IOP Institute of Physics

Physics in Food Manufacturing Conference

Session: Fats, lipids and nutrition

(Invited) Good fat, bad fat – how bad is bad?

K W Smith

Fat Science Consulting Ltd, UK

Current health recommendations inform us to reduce fat, especially bad, saturated fat, in our diet. Trans (partially hydrogenated) fats should be totally avoided and we should increase our intake of unsaturated fat, particularly omega-3. These guidelines are aimed at reducing cardiovascular disease, such as heart attack and stroke. Dutifully, many food companies have developed products that have lower fat levels and reduced saturated fat.

The growth of this type of advice began in the mid-fifties, but was challenged from the outset. It was only once it became a US Government recommendation that diets in the USA, and subsequently other countries, altered. However, increasing numbers of publications are challenging this advice. Even results from one of the largest studies in the diet and health area (Framingham Heart Study) gave rise to an observation at odds with expectation:

"...the more saturated fat one ate, the more cholesterol one ate, the more calories one ate, the lower the person's serum cholesterol."

"...the people who ate the most cholesterol, ate the most saturated fat, ate the most calories, weighed the least, and were the most physically active."

[1] William P. Castelli MD. Arch Intern Med, 1992, 152(7):1371-1372

So, is saturated fat bad for us? What is the truth?

A vast quantity of publications describes the negative health effect of fats and saturated fat, in particular. A careful review of the evidence was published recently:

"...dietary saturated fatty acids are not associated with [coronary artery disease] and other adverse health effects..."

"The adverse health effects that have been associated with saturated fats in the past are most likely due to factors other than SFAs..."

[2] G.D. Lawrence, Adv. Nutr. 2013, 4(3):294-302

In the UK, the percentage of calorie intake of both total fat and saturated fat has fallen over the last 3 decades, while carbohydrate intake has increased. Over this time, incidence of obesity has increased markedly (see DEFRA Family Food Surveys; NHS Statistics on Obesity, Physical Activity and Diet; and Stevens et al. Population Health Metrics 2012, 10:22).

It is clear that research, and interpretation of results, can be directed towards supporting a favoured hypothesis (perhaps unconsciously). However, it is also clear that conclusions are not as clear cut as we might anticipate.

Physics in Food Manufacturing Conference

New nanostructural insights into triacylglycerols in the molten state

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The study of triacylglycerols (TAGs) in their molten state is of fundamental importance for a deeper understanding of TAG-crystallization processes being highly relevant for both, manufacturing and medical applications. Whilst different models have been proposed to explain the nanostructured nature of the fluid state of TAGs, none of them are fully satisfactory. We propose a new model consisting of positionally uncorrelated lamellar TAG-assemblies embedded in an isotropic medium, that assist as pre-nucleating structures. This model was validated by applying a novel global fitting method, resulting in excellent agreement with the small angle X-ray scattering data [1]. Deeper analysis of the scattering patterns at different temperatures, both in cooling and heating direction, allowed us further to detect crystalline traces of TAGs even after heating to 40 °C, and record on cooling the onset of crystallization at 30-25 °C. The application of the presented novel model not only explains the outstandingly structured fluid of molten TAGs, but also lays the basis for analysing first crystallization steps in greater detail [2].

[1] Ladd Parada, M., Sadeghpour, A., Vieira, J., Povey, M., Rappolt, M. Global Small-Angle X-ray
[2] Scattering Data Analysis of Triacylglycerols in the α-Phase (Part II). *J. Phys. Chem. B*, Article ASAP (online).
[3] Sadeghpour, A., Ladd Parada, M., Vieira, J., Povey, M., Rappolt, M. Global Small-Angle X-ray Scattering Data Analysis of Triacylglycerols in the Molten State (Part I). *J. Phys. Chem. B*, Article ASAP (online).

Structuring edible oils using sterol olegelators

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Removing saturated fats from foods is desirable because of the health benefits that would be realised, but this is not trivial because solid fats contribute to the structure and texture of many common foods, such as baked goods, biscuits, butter, margarine and spreads and confectionery. However, saturated fats raise cholesterol levels in the blood, a risk factor for coronary heart disease. Replacing them with mono-or polyunsaturated oils is not feasible as these are liquid at ambient temperatures, and the food would lack the desired solid texture. Even foods branded as high in polyunsaturated fats, such as margarines and spreads must contain a relatively high proportion of saturated fat to give the correct texture by forming a network of fat crystals that trap and immobilize liquid oils in a semi-solid matrix. If food manufacturers are to develop foods with the saturated fat removed they will need to find alternative methods to form the semi-solid structure.

