Perfume Design, Performance and Classification & Sensorial Characteristics of Food Products

KEYWORDS: Perfume Design/ Aromatic profile/ Trail of Perfumes/ Sensorial characteristics/ Permeability/

A theoretical model based on Fick's second law for radial diffusion is proposed for modelling the radial diffusion of fragrances. Furthermore, a simple methodology is proposed to predict the sensory quality of flavoured products based on their gas phase composition, psychophysical models, and olfactory descriptors. The gas phase composition of each pure fruit juice was assessed using headspace and chromatographic techniques. A methodology was also proposed for modelling the diffusion of fragrances released from a moving source.

The volatile profile of industrially pre-treated soybeans defatted with ethanol was also assessed. It was intended to evaluate the impacts of industrial pre-treatment of the raw material and the different operational conditions of the alcoholic extraction process of soybean oil on the profile of volatiles contained in defatted solids and in protein concentrate obtained from these solids.

The studies regarding the aromatic profile of cocoa bean shells and fractions from the fat extraction process with hexane and alcoholic solvents aimed to evaluate the volatile compounds responsible for the aroma of the cocoa bean shells and the fractions obtained in the solvent extraction process.

Concerning the permeability coefficients and vapour pressure for fragrance materials, this study aims to correlate new experimental data relevant to the description of the combined evaporation/permeation process of fragrance systems applied to the skin.

Introduction and Objectives

Modelling diffusion of fragrances and Flavor Engineering

A fragrances mixtures containing odorants with different physicochemical properties (limonene, α-pinene, linalool, and geranyl acetate) were prepared. Their gas concentrations were experimentally measured using the diffusion tube and analyzed by means of gas chromatography with a flame ionization detector (GC-FID) (1D axial diffusion). From this point, an equivalence relation between the axial and radial diffusion models was found, as the diffusion tube only describes the 1D axial diffusion.

Additionaly, the headspace (i.e., the gas phase above the liquid mixture) of five commercial pure fruit juices (lemon, peach, pineapple, apple, and mango) was analyzed using dynamic headspace and gas chromatography coupled to mass spectrometry (DHS/GC-MS). Then, based on the gas concentrations of each component present in the fruit juice together with the odor and flavor thresholds we calculated the odor and flavor intensities. Thereafter, the family odor intensity model where relative weights were attributed based on the odor and flavor descriptors was created.

Perfumes are complex homogeneous liquid mixtures, composed of fragrant ingredients and solvents, that humans perceive through their olfactory system. Therefore, this work presents, for the first time, a study on fragrance release and diffusion from a moving source, with the objective of predicting the trail of a fragrance left by a person. Thus, a theoretical model (considering one-dimensional [1-D] and three-dimensional [3-D] diffusion) for predicting the diffusion of a perfume model from a moving source is proposed based on the extension of a solution for a stationary impulse source replacing the source position by the moving path of the source as a function of time.

Volatile profile of industrially pretreated soybean defatted with ethanol

The research project aimed to evaluate the impacts of industrial raw material pre-treatments (flaking and expansion) and different operational conditions in the alcoholic extraction process of soybean oil on the volatile profile contained in defatted solids and protein concentrates obtained from these solids. Thus, it was possible to evaluate whether ethanolic extraction favors the removal of off-flavors, improving the characteristic and undesirable odor of soy-based products, and aiming to increase the competitiveness of the alternative extraction process to replace the traditional process.

Evaluation of the aromatic profile of cocoa bean shells and fractions from the fat extraction process with hexane and alcoholic solvents

The extraction of lipids from plant matrices is commonly performed with commercial hexane due to its high efficiency in solubilising these compounds. However, it is a toxic solvent of fossil origin. In this way, several studies propose its replacement by alternative solvents, such as ethanol and isopropanol, which provide greater technological, economic, and environmental security to the process. The present project aimed to evaluate the volatile compounds responsible for the aroma of dry and roasted cocoa bean shells (CS) and the fractions obtained in the extraction process with hexane or alcoholic solvents.

Evaporation and Permeation of Fragrance Applied to the Skin

Based on the expertise of the research group in the development of methodologies on fragrance design, performance, and classification, this work intends to propose a simple method for modelling the diffusion rate of fragrances from skin based on a differential mass balance for each fluid phase and considering the skin as a sorption membrane. The experimental data for evaporation and permeation profiles were achieved using a Franz diffusion cell.

Current Development

Modelling diffusion of fragrances and Flavor Engineering

The developed model can efficiently predict the 1D radial diffusion of pure odorants and multicomponent fragrance mixtures. Additionally, the proposed 1D radial model presents advantages when compared to the 1D axial model, as it is able to predict the behaviour of odorants in a much more realistic way: the proposed 1D radial diffusion model provides relevant information not only about the gas concentration of each component at a certain distance from the scented source but also in any direction.

The results showed that the developed methodology describes well the dominant family of the odor and flavor of both pure and combinations of fruit juices and provides valuable information about the dominant fruit of the mixture. Furthermore, the predicted sensory description of pure fruit juices and respective mixtures matched that given by consumers for the main olfactory family and most of the

studied cases. Based on the results, this approach of characterizing the odor and flavor of beverages is a powerful tool for the food industry by reducing the time required for the development of new products and improving quality control of not only beverages but also other flavored products.

