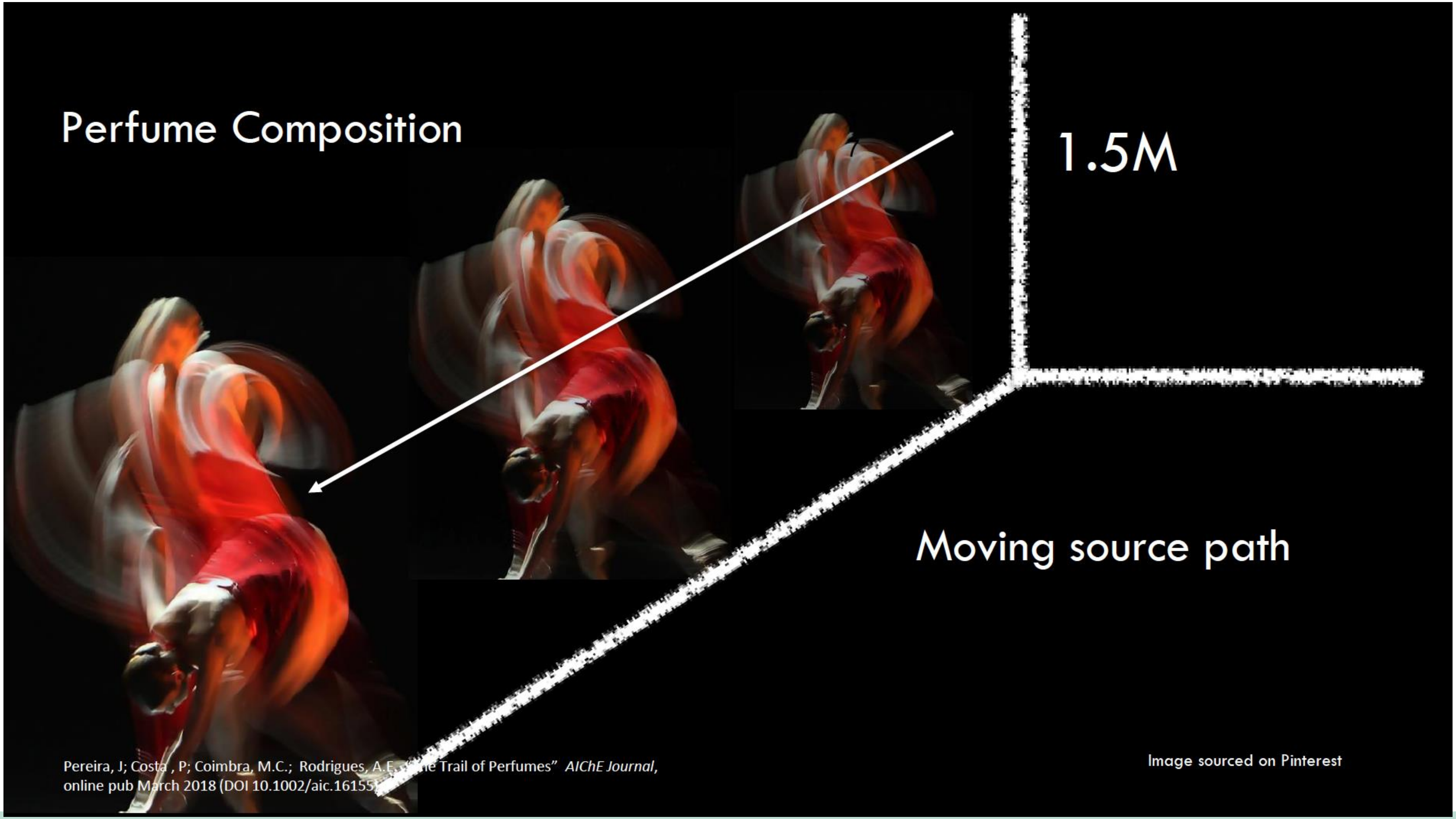
• After 60seg



Osmoz	Scent Direct	iPerfumer (Givaudan)	SFP	LT & TS	Fragrantica.com	Perfume intelligence
Oriental-woody	Oriental-fresh	Oriental-Woody-Floral	Floral-woody-amber	Amber rose	Oriental-woody	Floral-oriental

Teixeira, M.A., Rodríguez, O., Rodrigues, A.E., Ind. & Eng. Chem. Res., 49,11764-77, 2011.