It has been known for several years that phytosterols β-sitosterol and γ-oryzanol are able to solidify triglyceride oils by forming a so-called oleogel. SANS studies of the system suggest the molecules self-assemble to form hollow fibrils with a diameter of about 9-10nm. It is believed sitosterol and oryzanol form a dimer in oil, stabilised by a hydrogen bond (based on molecular mechanics modelling and FTIR spectroscopy). This wedge shaped dimer then self-assembles into a helical fibril. It is unclear what drives the self-association of the dimer into a fibril. Molecular docking of the phytosterols confirms the presence of an H-bond and shows that the dimer adopts a staggered conformation due to the presence of an orthoganol methyl group that prevents parallel alignment of the sterane cores. This wedge shape, we believe, is a

feature that directs formation of a helical tubule as it creates a twist when consecutive dimers align. *De-novo* synthesised sterol ester analogues of oryzanol that lack this methyl group do not gel, lack the hydrogen bond and the orthogonal methyl, thus forming a parallel dimer. Once formed tubules further associate into bundles. Raman, UV-Vis and CD spectroscopy show bundle formation is associated with vibrational modes in ferulic acid ester groups attached to oryzanol suggesting that these start to aggregate. MD simulations of two tubules shows that ferulate groups of oryzanol stick out from the surface of tubules, and that pi-stacking, vdW and H-bond interactions between the ferulates stick tubules together. Using a combination of AFM, spectroscopy and theoretical modelling we have elucidated some of the molecular features that allow phytosterols to act as oleogelators. With this knowledge, we hope to be able to design and synthesise new olegelators *de-novo* to allow greater control over oleogel structure and properties.

Applications of ultrasound in food science – novel control of fat crystallization and structuring

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It is well known that high power ultrasound (>10 kW m-2) has significant material altering properties and impacts on crystal nucleation and growth. However, there are many disadvantages in the case of many foods including off-flavours arising from lipid oxidation, contamination of product due to cavitational erosion of sonotrodes, wear and short lifetime of apparatus arising from cavitation, production of high levels of free radicals and the chaotic nature of cavitation which makes control difficult. The aforementioned make process development of high-power ultrasound equipment difficult to achieve. We have shown that low power (<1 kW m-2) ultrasound can control crystal nucleation, opening new fields of application in food processing. Here we examine how such low power ultrasound methods may be used to manipulate structure from the molecular level up to the bulk product.

[1] Povey, M. J. W. (2017) 'Applications of ultrasonics in food science - novel control of fat crystallization and structuring', Current Opinion in Colloid and Interface Science. Elsevier Ltd, 28, pp. 1–6. doi: 10.1016/j.cocis.2016.12.001.

(Invited) Entropy, the second law of thermodynamics and why 'a calorie may not be a calorie'

A Preece

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UK overweight and obesity rates have increased significantly in recent years. This apparent upward trajectory appears set to continue and could have wide-ranging undesirable consequences for the UK economy, notably the NHS, if not arrested. Many public health efforts to address this overweight phenomenon are founded on dieting for weight loss notions based on the first law of thermodynamics and calorie restriction and/or energy balance management. Some scientists are questioning these approaches, suggesting they inappropriately disregard the second thermodynamic law (entropy), better suited to account for metabolic realities. Also, any self-deterministic conscious control approach to dietary restriction effectively flouts free-living actualities, overriding evolved and autonomic energy homeostasis functions in humans, established through experiential learning (eating occasions) and subconscious perceptions of expected satiety and satiation. Indeed, these 'expected fullness cues' are here proposed as planned dietary ingestion outcomes worthy of consideration in the design of manufactured food and, possibly, in the information contained in food product labelling. Furthermore, it is proposed the likely continued rise in quantified-self biomarker technologies (for example continuous blood glucose, heart rate variability, blood pressure and other

monitors), alongside advancing food environment and contextual interpretation technologies (such as camera-based automatic food volume and nutrient profile estimations and recording of eating occasions), may reveal additional personal insights to individuals, regarding the impact of their lifestyle and food ingestion choices on their particular physiology. Whilst such awareness and associated change in food choices might be seen as a potential threat to the success of some current food products, it also offers opportunities for physicists to influence the design of new products targeting metabolic health, thereby supporting both the wellbeing needs of individuals and wider public health aspirations.

Session: Physics of Food Microstructure

(Invited) Cereals and physics: windows on fundamental realities

G Campbell

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"No man qualifies as a statesman who is entirely ignorant of the problems of wheat." – Socrates

CP Snow in his 1959 lecture on The Two Cultures lamented of "educated" people: "Once or twice I have asked the company how many of them could describe the Second Law of Thermodynamics. The response was cold: it was also negative. Yet I was asking something which is the scientific equivalent of: Have you read a work of Shakespeare... So the great edifice of modern physics goes up, and the majority of the cleverest people in the western world have about as much insight into it as their neolithic ancestors would have had."

By a similar token, Socrates reminds us that an awareness of cereals, which feed the world and dominate human history, technology, politics and international relations, ought to feature within the purview of an educated person. Yet the majority of people are unaware of the role of cereals as the source and ongoing basis of civilisation, and could not even name the major cereals, let alone recognise them. But an appreciation of cereals, like an appreciation of physics, opens up new vistas of understanding that are both edifying and useful. Cereals feed the body, but they also challenge social systems, inspire technological advances, and enrich the soul. Like one of their most celebrated products, in educational terms cereals reach the parts other disciplines don't reach.

"What other food could do all this symbolic work and yet still reliably fill human bellies? No wonder long stretches of European history can be told as the story of bread." – Michael Pollan (2013)

Wheat is the king of grains and the world's most important cereal because wheat, uniquely, gives us raised bread. And bread is the world's most important food because of its aerated structure. In these two statements lies half of all that is important about cereals. The aesthetic appeal of bread, its practical challenges and its mystery and symbolism all derive from its bubbles. And the behaviour of bubbles in bread is a topic to which physicists, and indeed chemical engineers, have distinctively valuable perspectives to offer.

