Development of Partial Least Square models for the prediction of the concentration of a gustative stimulus in water from physiological data

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GWENAELLE HAESE[1], PHILIPPE HUMEAU[1], FABRICE DE OLIVEIRA[1], PATRICK LE CALLET[2], PIERRE LE CLOIREC[3]
[1]CSTB, AQUASIM, 11 rue Henri Picherit, BP 82341, 44323 Nantes Cedex 3, France
[2]IRCCyN lab. Polytech'Nantes, Rue Ch. Pauc, BP 50609, 44306 Nantes, France
[3]Ecole Nationale Supérieure de Chimie de Rennes, CNRS, UMR 6226, 11 allée de Beaulieu, CS 50837, 35708 Rennes Cedex 7, France

Introduction:
Classical physicochemical or sensory methodologies are often inadequate to describe the perception of water and their correlation is complicated. Indeed, the taste of water is difficult to describe due to low concentrations of sapid molecules. The aim of this work was to combine sensory and physiological measurements in order to correlate data with chemical properties of sapid solutions.

Methods:
Eighteen subjects out of 43 were selected from their performances in taste recognition tasks. The four basic tastes (sweet, salty, acid and bitter) were used at four different concentrations (Table 1) in Evian water used as a standard solution.

Table 1: Threshold values and concentration ranges of the taste stimuli (g.L^{-1})

Taste	Chemical	Detection threshold	Solutions 1	2	3	4
Acid	Citric acid	0.384	0.31	0.38	0.48	0.60
Bitter	Caffeine	0.05-0.35	0.14	0.17	0.22	0.27
Salty	NaCl	0.584	0.69	0.98	1.40	2.00
Sweet	Sucrose	6.846	2.59	4.32	7.20	12.00

Non-invasive physiological methodologies were applied such as electrodermal, heart rate variations and skin blood flow measurements, recorded in real-time during tasting tests. A questionnaire about the intensity and pleasantness of the stimuli was filled by subjects. Six repetitions were made. Physiological parameters were extracted from the signals (Figure 1).

a) b)

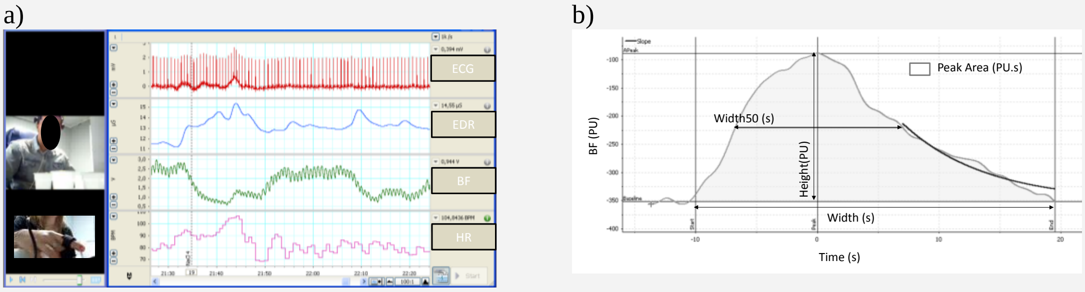

Figure 1: Acquisition screen of the physiological signals(a) and example of parameters extraction from a peak analysis (b)

Analyses were individual because each subject has his own "preferential channel".
ANOVA measuring the product effect on the physiological parameters enabled the determination of discriminant parameters, used in the PCA for visualizing the product space.

Results:
The individual product space was used as a reference map for basic taste stimuli in water at known concentrations. The Partial Least Square models were built on this reference data, for each taste.
Then, new physiological measurements were performed on taste stimuli (Exp2 – 2 repetitions). They have been projected on the PCA reference map (Figure 1) and their concentrations in sapid molecules was predicted from the PLS models developed previously (Table 2).