Sillage in perfumery C Benaim and J Brahms, IFF – WPC 2018, Nice



Sillage in perfumery C Benaim and J Brahms, IFF – WPC 2018, Nice

Aura of aroma

Observations: the amount of certain materials found in headspace over mixtures on skin was over-represented vs liquid phase concentration:

- Under-represented materials – limonene, hedione , benzyl sal
- Over-represented materials: linalool, linalyl-acetate, cashmeran and coumarin and ethyl vanillin

"Aura of Aorma®: A Novel Technology to Study the Emission of Fragrance from the Skin" Mookerjee, B. D.; Patel, S. M.; Trenkle, R. W.; Wilson, R. A.; in Flavours and Fragrances Karl A.D. Swift ed. Elsevier, 1997, Cambridge, UK. pp 36-47.

Image sourced on Pinterest

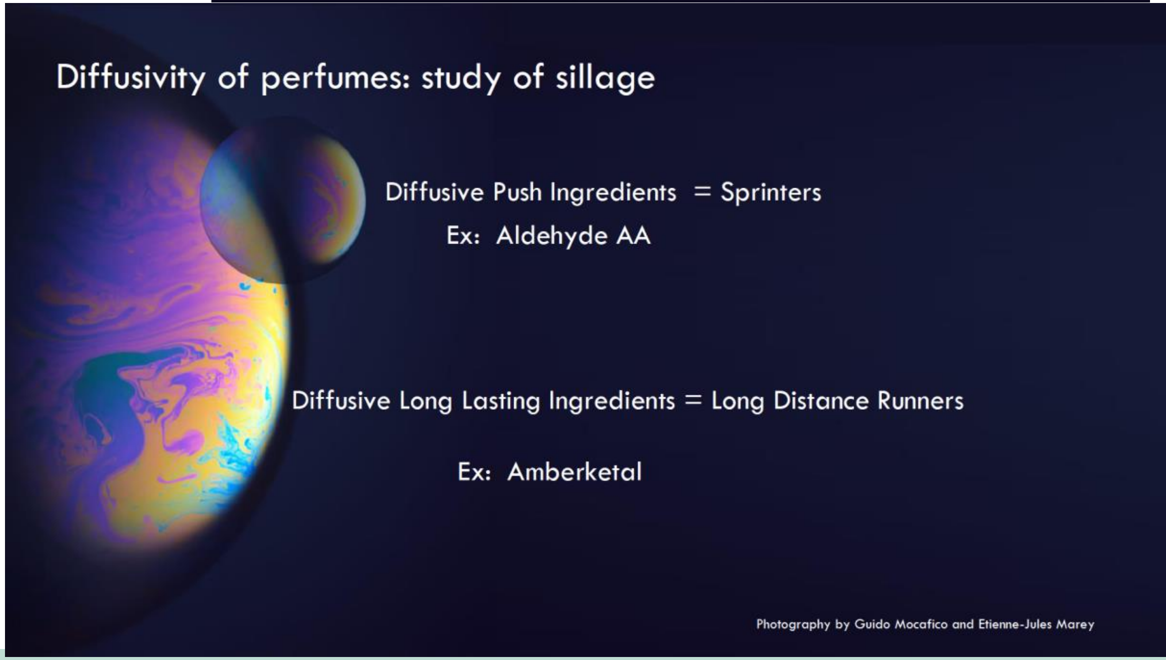
Aura of aroma

Technical study of aura: oriental scent skin vs oil

Component		Oil %	Aura on skin %
Limonene	Topnote	30.0	20.4
Linalool	Topnote	1.7	17.9
Linalyl Acetate	Topnote	9.9	21.6
Ethyl Vanillin	Middle Note	0.2	1.6
Coumarin	Middle Note	1.7	7.8
Methyl Ionone	Middle Note	1.1	2.1
Musk Xylol	Bottom Note	trace	0.3