"Aside from hydrocarbons, grains are the most concentrated form of true wealth—sun energy—to be found on the planet." Richard Manning (2004)

As we face the diverse and daunting challenges of oil depletion and climate change in the 21st century, cereals are again on the frontline, as they have always been. Maintaining and increasing production, in the face of climate change and population growth, exercises governments and agronomists; efficient processing into safe, secure and nutritious foods exercises cereal scientists and food manufacturers; and exploiting cereals as a renewable feedstock, to meet our chemical and energy needs as well as our food needs,

exercises biorefinery engineers. Systems thinking that appreciates the foundational and diverse roles of cereals is needed to address these highly interconnected issues. One might surmise that a Theory of Everything for cereals would truly stretch the intellect and create genuinely educated people capable of addressing the pressing needs of the world.

Effect of storage temperature and relative humidity on reconstitutable freeze-dried oil-in-water emulsion stabilised by hydrophobically modified starch

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Dried emulsions with good level of stability post reconstitution have great potential in many industries including food manufacturing and are of significant interest in that the dry formulations can easily be stored and more cheaply transported. Extensive attention has been paid to encapsulation and drying of emulsions, but reconstitution of dried emulsions is rarely studied, let alone the effect of storage on the properties and colloidal stability of reconstituted dried emulsions. The influence of storage time and conditions on the colloidal stability of oil-in-water (O/W) emulsion stabilised by modified starch has been examined here. Emulsion systems of 20% O/W were prepared with initial mean droplet size (d43=460 nm) using hydrophobically modified starch as the emulsifier. These were subjected to freeze drying, and then up to 3 weeks of storage under different storage conditions, varying in relative humidity and temperature. Reconstitution was performed at specific time intervals during storage for each set of samples. The change in droplet size and morphology of the reconstituted emulsion showed that storage temperature has a major effect on the stability of reconstituted emulsions. Lower temperatures are more stable and a generic degradation pattern was observed in most temperatures studied. Freeze dried emulsion stored at -30±1°C for at least 3 weeks, once reconstituted, gave liquid emulsions that were stable for at least another 2 weeks (and in some cases even longer). In contrast, flocculation was observed upon reconstitution when the dry sample was stored at relatively high storage temperatures (4˚C and 20˚C), but neither creaming nor coalescence was present. It is often assumed that little change to the colloidal state of the system during storage occurs, once the system has been dried. Our results show this not to be the case. Even in the solid dried form, the emulsion droplets still undergo substantial changes in their size, impacting their subsequent stability during and post reconstitution. This already has major commercial potentials such as the possibility of mass production of the dried emulsions in a central site, shipment of the dried powder to other locations, and storage and rehydration of these as when required. However, with further studies and optimisation of these additional parameters, the realisation of even smaller but stable sub-micron reconstitutable emulsions is not far behind.

Wetting, dispersion and dissolution of food powders at different length scales

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This contribution will present an overview of our recent studies to understand the physical mechanisms conditioning the wetting, dispersion and dissolution of food powders at different length scales: (i) the bulk powder, (ii) the powder grains, (iii) and the heterogeneities on the powder surface.

The scaling laws governing the stability of a powder island on a liquid surface, and governing the wicking of the wetting liquid into the interparticle pores as a function of the Bond number, provide a physical justification for the agglomeration processes commonly used in the food industry.

Drying processes cause surface heterogeneities (e.g. consisting of surface fat) that we consider at the macroscopic level through a lumped contact angle. We also study heterogeneities at the microscopic level through wetting experiments on soluble thin layers of polysaccharides micro-patterned with fat droplets.

These studies can contribute to designing powders with improved dissolution properties, but can also inspire more effective processes to dissolve demanding food powders. This is of high importance to facilitate the ongoing efforts to reduce sugar without compromising on the quality attributes of dehydrated food products.

Fragmented proteins as steric stabilisers and emulsifiers in food colloid formulations

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Animal proteins, in particular milk-based proteins, remain the obvious emulsifiers of choice in many food emulsion formulations. However, the increasing use of such proteins in other industries (e.g., adhesives), high costs associated with the production of animal-based proteins and the increasing preference of consumers for phasing out of certain animal products, all necessitate the development of edible, non-animal-based alternatives. Vegetable proteins, due to their rather globular and aggregated nature are not particularly efficient emulsifiers. Furthermore, the sequence of hydrophobic and hydrophilic amino acids in vegetable proteins is often far from that expected for an ideal emulsifier or a good colloid steric stabiliser.

It has been suggested that while native vegetable proteins may not be suited to emulsification, certain sections of such proteins may have much more favourable primary structures for this purpose. However, the initial costs of developing the required biotechnology for producing (via selective proteolysis) and isolating such polypeptides is very high, especially given the large combinations of polypeptide fragments possible. Thus, there is a need to pre-select and focus experimentation on a few potentially most promising polypeptides. To this end, we have used the Self-Consistent-Field methodology, frequently used in the fields of polymer Physics and Chemistry, to select and study the surface properties of polypeptides that in principle could be produced from various sources. Such calculations not only provide information on the efficiency of adsorption but also the thickness and extent of the adsorbed layer. Furthermore, it is possible to calculate the strength and the nature of interaction forces between emulsion droplets arising from the overlap of the polypeptide layers on the droplet surfaces.

