Food Chemistry 151 (2014) 487–499

Contents lists available at ScienceDirect

Food Chemistry

journal homepage: www.elsevier.com/locate/foodchem

Interpretation of psychophysics response curves using statistical physics

S. Knani [a,*], M. Khalfaoui [a], M.A. Hachicha [a], M. Mathlouthi [b], A. Ben Lamine [a]

[a] Unité de Recherche de Physique Quantique, Faculté des Sciences de Monastir, Tunisia
[b] Laboratoire Chimie Physique Industrielle, UMR FARE 664, Université de Reims Champagne Ardenne, Faculté des Sciences, BP 1039, F-51687 Reims Cedex 2, France

ARTICLE INFO

Article history:
Received 30 December 2012
Received in revised form 11 October 2013
Accepted 20 November 2013
Available online 28 November 2013

Keywords:
Taste
Statistical physics
Psychophysical curves
Entropy

ABSTRACT

Experimental gustatory curves have been fitted for four sugars (sucrose, fructose, glucose and maltitol), using a double layer adsorption model. Three parameters of the model are fitted, namely the number of molecules per site n, the maximum response $\Re_M$ and the concentration at half saturation $C_{1/2}$. The behaviours of these parameters are discussed in relationship to each molecule's characteristics.

Starting from the double layer adsorption model, we determined (in addition) the adsorption energy of each molecule on taste receptor sites.

The use of the threshold expression allowed us to gain information about the adsorption occupation rate of a receptor site which fires a minimal response at a gustatory nerve.

Finally, by means of this model we could calculate the configurational entropy of the adsorption system, which can describe the order and disorder of the adsorbent surface.

1. Introduction

In a previous study (Knani, Mathlouthi, & Ben Lamine, 2007), we tried to derive an analytical expression of the gustatory response using statistical treatment and the adsorption hypothesis. Quantitative psychophysical information about perceptual characteristics of sweet molecules was established through the determination and the modelling of their concentration–response curve. A SMURF (Sensory Measuring Unit for Recording Flux) device was used to obtain our experimental curves, giving the response against the concentration of four substances (sucrose, fructose, glucose and maltitol).

The aim of the present work is to derive interpretations which are related to the taste mechanism of four sweet molecules on the basis of numerical simulation of the psychophysical curves. The physicochemical parameters introduced in the theoretical model, and interpreted physically, can produce information associated with the binding of stimulus to receptor site at equilibrium. We now attempt to interpret results obtained by the fitting of the psychophysical response curves with the bilayer adsorption model. Using the established expression model, we have determined the rate of occupation at minimal concentration, which elucidates a response at the gustatory nerve. This concentration is linked to the adsorption energy of the sweet molecule. Calculation of configuration entropy provides information about order and disorder during molecular arrangement at the adsorbent surface.

We are not trying, with our model, to explain the biological phenomenon of sweet sensation. Rather, we are interested in the adsorption process which governs the gustatory phenomenon and by which we can interpret some aspects of the gustatory response as a stereographic and energetic one in relation to the intensity of the sweetness.

The present work is useful in the comprehension of the behaviour of sweet molecules versus the sensitive membrane. Moreover, studying a great number of sweet molecules or any other different types of molecules could reveal similar features, such as conformational or energetic features, in order to recognise (in advance) gustatory properties of a molecule.

2. Materials and methods

2.1. General

Recording of the intensity–time curves was carried out using the SMURF technique (sensory measuring unit for recording flux) (Knani et al., 2007). This device is composed of a potentiometer connected to a recorder. During the recording of the intensity response, it is requested that the taster move the cursor according to the perceived intensity. This method of recording has the advantage of reducing the reaction time; in fact the taster records the amplitude of the intensity of the sugars as he feels it.

The recording of the psychophysical curves was carried out in three steps: selection of panellists, training them to use the SMURF technique and recording sessions. The selection of the assessors

* Corresponding author. Address: Faculty of Sciences of Monastir, Boulevard de l'Environnement, 5019 Monastir, Tunisia. Tel.: +216 73 500 276; fax: +216 73 500 278.
E-mail address: knanisalah@yahoo.fr (S. Knani).

0308-8146/$ - see front matter © 2013 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.foodchem.2013.11.114

was based on the aptitude of candidates to detect sweetness (Knani et al., 2007). Nine candidates with a good ability to detect sweetness were selected. The candidates were given an outline of the work objectives, but with no information on the type of the sweeteners.

Training of the panellists in using the SMURF technique was held in several sessions and, when necessary, extra training sessions were given. To help the taster in evaluation, we gave him/her a reference solution of sucrose (50 g/l) and he/she matched 50 graduations on the 0–100 scale of the potentiometer. These graduations are the values given to standardise the intensity of the sample (Knani et al., 2007). Practice sessions were held to record the intensities of several solutions.

The solutions used for recording the intensity according to sugar concentration were 4.6, 6.9, 9.2, 18.4, 23, 46, 69 and 92 g/l. During a tasting session, four concentrations were presented to the taster. These concentrations were contained in odour-free plastic cups coded with randomly selected three-digit numbers. A fifth sample, containing sucrose (50 g/l), was presented as a reference solution. The panellists started by rinsing their mouths with water. They tasted the reference solution; then they were instructed to score the sweetness intensity continuously over time by moving the cursor of the potentiometer from sipping the whole sample through to expectoration, when the perception of the sweet taste is maximal, until extinction of the sweet sensation.