"Aura of Aorma®: A Novel Technology to Study the Emission of Fragrance from the Skin" Mookerjee, B. D.; Patel, S. M.; Trenkle, R. W.; Wilson, R. A.; in Flavours and Fragrances Karl A.D. Swift ed. Elsevier, 1997, Cambridge, UK. pp 36-47.

Image sourced on Pinterest



Pereira et al, AIChEJ The trail of perfumes(2018)

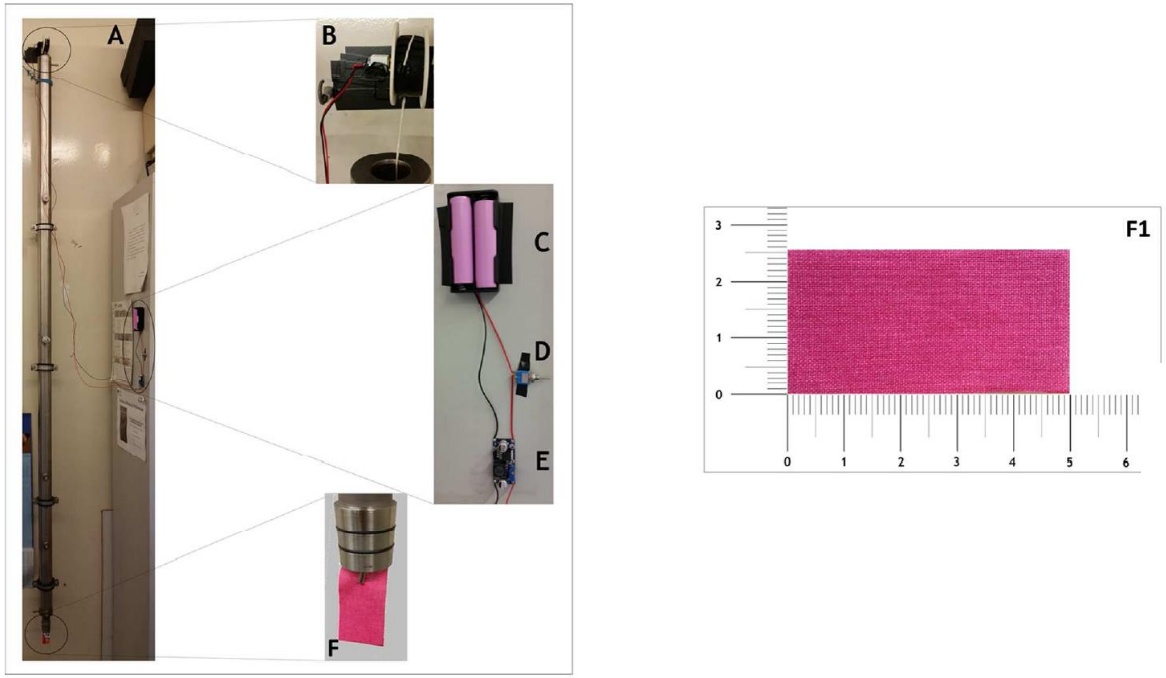


Figure 2. System developed in the laboratory; F1 – Zoom of the textile used as the source, and t respective dimensions.