We demonstrate the principles here by comparing the surface adsorption and colloidal steric stabilising properties of a polypeptide fragment, which potentially is derivable from hydrolysis of “Soybean β-Conglycinin alpha Prime Homotrimer” protein, with that of the milk protein as1-casein. This plant

polypeptide consists of 145 amino acid residues and was deliberately chosen due to its structural resemblance to as1-casein. We find that surface properties of the fragmented protein are indeed very similar to as1-casein at appropriate pH values relative to the iso-electric point (pI) of each respective protein (The pI of the plant polypeptide is close to 7.7, whilst that for as1-casein is close to 4.6). This potentially allows the plant protein to provide better emulsion stabilising properties than as1-casein at the relatively low pH range between 4 to 5, which is often desirable in foods.

(Invited) Structure and dynamics of lipid assemblies

A Tyler

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Lipids exhibit rich polymorphism in water and can adopt phases that may possess 1- (lamellar sheets), 2- (hexagonally arranged cylinders) or 3-dimensional periodicity (cubic phases). Here we present examples of novel lipid lyotropic liquid crystalline phases, as well as the generation and control of highly swollen interconnected cubic lipid structures which have enormous potential for encapsulation and controlled release of bioactive molecules, and large membrane protein crystalisation.

Controlling the structure and out-of-equilibrium dynamics of such soft matter systems is vitally important in a wide variety of critical research areas including the pharmaceutical and biotechnological industries. Despite the huge importance of this field, there remain significant barriers to its study, primarily the ability to control the size, shape and stability of soft matter systems and their dispersions, as well as triggering their structural evolution and time-resolved probing of dynamic structures. Although a plethora of equilibrium phase diagrams have been published, there is a scarcity of knowledge regarding the kinetics and mechanisms of lyotropic phase transitions. If we are to further our knowledge of events such as bioactive delivery then a comprehensive understanding of the processes governing phase transitions, the type of intermediates formed and the mechanism by which a transition occurs are vital.

A superb technique for monitoring and initiating the structural evolution of such systems, in the millisecond regime, is time resolved X-ray diffraction, using pressure or pH as the trigger mechanism. We have employed this technique to investigate transition kinetics in various lipid mixtures.

Session: Physical Measurement of Foods

(Invited) Lighting up the world of food security with raman spectroscopy

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It's not a question of if food fraud will occur, it's unfortunately a case of when and how badly the food supply chain will be disrupted, and whether this disruption is deliberate or accidental and if this is potentially dangerous to human and animal health. Major food adulteration incidents occur with alarming frequency and are episodic, with multiple incidents reinforcing this view. Thus capable guardians are needed to 'police' the food supply chain. Most often these are based on chromatography usually coupled with mass spectrometry and these are employed within centralised food testing laboratories (Ellis et al., 2016). They therefore give retrospective results and cannot easily be deployed on site. We believe that so called point-and-shoot approaches based on Raman spectroscopy are attractive as these are handheld and can be used for rapid in situ through-container analysis and thus do not damage the sample or the container/wrapper during analysis.

This keynote will first highlight the need for capable guardians (sensing technologies) within the food supply chain (Ellis et al., 2012, 2016) and introduce Raman spectroscopy as an approach for non-destructive on-site analysis (Ellis et al., 2015) that generates food fingerprints (Ellis et al., 2012). This will then be followed by examples where we have recently developed Raman and related techniques:

- The development of surface enhanced Raman scattering (SERS) for trace detection of off-flavour components and banned substances within complex food matrices (Cheung et al., 2010; Sørensen et al., 2015).
- For the detection of coconut water stretching with water disguised with sugars to keep the soluble solids contents equivalent (Richardson et al., 2019).

[1] Handheld spatially offset Raman spectroscopy (SORS) for through-container analysis, which was used to detect the adulteration and counterfeiting of Scotch whisky, and other spirit drinks (Ellis et al., 2017).

[2] Cheung, W., Shadi, I.T., Xu,Y. & Goodacre, R. (2010) Quantitativeanalysis of the banned food dye Sudan-1 using surface enhanced Raman scatteringwith multivariate chemometrics. The Journal of Physical Chemistry C114, 7285-7290.

[3] Ellis, D.I., Brewster, V.L., Dunn, W.B., Allwood, J.W., Golovanov, A.P. & Goodacre, R. (2012) Fingerprinting food: current technologies for the detection of food adulteration and contamination. Chemical Society Reviews 41, 5706-5727

[4] Ellis, D.I., Eccles, R., Xu, Y., Griffen, J., Muhamadali, H., Matousek, P., Goodall, I. & Goodacre, R. (2017) Through-container, extremely low concentration detection of multiple chemical markers of counterfeit alcohol using a handheld SORS device. Scientific Reports 7: 12082

[5] Ellis, D.I., Muhamadali, H., Allen, D.P., Elliott, C.T. & Goodacre, R. (2016) A flavour of omics approaches for the detection of food fraud. Current Opinion in Food Science 10, 7-15

[6] Ellis, D.I., Muhamadali, H., Haughey, S.A., Elliott, C.T. & Goodacre, R. (2015) Point-and-shoot: rapid quantitative detection methods for on-site food fraud analysis – moving out of the laboratory and into the food supply chain. Analytical Methods 7, 9401-9414.