A theoretical 1-D diffusion model was proposed for predicting the trail of perfumes. This methodology considers a scented source moving through space and a continuous fragrance release from the moving source. The trail of a perfume model α-pinene was simulated, and the 1-D experimental data showed good agreement with the numerical simulation, which allows concluding that the presented model is suitable for modeling the diffusion of fragrances when applied in a moving source. Regarding the 3-D diffusion model, where the same perfume model α-pinene was used, we studied the effect of turbulent diffusion to account for the movement of the scented source—a person walking in a room or corridor indoor at 1.34 m/s; the influence of the diffusion coefficient values on the gas concentration profiles (trail), as a function of time and distance.

Volatile profile of industrially pretreated soybean defatted with ethanol

It was verified that certain soybean processing conditions increased the content of volatile compounds responsible for undesirable odors, such as expansion pre-treatment and oil extraction processes using ethanol as a solvent. The high temperatures used in the soybean pre-treatment and alcohol use possibly led to the denaturation of proteins, resulting in greater interaction between undesirable compounds and the solid matrix. In this context, it is necessary to adequately evaluate the employed operational conditions, as the reduction of undesirable odors may occur at the expense of structural changes and, consequently, functional properties. However, regarding odor intensity, it can be inferred that the use of alcoholic solvent in the oil extraction, as well as the use of high temperatures in the pre-treatment of oilseeds, off-flavors in soybean-based products.

Evaluation of the aromatic profile of cocoa bean shells and fractions from the fat extraction process with hexane and alcoholic solvents

Regarding the evaluation of the aromatic profile of CS, it was possible to conclude that they present volatile compounds characteristic of cocoa aromas, such as aldehydes and pyrazines, in addition to alcohols, terpenes and ketones. The main difference between the volatile fractions of CS and natural cocoa powder was observed in the lower percentage of pyrazines and the greater presence of acetic acid in CS. The proposed study added information about the sensory characteristics of CS and the effect of the type of solvent used in the extraction process, allowing the evaluation of the applicability of the fractions evaluated as substitutes for commercial materials, such as butter and cocoa powder.

Evaporation and Permeation of Fragrance Applied to the Skin

A novel model was developed aimed at describing the evaporation and permeation profiles of fragrance systems (α-pinene, limonene, and linalool diluted in ethanol) from porcine skin using a Franz diffusion cell. The proposed model is based on Fick's first (permeation) and second (evaporation) laws of diffusion. The model described well the behaviour of all tested fragrance systems, being more effective for those containing limonene and α-pinene as odorants. An in vitro methodology is proposed, capable of predicting the evaporation and permeation of fragrances on the skin and which can contribute positively to the perfume and cosmetics industries, allowing the development of new and/or more efficient fragrance formulations

.Future Perspectives

More than two decades have past since research on perfume engineering started at LSRE: perfumery ternary diagram (PTD) and extension to quaternary and quinary systems (PQD and PQ2D), prediction of odor thresholds and VLE, performance of perfumes—1D and 3D diffusion models—and trail of perfumes, classification of perfumes—perfumery radar, effect of matrix and skin, extension to flavor/taste engineering.

The methodology of perfumery ternary diagram (PTD) was a pioneering idea that can be extended to fragrance mixtures of N components to find compositions delivering a certain smell. It can be further elaborated to include the effect of skin on the evaporation of perfumes. The Perfumery Radar can be extended to other areas (wines) and the methodology extended to taste/flavor engineering.

Related Sustainable Development Goals

Outputs

PhD Theses

[1] Rafael Nolibos Almeida, Estudo Fenomenológico da Difusão de fragrâncias, PUCRS, Brazil, PDEQB, FEUP, 2019

Master Dissertations

[1] Sofia Lopes, Long lastingness of a fragrance, MIEQ, FEUP, 2017
[2] Joana Pereira, The trail of fragrances, MIEQ, FEUP, 2017
[3] Ana Monteiro, Taste Engineering, MIEQ, FEUP, 2017

Selected Publications

[1] Rafael N. Almeida, A.E. Rodrigues, Rubem M.F. Vargas and Eduardo Cassel, AIChEJ. 67,17351 (2021)
[2] A.E. Rodrigues, I. Nogueira and Rui Faria, Molecules. 26, 3095 (2021)
[3] Rafael N. Almeida, J. G.M. Hartz, Patrícia Costa, A.E. Rodrigues, R. M.F. Vargas and E. Cassel, Int. Journal of Cosmetic Science. 43, 225 (2021)
[4] Sofia Lopes, Catherine Pinheiro, P. Costa, I. Fernandes; F. Barreiro; A.E. Rodrigues, INDCROP. 139, 111407 (2019)
[5] Rafael Almeida, Patricia Costa, Joana Pereira, Eduardo Cassel, A.E. Rodrigues, Ind Eng Chem Res. 58, 9644 (2019)
[6] Joana Pereira, Patrícia Costa, J. M. Loureiro, A. E. Rodrigues, CJChE. 97, 351 (2019)
[7] Ana Monteiro, Patricia Costa, J.M. Loureiro and A.E. Rodrigues, Ind Eng Chem Res. 57, 8115 (2018)
[8] Joana Pereira, Patricia Costa, M.C. Coimbra, A.E. Rodrigues, AIChEJ. 64(7) 2890 (2018)

Team

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