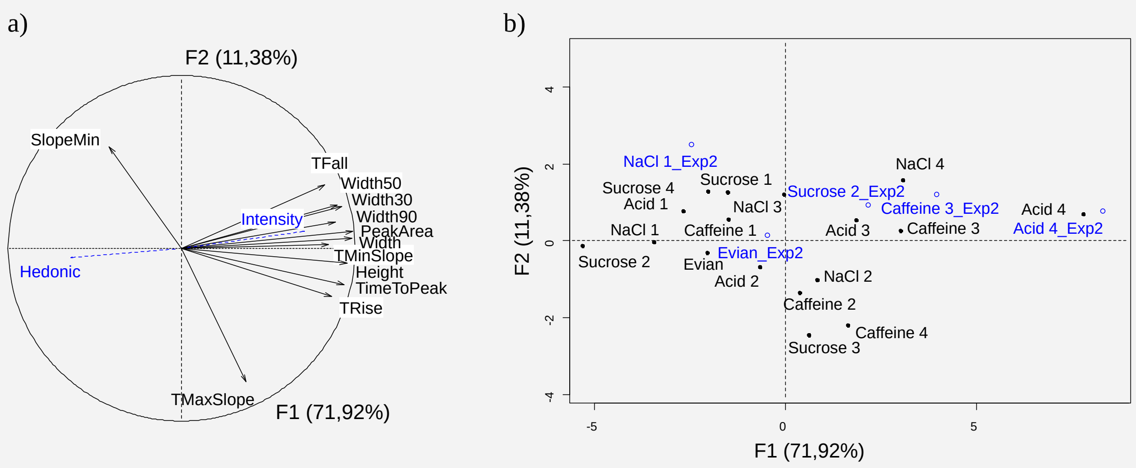

Figure 2: Representation of the variables (continuous black line for active variables, dotted blue line for illustrative ones) (a) and of the gustative stimuli (black dots for active individuals, blue dots for illustrative ones) (b) from the PCA (F1-F2) on blood flow data obtained with one subject.

Table 2: Comparison between the real concentrations and the predicted ones by the PLS models developed for each taste

	Concentration ($g.L^{-1}$)	
	real	**predicted**
Acid 4_Exp2	0.60	0.65 ± 0.01
Caffeine 3_Exp2	0.22	0.25 ± 0.03
NaCl 1_Exp2	0.69	0.87 ± 0.02
Sucrose 2_Exp 2	4.32	14.31 ± 4.21

Discussion:

A reliable model for predicting the concentrations of flavouring substances in water was proposed directly from the physiological responses of a subject. This prediction is more realistic and stable with negative hedonic valence stimuli, due to strongest and more easily identifiable physiological responses. Furthermore, models are applicable with low concentrations close to detection thresholds.

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CONTEXT AND OBJECTIVES

Classical physicochemical analysis or sensory methodologies are often inadequate to describe the perception of tastes and odors of water, the taste of water is difficult to describe due to low concentrations of sapid molecules.

An alternative way would be to reach the involuntary and unconscious responses *via* the study of the nervous system responses to assess the emotional reactions to the tastes and odors of water.

The first aim of this study was to combine sensory and physiological measurements in order to correlate data with chemical properties of sapid solutions.

The second objective was to obtain a reliable prediction of the chemical characteristics of a stimulus based on physiological responses.

MATERIALS AND METHODS

1 | Panel and products

18 naïve subjects were selected from 43 volunteers because of their high performances in three taste recognition tasks:
> Ranking
> Detection
> Matching
Attribution of a score.

4 basic tastes:
> Acid
> Bitter
> Salty
> Sweet

X 4 concentrations (1: low to 4: high)
In Evian water also used as a reference and as a blank.

Table 1: Concentrations for each basic taste ($g.L^{-1}$)

Taste	Chemical	Detection threshold	Solutions 1	2	3	4
Acid	Citric acid	0.384	0.31	0.38	0.48	0.60
Bitter	Caffeine	0.05-0.35	0.14	0.17	0.22	0.27
Salty	NaCl	0.584	0.69	0.98	1.40	2.00
Sweet	Sucrose	6.846	2.59	4.32	7.20	12.00

2 | Protocol

16 stimuli in randomized order but balanced for the intensity levels and with an Evian water sample as a reference

Sensory questionnaires: Intensity and hedonic scales

Physiological responses: Electrodermal responses (EDR), skin blood flow (BF) and heart rate (HR)

Extraction of parameters (statistics, spectral and shape parameters) and normalization

Correlations (Pearson)?