[7] Richardson, P.I.C., Muhamadali, H., *Ellis, D.I. & *Goodacre, R. (2019) Rapid quantification of the adulteration of fresh coconut water by dilution and sugars using Raman spectroscopy and chemometrics. Food Chemistry 272, 157-164

[8] Sørensen, K.M, Westley, C., Goodacre, R. & Engelsen, S.B. (2015) Simultaneous quantification of the boar-taint compounds skatole and androstenone by surface enhanced Raman scattering (SERS) and multivariate data analysis. Analytical and Bioanalytical Chemistry 407,7787-7795.

Raman imaging of chocolate and other confectionary

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In this work, we characterise the distribution of chemical ingredients in confectionary samples using Raman spectroscopy. Applying this technique to samples of chocolate it was possible to characterise the distribution of lactose, sucrose and fats, even from highly fluorescent samples such as milk chocolate. Understanding the distribution of fats and sugars in chocolate can lead to changes in formulation and production methods that give improvements in the flavour, feel and stability of chocolate products.

We also show Raman analysis of bubble gum; from identifying the ingredients of the gum to imaging their distribution. Differences were observed in the distribution of the ingredients on the outside of the gum relative to the inside of the gum. The distribution of these ingredients affects the gum's taste, function and stability during storage.

Raman spectroscopy is a non-contact, non-destructive tool that provides sub-micrometre information on the chemical and crystal structure of materials, allowing individual ingredients/components to be identified and quantified. Recent advances in Raman instrumentation have enabled breakthroughs that make it very friendly for food analysis. These include high speed mapping allowing spectral acquisition at rates greater than 1000 spectra per second and automatic surface tracking, enabling samples with complex geometries to be mapped without manual intervention.

Investigation of the reconstitution, structure and formation of dairy systems and gels: Use of Super-resolution microscopy and Ultrasound Spectroscopy

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The structure and formation of dairy products provide systems in which nano-scale components undergo complex interactions to form structures with a multitude of macroscopic properties. A combination of Super-resolution imaging and Ultrasound spectroscopy has been applied to obtain an overview of the dynamics, interactions and structural properties of reconstituted dairy products to achieve unprecedented spatial and temporal resolutions, under given conditions.

Stimulated Emission Depletion (STED) microscopy has been used to image dairy gels from fresh and reconstituted skim milks. Protein structures have been resolved to 100 nm after an imaging protocol that does not require sample preparation except for fluorophore addition. Quantitative image analysis has been developed using an empirically validated model to extract the size of protein domains, pore size, fractal dimension and degree of co-localisation of two distinct component. This image correlation-based analysis method has many potential applications to quantifying different porous, fractal or multi-component system. Coherent Anti-Stokes Raman Scattering (CARS) microscopy provides a label free negative control for the use of a fluorescent dye required for STED imaging.

The speed of sound and acoustic attenuation are dependent on a materials physical properties therefore information can be obtained about the dynamic changes in the sample. Ultrasound Reflection Spectroscopy has been used to monitor the changes in the dissolution of dairy derived powders. The frequency dependent attenuation spectrum provides unique measurements on concentrated colloidal dispersions without dilution. Effective combination of these techniques provides a unique insight into the entire process of characterising a reconstituted dairy derived gel with novel temporal and spatial resolutions.

Hyperspectral Imaging: Machine Vision and AI for use in food sorting applications

J Gilchrist

Camlin Photonics, UK

Over the last thirty years Hyper-Spectral Imaging (HSI) has become an important technology in food, agriculture and environmental monitoring applications. The linking technology to enable HSI to be successful in such applications is the use of pre-processing the data and machine vision analysis techniques now recently coupled with Artificial Intelligence will be discussed

(Invited) Mapping food composition by hyperspectral imaging

M Whitworth

Campden BRI, UK

Hyperspectral imaging provides spectroscopic data for each pixel in an image. This can be used to classify different regions within a scene or to measure the spatial distribution of properties. At visible wavelengths, the approach can be used to discriminate features of otherwise similar colour. Potential applications for food include identification of adulterants in dried herbs, or online detection of foreign bodies. At Near infrared (NIR) or Short wave infrared (SWIR) wavelengths, the method provides information on technologically relevant aspects of food composition. NIR spectroscopy is already widespread for rapid analysis of bulk food composition, for both laboratory and online use. Hyperspectral NIR imaging enables the spatial distribution of composition also to be mapped. This provides a useful method to measure the distribution and migration of components such as fat and moisture, and to analyse specific regions of complex multi-component products.

Campden BRI uses hyperspectral NIR imaging for product characterisation as part of a suite of methods for assessment of product colour, structure and composition. A common requirement is to assess trial samples in support of product development, to assess the effects of processing conditions and storage. Examples will be presented for laboratory and at-line measurements for a range of different food applications, using a pushbroom HgCdTe instrument.

Quantitative measurements can be obtained using multivariate calibrations developed using reference samples. Where this is not practical, qualitative information can in some cases be obtained by assessment of specific absorbance bands. Examples are presented for confectionery and for fat distribution in chips in relation to processing conditions.

A common application is measurement of moisture distributions, after production or for storage trials. Results will be presented for bread, biscuits and custard tarts, using calibrations and classifiers based on partial least squares regression, including spectral pre-treatments. An overview of the analysis approach will be given.