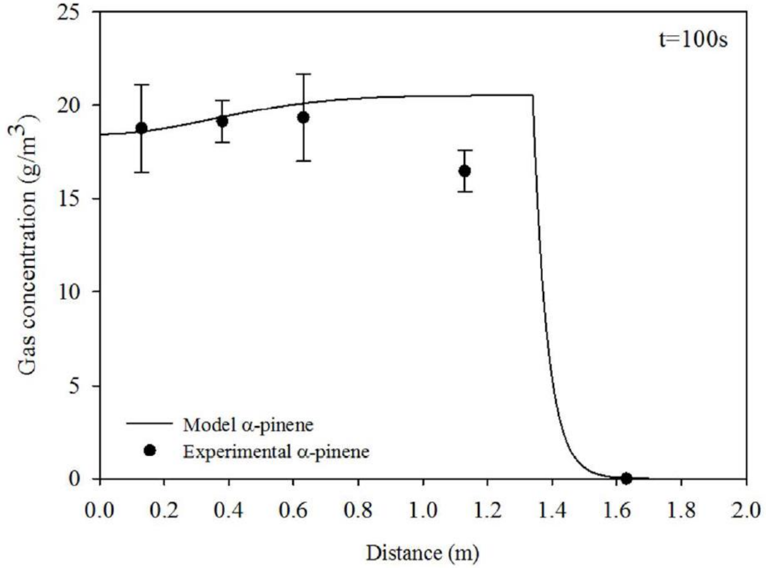


Figure 3. Theoretical and experimental gas concentration profiles of α-pinene over distance, at a fixed time of 100 s, of a source moving at 1.34×10^{-2} m/s, and $D_{\alpha\text{-pin}}=6.04 \times 10^{-6}$ m^2/s.

Conclusions

PTD® and PQ2D® methodologies

Valuable tools for the prediction of the odor elicited from mixtures

Easily extended to n components

Evaporation/release of fragrance mixtures

Predicted odor character agreed in 95.4% with experimental measurements

Propagation of odorants in air and performance

Evaluation and simulation of the perceived odor over time and distance

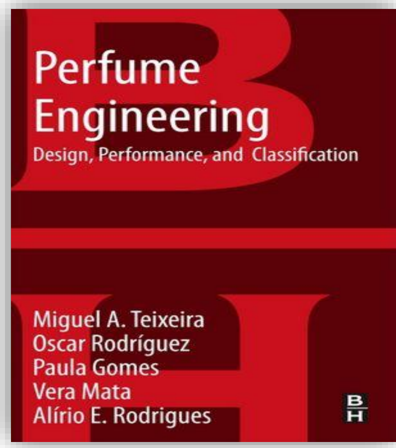
Perfumery Radar

Accurately predicts and classifies perfumes into olfactory families

Trail of perfumes (sillage)

Need for experimental research on measuring diffusivities

The role of AI….



Teixeira, M. A.; Rodriguez, O.; Gomes, P.; Mata, V.; Rodrigues, A., Elsevier: Oxford, UK, 2013.

Acknowledgments

- To Dr **Vera Mata**-I started Perfume Engineering at LSRE with my pos-doc Vera Mata –predicting smell with engineering tools (Perfumery Ternary Diagram)and later PhD student *Paula Gomes*
- To **Miguel Teixeira** who came as PhD student extending PTD to quaternary and quinary mixtures, created the Perfumery Radar and evaluated perfume performance with diffusion tube…and after years with IFF he is back in Portugal
- To Dr **Patrícia Costa who** came as pos-doc and developed the effect of matrix on fragrance behavior and studied the effect of skin of fragrance release with *Rafael Almeida* from PUCRS using Franz-diffusion cell
- To the trainees from Lyon, Montpellier, Poland, Spain, Brazil…pos-docs Daniel Gonçalves
- To PhDs and colleagues involved in microencapsulation of perfumes and aromas (Sofia Teixeira, Isabel Martins, Asma Sharkawy, Filomena Barreiro)
- To the MSc from ChE Department of FEUP who worked on the Trail of Perfumes (Joana Pereira), Taste Engineering (Ana Monteiro) and Perfume encapsulation (Sofia Lopes)

Porto and FEUP