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Main individual and product characteristics influencing in-mouth flavour release during eating masticated food products with different textures: Mechanistic modelling and experimental validation

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HIGHLIGHTS

- The mechanistic model includes both physiological and physical mechanisms.
- The most influent parameters for the intensity and the dynamics of the release were identified.
- The modelling approach highlighted aroma retention by lubricated mucosa.

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ABSTRACT

A mechanistic model predicting flavour release during oral processing of masticated foods was developed. The description of main physiological steps (product mastication and swallowing) and physical mechanisms (mass transfer, product breakdown and dissolution) occurring while eating allowed satisfactory simulation of *in vivo* release profiles of ethyl propanoate and 2-nonanone, measured by Atmospheric Pressure Chemical Ionization Mass Spectrometry on ten representative subjects during the consumption of four cheeses with different textures. Model sensitivity analysis showed that the main parameters affecting release intensity were the product dissolution rate in the mouth, the mass transfer coefficient in the bolus, the air–bolus contact area in the mouth and the respiratory frequency. Parameters furthermore affecting release dynamics were the mastication phase duration, the velopharynx opening and the rate of saliva incorporation into the bolus. Specific retention of 2-nonanone on mucosa was assumed to explain aroma release kinetics and confirmed when gaseous samples were consumed.

1. Introduction

The release of aroma compounds from food products during eating is a key step for their perception and ultimately for the acceptance of the product by the consumer. Food oral processing is complex (Chen, 2009) and flavour release induced by this processing depends on both the physiology and experience of subjects and on product properties. To identify what are these main properties explaining flavour release, it is necessary to develop an approach allowing the dissociation of mechanisms occurring during food oral processing. Mathematical modelling can help improving the understanding of the limiting mechanisms by pointing out the most important parameters related to the product and to the individual and allowing quantitative predictions of release dynamics. Therefore, models can help design the food products in a rational way, possibly targeted towards particular consumer groups such as young children, elderly or people with specific disorders.

The mechanistic modelling of aroma compound release during food consumption allows one to calculate, from known physical laws, the amount of aroma compounds transferred over time in each anatomical compartment involved during food oral processing (mouth, nasal cavity, pharynx).

The first mechanistic models have focused on predicting the release of aroma compounds from a two-phase emulsion (water, oil) in contact with gas (Harrison et al., 1997). They were based on physico-chemical principles governing the release of volatile molecules from a food matrix: (i) the mass conservation of