A further application is to measure the distribution of properties for individual grains in a sample. Examples will be presented for protein content and alpha-amylase activity in wheat grains, moisture, lipid, sucrose, caffeine and trigonelline content in green coffee beans, and fermentation index, polyphenol content and antioxidant activity in cocoa beans.

Further applications will be presented for meat quality and fish freshness. For meat, foreribs of beef were analysed for fatty acid composition and to predict texture based on spectra for segmented fat and lean regions. For fish, NIR and colour measurements were made for several regions of whole cod and fillets to identify the best predictors of freshness.

In addition to the examples presented, Campden BRI has developed dedicated calibrations for several clients' products. In combination with other imaging and product assessment methods, these provide an invaluable method to study the distribution of composition in support of product and process development activity, or for translation to online inspection.

Session: Physical and data modelling of foods

(Invited) Meso-scale modelling and applications in foods

J Yeomans

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Foods are complex systems which leads to challenges in modelling. Many different processes and length scales may be important, and not all of them can be included in a single simulation. Meso-scale modelling aims to include enough physical detail to be able to answer realistic questions, but not so much that the simulations become infeasible. It is best suited to the length scales of colloids, polymers and bacteria.

I shall focus on two mesoscale simulation methods, multiparticle collision dynamics and free energy lattice Boltzmann approaches. Using examples from our recent work I shall illustrate where these techniques have proved helpful in gaining new understanding of increasingly complex soft and active materials.

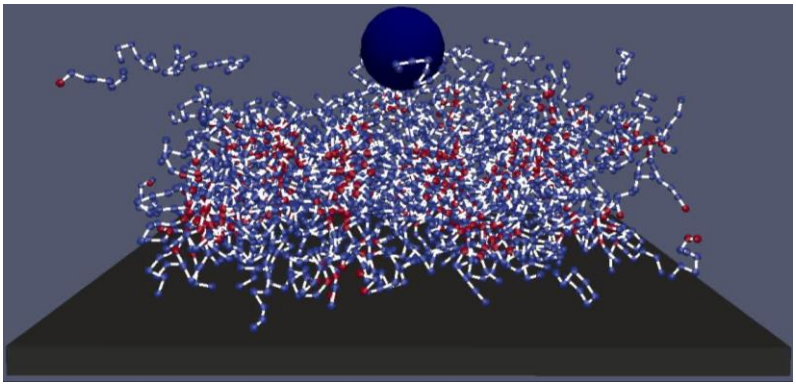

Fig 1: Multiparticle collision dynamics simulations of a bacterium swimming through a dense biopolymer suspension (A. Zoettl)

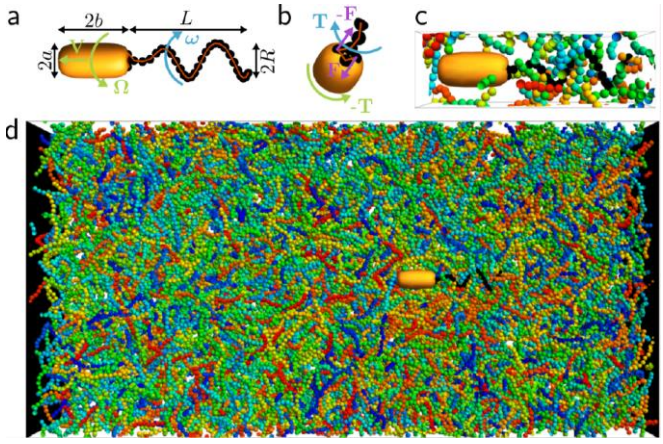

Fig 2: Modelling a colloid crossing a mucus layer (A. Doostmohammadi

Outdoor 3D imaging of wheat for phenotyping

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The food industry has experienced an increase in production quality and efficiency due to the help of ever improving imaging and measurement technologies. Some of these same technologies are beginning to find usage at the other end of the food production process, namely: farming.

Wheat is a globally important crop, making up 20% of all calories consumed on Earth. Improvements in farming practices have allowed wheat yield to be increased 3× between 1960 and 2000. Post-2000 this increase has slowed, and in some parts of the world like the UK, has even plateaued. To ensure future demand can be met, it is estimated that by 2050 a 60% increase in wheat production is required. To meet this goal, better varieties of wheat are created by cross-breeding different varieties that have traits or "phenotypes" that are desirable e.g. drought and disease resistance, high yield and growth rate. For the phenotyping process to be efficient, these traits must be measured in a quantifiable and accurate manner.

Currently as part of field trials, new varieties of wheat are grown outdoors in small test patches. Data collection on certain phenotypes e.g. wheat ear size and wheat height must be carried out manually in-field. Some researchers are interested in the use of point clouds produced via 3D imaging technologies to obtain such dimensional and physiological data. We investigate the use of a several 3D imaging technologies, some of which are more commonly used in controlled indoor environments such as factories, and their ability to produce point clouds of wheat growing outdoors suitable for dimensional measurements.

Modelling molecular release during coffee brewing

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The brewing of coffee involves the release into the brew of a wide range of molecular, oligomer and polymeric species. Coffee flavour evolves during brewing due to the differences in time scales of release. Despite this complexity physical modelling can bring some insight. Although work in progress, a model for coffee brewing is developed which includes both diffusion and interactions within coffee particles; it includes partitioning between water and oil phases, and adsorption/desorption on cell-wall polysaccharides. It is used to fit data for total yield, caffeine, trigonelline, chlorogenic acids and melanoidins. It is used to predict and compare against literature data on how molecular polarity effects release. The sourness of coffee is a key aspect of quality, it will be shown that this is related both to the acid and mineral content of coffee particles. Using a model for the total yield the release of individual species against total yield can be modelled. Composition (relative proportions of individual species) and yield are not one to one, coffee prepared to the same yield can have different compositions.