They then rinsed their mouths again, tasted the first sample, evaluated its intensity and simultaneously recorded the corresponding time–intensity curve compared to the reference sample. Evaluation of the remaining samples was conducted in a similar way (Knani et al., 2007).

We used the intensity–time recordings to obtain response–concentration curves which are the subject of the current work. Hence, we retain the maximum values of the intensity–time curve corresponding to a suitable concentration. These values, compared to the intensity of the reference solution (sucrose 50 g/l), represent the response of the subject to this concentration.

To get a relationship between the psychophysical response and the concentration of stimulus, we suppose that the interaction between sweet molecule and receptor site is merely summed up to adsorption (Hoopman, Birch, Serghat, Portmann, & Mathlouthi, 1993; Knani et al., 2007; Lindemann, 2001; Portmann & Kilcast, 1996). Hence our system may be considered as composed of three parts: the adsorbate (dissolved sugar molecule in water), the adsorbent (receptor site in gustatory cells) and the complex formed between stimulus and receptor at equilibrium with the free state. Investigation of the exchange of particles from non-adsorbed to the adsorbed state requires use of the grand canonical ensemble in statistical physics (Khalfaoui, Baouab, Gauthier, & Ben Lamine, 2002; Knani, Khalfaoui, Hachicha, Ben Lamine, & Mathlouthi, 2012; Knani et al., 2007).

In the analytical expression of the gustatory response, we have introduced at least three physicochemical parameters intervening in the adsorption process, namely the number of molecules per receptor site (n), the density of receptor sites (N_M) and the concentration at half saturation ($C_{1/2}$). This last parameter is a function of the adsorption energy. The model giving the gustatory response versus the concentration of sugars in solution allows the shapes of the experimental curves to be interpreted using established methods in statistical physics. Yet we demonstrated, in a previous study (Knani et al., 2007), that some models can fit the experimental curves with a good correlation. Therefore, this method allowed us to achieve a physical interpretation from parameter behaviour.

Development of the expression of the model, using statistical physics, allowed the assigning of a physical meaning to the constants and facilitated interpretation of the sweetness perception mechanism at the microscopic level. Understanding of physicochemical parameters, namely density of receptor sites, number of molecules per site and the adsorption energy, yields a convenient tool for interpretation of the adsorption process and, consequently, for characterisation of stimulus–receptor interaction at a microscopic level.

2.2. Selection of the adequate model

We have developed, in a previous paper (Knani et al., 2007), some expressions of theoretical adsorption models, based on the canonical ensemble in statistical physics, with the aim of selecting an adequate mathematical model of the gustatory response and stimulus concentration in water. The fitting of the experimental curves demonstrates that some proposed models present a good correlation with the experimental curves, especially when our hypotheses are improved with supplementary parameters (Knani et al., 2007). Thus, we can adopt these more elaborated models for the description of the experimental psychophysics curves. Nevertheless we can use a model with a reduced number of parameters in order to easily interpret the adsorption process. In this case we regard these parameters as average values of the more elaborated model parameters. Hence, we choose a model that we have called the "double layer model" (Knani et al., 2007) to characterise the stimulus–receptor site interaction. This choice is due to the simplicity of interpretation since the double layer model has only three parameters. The more elaborated models have at least two energy levels. The parameters of the double layer model give information about the number of molecules per site, the density of receptor sites, the adsorption energy and the number of formed layers. We summarise theses parameters in two categories; on the one hand a steric (n) parameter, reflecting the properties of anchorage between adsorbed molecules and receptor sites related to the geometry of molecule (for example), and on the other hand, an energetic parameter giving the adsorption energy which characterises the binding between stimulus molecule and receptor site. The study of the effects of these parameters on adsorption yields information on the peripheral taste mechanism.

We consider that a various number of molecules are adsorbed onto N_M receptor sites per unit of surface with the same energy ($-\varepsilon$). We suppose that the response at the gustatory nerve level occurs when an equilibrium between adsorbed sweet molecules (S) and receptor site (R) is reached (Knani et al., 2007; Lindemann, 2001). This is represented by the following equation:

$$nS + R \leftrightarrows S_nR \tag{1}$$

where n represents the number of adsorbed molecules per site R and S_nR is the formed stimulus–receptor complex.

The grand canonical partition function of one receptor site can be written as (Knani et al., 2007),

$$z_{gc}(T,\mu) = \sum_{N_i=0,1,2} e^{-\beta(-\varepsilon-\mu)N_i} = 1 + e^{\beta(\varepsilon+\mu)} + e^{2\beta(\varepsilon+\mu)} \tag{2}$$

where μ is the chemical potential of the adsorbed molecule, β is defined as $1/k_BT$; k_B is the Boltzmann constant and T is the temperature in Kelvin and N_i is the receptor site occupation state; μ takes the value 0 if the site is empty, the value 1 if the site is occupied by n molecules and the value 2 when it is occupied by $2n$ molecules.

The grand canonical partition function related to the total N_M receptor sites per unit of surface is written as (Knani et al., 2007):

$$Z_{gc} = \prod_{i=1}^{N_M} Z_{gc}(T,\mu) = \left(z_{gc}(T,\mu)\right)^{N_M} \tag{3}$$

The average number of the occupied sites is given by (Knani et al., 2007):