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Nomenclature

A	product/saliva contact area (cm²)
A_{FAL}	air/liquid bolus contact area in the pharynx (cm²)
A_{OAL}	air/liquid bolus contact area in the oral cavity (cm²)
A_{NAM}	air/lubricated mucosa contact area in the nasal cavity (cm²)
A_{OLP}	liquid bolus/product contact area in the oral cavity (cm²)
A_{OLP}	liquid bolus/product contact area in the oral cavity just before swallowing (cm^2)
C_{FA}	aroma concentration in the air in the pharynx (g/cm^3)
C_{FL}	aroma concentration in the liquid bolus in the pharynx (g/cm^3)
C^*_{FL}	aroma concentration at the air/liquid bolus interface in the pharynx (g/cm^3)
C_{NA}	aroma concentration in the air in the nasal cavity ($g/cm^{3)}$
C_{NM}	aroma concentration in the lubricated mucosa in the nasal cavity (g/cm^3)
C_{OA}	aroma concentration in the air in the oral cavity (g/cm^3)
C^*_{OAL}	aroma concentration at the air/liquid bolus interface in the oral cavity (g/cm^3)
C_{OL}	aroma concentration in the liquid bolus in the oral cavity (g/cm^3)
C_{OP}	aroma concentration in the product in the oral cavity (g/cm^3)
C_{Psalt}	salt concentration in the solid product (g/cm^3)
C_{Ssalt}	salt concentration in artificial saliva (g/cm^3)
C_{TA}	aroma concentration in the trachea (g/cm^3)
e_{NM}	layer thickness of the lubricated mucosa in the nasal cavity (cm)
F_R	respiratory frequency (number of cycles/s)
$fr_{masticatory}$	masticatory frequency (number of chews/s)
$fr_{opening}$	opening frequency of the velopharynx (occurrence number/s)
HM_{bolus}	moisture content of the bolus (%)
HM_{cheese}	moisture content of cheese product (%)
K_{FAL}	air/liquid bolus partition coefficient in the pharynx
K_{NAM}	air/mucosa partition coefficient in the nasal cavity
K_{OAL}	air/liquid bolus partition coefficient in the oral cavity
k_{FL}	mass transfer coefficient in the liquid bolus in the pharynx (m/s)
k_{NM}	mass transfer coefficient in the lubricated mucosa in the nasal cavity (m/s)
k_{OA}	mass transfer coefficient in the air phase in the oral cavity (m/s)
k_{OL}	mass transfer coefficient in the liquid bolus in the oral cavity (m/s)
R	average radius of particles in the bolus (m)
r_L	mass fraction of liquid bolus remaining in the mouth after deglutition (g/g)
r_{cs}	cheese/saliva mass ratio (g/g)
t_{deg}	swallowing moment (s)
Q_{NA}	air flow rate coming from the nasal cavity (cm^3/s)
Q_{OA}	air flow rate coming from the oral cavity (cm^3/s)
Q_{OS}	average rate of saliva incorporation in the bolus (cm^3/s)
Q_{TA}	air flow rate coming from the trachea (cm^3/s)
v	product dissolution rate in the saliva (cm/s)
V_{FA}	volume of air in the pharynx (cm^3)
V_{FL}	volume of liquid bolus in the pharynx (cm^3)
V_{NA}	volume of air in the nasal cavity (cm^3)
V_{NM}	volume of lubricated mucosa in the nasal cavity (cm^3)
V_{OA}	volume of air in the oral cavity (cm^3)
ΔV_{OA}	amplitude of mouth volume variation during mastication (cm^3)
V_{OL}	volume of liquid bolus in the oral cavity (cm^3)
V_{OP}	volume of product in the oral cavity (cm^3)
v_{OPini}	initial volume of product in the oral cavity (cm^3)
V_{OPD}	volume of dissolved product in the liquid bolus of the oral cavity (cm^3)
V_{OS}	volume of saliva in the bolus (cm^3)
$V_{Salivadeg+}$	volume of saliva usually present in the oral cavity after swallowing (cm^3)
V_T	tidal volume (cm^3)
ϕ_{FAL}	volatile mass flux between the air and the liquid bolus in the pharynx (g/s)
ϕ_{NAM}	volatile mass flux between the air and lubricated mucosa in the nasal cavity (g/s)
ϕ_{OAL}	volatile mass flux between the air and the liquid bolus in the oral cavity (g/s)
ϕ_{OLP}	volatile mass flux between the product and the liquid bolus in the oral cavity (g/s)
ϕ_{salt}	salt mass flux between the product and saliva (g/s)
Remark	The solid part of the bolus consists of the non-dissolved part of the food product.

volatile compound, (ii) the mass transfer at the emulsion–gas interface (interfacial penetration theory), (iii) equilibrium properties at the emulsion–gas interface (Overbosch et al., 1991). First-order chemical kinetics have also been included in some models to describe reversible interactions between aroma compounds and non-volatile compounds such as macromolecules (Harrison et al., 1997). However, these first models are not really representative of *in vivo* phenomena because the geometry of the system (surfaces and volumes) is assumed constant (which is not the case during food consumption) and they do not consider dynamic phenomena such as the dilution with salivary flow or the cyclic breathing of the subject. In addition, some of these models do not include any comparison with experimental data release (Harrison et al., 1997).

Further development of these pioneering models has led to a better representation of *in vivo* conditions occurring during food consumption, by including notably parameters related to individual physiology, such as salivary flow, periodic breath, *etc.* (Normand et al., 2004; Wright and Hills, 2003a). In addition, one of the major improvements in these models was to consider the aroma persistence phenomenon *i.e.* aroma release from bolus deposit covering the pharyngeal mucosa after swallowing. These models showed the relative roles of product and consumer characteristics and were validated against experimental data.

The first model including physiological data was proposed by Normand et al. (2004) in the case of liquid products and highlighted two main release regimes: (i) release due to equilibrium batch extraction (only pertinent for few breaths after swallowing) and (ii) release from lubricated mucosa (persistence phenomena). In the case of semi-liquid food, the most comprehensive model to date is the one developed by Trelea et al. (2008) and further developed by Doyennette et al. (2011a) coupling aroma release in the mouth and in the pharynx.

Mechanistic models describing aroma release from masticated foods are far less available in the literature, mostly because of the difficulty to understand the complex mechanisms which are involved during the consumption of those foods. Compared to