Electronic inspection of the inner pressure of bottled & canned food or beverages. How convex sets theory defines its limits

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In the Food and Beverage packaging industry it is of paramount importance to assure the safety of packaged products. A range of solutions are given by the automated quality assurance (QA) analytical inspection technologies, relying on electromagnetic interactions between detector and packaged product.

Convex Set Theory defines the upper limits of the performances of the ultrasound inspections (US) in the modern Food and Beverage Packaging Line environment, as outcome of the analyses of the acoustic reaction of a closure stimulated by ultrasounds. Allowing to determine if a container has any or more of the typical containers' defects: leaking, deformed, punctured, cocked, missing sealing compound, etc.

The Inner Pressure Inspection by Ultrasounds considers closures like ideal circular membranes whose oscillation characteristic values (eigenvalues) are defined by its diameter, surface tension and superficial density. Signals processed assuming a basic model ignoring physical properties relevant for the real membranes (crown-corks closures, lids and threaded caps). Properties like bending stiffness, material non-uniform density, atmospheric pressure, etc.

But the problem it is tasked to solve regards what information about a convex compact body, closed by a clamped membrane, can be obtained from the sequence of eigenvalues of the eigenvalue problem applied to a Helmholtz wave equation. In 1911 the physicist Hermann Weyl showed that the sequence of its eigenfrequencies determines the area of a plane vibrating membrane. As a consequence, it was later conjectured that the shape of the membrane could also be determined by this sequence.

Challenging that conjecture we could ask ourselves: is it possible to conceive two drum heads whose shape is different but with the same set of eigenfrequencies?

A serious problem, because apart exceptions accounting for <0.001% of them, the closures adopted by the Food & Beverage industry have similar areas. But, in the Food & Beverage Packaging lines, the defective

closures are observed mainly differing by the population in their shape. Common sense suggests that a round drum will sound differently than a square or octagonal. Every metal cap shape signing with its own signature. A superposition of terms of amplitude y and non-harmonic overtones at frequency is what the industry considered true thirty years ago.

Seamed cans and crown-cork closed bottles represent examples of the general concept of convex manifold. A positive answer to the question above implies that they could exist differently shaped iso-spectral manifolds, proving the existence of a natural limit preventing False Positives' minimisation. A question unsolved until 1992 when Gordon, Webb, and Wolpert conceived two polygons with an identical set of eigenvalues. Making sense of the main limit affecting all Inner Pressure inspections. False Positives caused by defective closures having the same area of an actually correctly closed, only differing in their shape.

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Getting the most out of physics based modelling in the food industry

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Many different modelling techniques are exploited in the food industry to help validate, optimize and scale-up food processes and, where possible, industrial CFD, FEA and DEM codes are used to solve problems involving the effect of geometry and structure on the transformation of liquid, solid and powdered products based on measured material and transport properties.

In many cases, however, the transformations occur on several scales making the explicit modelling of these processes prohibitively expensive unless they are separated into simpler sub-models and coupled to each other through boundary conditions (e.g. using sorption isotherms, Henry's law, . . .) and integrated properties (e.g. bulk density, enthalpy, . . .).

Some examples of this approach include:

- The multi-cell counter current sorption of critical compounds from a concentrate into activated carbon. Here the concentration is computed on several levels: 1) in the flow through a line of cells with periodically changing connectivity, 2) in the flow through a fixed bed in each cell and 3) in the diffusion & sorption of compounds along the micro-channels within the carbon particles.

- The sorption of injected gas bubbles into a concentrate under pressure is another. Here the changing flow conditions of a gassed concentrate is computed along a production line together with the evolution of the coupled bubble distribution to determine the level of dissolution under different operating conditions.

- By including the phase-change of moisture into vapor, the reverse process can also be modelled to predict the vapor expansion of extruded concentrates.

- Spray drying is another process that can be broken down into several connected steps & scales to predict: 1) the flow conditions at the outlet of a pressure swirl nozzle; 2) the break-up of the spray into a distribution of droplets via the Kelvin-Helmholz instability and 3) the drying of the droplets via Lagrangian particle tracking with two way coupling. The radial diffusion of heat and mass within each particle makes the simulation very heavy so it is often approximated with a normalized drying curve

approach instead. The model can be extended to include agglomeration of particles by coupling with a population balance model with a suitable kernel function.

These are just a few of the processes that are modelled in industry by breaking down the process into a series sub processes solved on different scales. In most cases, the models are either solved as a lumped system or solved as a sequence of PSTR's to approximate a plug flow. But with the availability of powerful computer clusters, multiscale models are now coupled with 3D CFD simulations to make predictions with much higher geometric accuracy.

In this talk a brief overview of modelling activities will be given followed by some modelling applications to illustrate the diversity in how physics based modelling is exploited in the food industry and how multiscale models are used in particular.