3 | Physiological measurements and parameters extractions

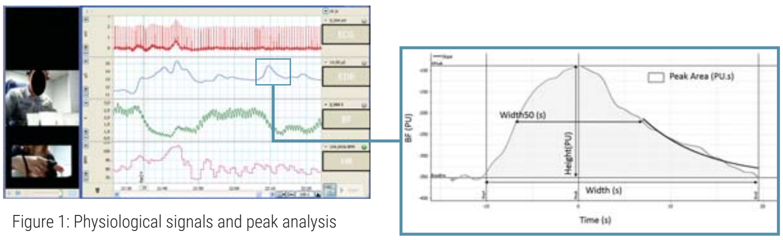

Figure 1: Physiological signals and peak analysis

4 | Statistical analysis

Specific analysis was carried out for each subject as he/she has his/her own "preferential channel".

The **ANOVA**, which measures the product effect on the physiological parameters, enabled the determination of **discriminant parameters** used in the **PCA** for visualizing the product space.

MAIN RESULTS

The individual product space was used as a reference map for basic taste stimuli in water with known concentrations.
The Partial Least Square models were built on this reference data, for each one of the 4 basic tastes (Figure 2)

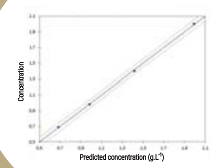

Figure 2: Regression line between the real concentration and the predicted one for NaCl

Then, new physical measurements were performed on taste stimuli (Exp2-2 repetitions). They have been projected on the PCA reference map (Figure 3).

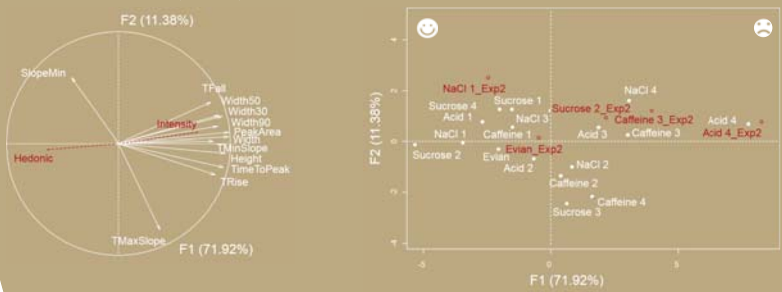

Figure 3: Representation of the variables (Continuous white line for active variables, dotted red line for illustrative ones) (a) and of the gustative stimuli (White dots for active individuals, red dots for illustrative ones) (b) from the PCA (F1-F2) built from blood flow data obtained with one subject.

The concentrations in sapid molecules of these new stimuli were predicted from the PLS models previously developed (Table 2).

	Concentration ($g.L^{-1}$) Real	Predicted
Acid 4_Exp2	0.60	0.65 ± 0.01
Caffeine 3_Exp2	0.22	0.25 ± 0.03
NaCl 1_Exp2	0.69	0.87 ± 0.02
Sucrose 2_Exp2	4.32	14.31 ± 4.21

Table 2: Comparison between the real concentrations and the predicted ones by the PLS models developed for each taste.

CONCLUSION AND PERSPECTIVES

1. A reliable model for predicting the concentrations of flavoring substances in water directly from the physiological responses of a subject is proposed.

2. This prediction is more realistic and stable with negative hedonic valence stimuli, due to stronger and more easily identifiable physiological responses.

3. Furthermore, models are applicable with low concentrations, close to detection thresholds.

CONTACT
Gwénaëlle HAESE
Research and Consulting Engineer in Sensory Analysis and Physiology
Tel.: +33 (0)2 40 37 20 65 / gwenaelle.haese@cstb.fr

CENTRE SCIENTIFIQUE ET TECHNIQUE DU BATIMENT
Tel.: +33 (0)2 40 37 20 00 – Fax: + 33 (0)2 40 37 20 60 – www.cstb.fr
11 Rue Henri Picherit, 44323 Nantes France
MARNE-LA-VALLÉE / PARIS / GRENOBLE / NANTES / SOPHIA ANTIPOLIS

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