Poster programme

P1. Ultrasound assisted extraction of rice bran protein and its functional properties

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Rice bran is an undervalued and underutilized by-product from rice milling, contains about 10-15% protein which is comprised of 24-39% water-soluble, 33-42% salt-soluble, 1-4% alcohol-soluble, and 26-30% alkali-soluble protein fractions1. The rice bran protein has been intensively studied for the last few decades and it has immense potential in food and pharmaceutical applications due to its superior quality comprising hypoallergenicity and anti-cancer activity. Rice bran protein concentrate has been used as a nutritional supplement and functional ingredient in food processing. The emulsifying and foaming properties of rice bran protein concentrates have been reported to be quite good in the formulation of various food products2. Extraction of rice bran protein is considered to be advantageous due to the increasing demand for relatively inexpensive sources of protein which can be incorporated into value-added food products. Extraction methods that have been developed so far still remain a challenge to for the commercial production of protein concentrate or isolate from rice bran in terms of efficiency and cost-effective. In this study, a standard ultrasound-assisted extraction (UAE) process has been developed at NCEFE for extracting and isolating various protein fractions (albumins, globulins, glutelins, and prolamins) in rice bran. UAE is considered to be advantages with better penetration of the solvent into the cellular material, improvement in mass transfer, better release of the extract due to the disruption of the cell wall. This UAE, a physical method is more desirable than chemical or enzymatic methods in food processing as they induce lesser alterations in foods and lesser health concerns. UAE of protein from defatted rice bran in an aqueous solution was performed under alkaline condition (pH 11) and an increase in ultrasonic power is found to significantly reduce the extraction time. The objective of this study includes the effects of UAE variables (e.g. sonication power and time) on the protein yield; the extraction kinetic parameters (extraction time) and a comparative study on functional properties of rice bran protein concentrate obtained from UAE and conventional extraction. The results depict that the protein yield is higher using UAE compared to the conventional extraction, and it shows excellent functional properties.

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P2. Ultrasound spectroscopy techniques for the characterization of edible oleofoams

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Because of the dramatic rise of obesity in UK in the last three decades, several food companies have committed to design and manufacture healthier foods with reduced caloric content. A critical food sector that needs improvement is confectionery. Sweets, candies and chocolate contain substantial amounts of sugars or fats, and their consumption is significantly contributing to the obesity problem. An effective way of reducing calories is to use edible oil-based foams (oleofoams) to prepare aerated food (e.g., aerated chocolate bars or mousses) [1]. The main constituents of edible oleofoams are a liquid oil phase, air bubbles and a further high-melting, crystalline fat phase, which stabilises the bubbles acting via a Pickering effect. Such complex microstructure determines the macroscopic chemical, physical and nutritional properties of oleofoams [2]. Therefore, continuous monitoring and control of oleofoams microstructure during manufacturing is essential to ensure the quality of the final food product. Ultrasound spectroscopy is a fast and affordable monitoring technique, characterized by non-intrusiveness and non-destructive behaviour, which is particularly promising for online, in situ characterization of oleofoams. Short, low-intensity ultrasound pulses can be propagated through the sample and give useful information about oleofoams microstructure.

In this work, several oleofoams with varying lipid composition, crystallisation and aeration protocols and age have been analysed using broadband ultrasonic transducers, both in reflection mode – using an airborne acoustic microscope – and in transmission mode. The aim of the work is to find a correlation between the measured acoustic properties (speed of sound and attenuation) with the foam physical properties and microstructure. The experimental results show how ultrasound spectroscopy can be a valuable tool for determining bubble size distribution, which is a central feature for characterizing an oleofoam.

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P3. Quantifying the effect of natural antimicrobials and ultrasonic treatment on the stress adaptation and antimicrobial resistance of *listeria* in viscoelastic gels

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Minimally processed foods retaining their nutritional content, natural colouring, taste and texture are in increasing demand, hence minimal food processing techniques for microbial decontamination, e.g. natural antimicrobials are of interest(1). These techniques can be combined with non-thermal processes such as ultrasounds, which can have a synergistic effect and act as a hurdle for the growth of bacteria, thereby increasing processing efficiency(2). However, they are milder than classical methods and may present a mild, sublethal stress, allowing for post-treatment survival, stress adaptation, and potential antimicrobial resistance (AMR) development(3). This is concerning for *Listeria*, a pathogen associated with ready-to-eat foods and high mortality(4).

Additionally, cells grown as colonies in solid(like) food systems experience a significantly different biochemical and structural environment in comparison to planktonic growth in liquid systems. Diffusional limitations of oxygen/nutrients and accumulation of (acidic) metabolic products around the colony can cause a self-induced (acid) stress that may affect the microbial kinetics and the microbial environmental response(5). Microorganisms could also display a different level of AMR development due to environmental stress adaptation and cross protection(6). Most available studies on the inactivation of food-related pathogens (including *Listeria*) by natural antimicrobials and/or ultrasounds are conducted in liquid broth systems, or in real liquid food products. However, many food products are solid(like) e.g. soft cheeses, meats, and studies in real food products are informative only for the specific product studied. A fundamental study on microbial inactivation by ultrasound and/or natural antimicrobials in structured systems is lacking.

Methods and results: The present work is a systematic comparative study on the effect of novel food processing technologies (ultrasound and/or nisin) on the inactivation of *Listeria*, in viscoelastic systems which can mimic real food products. A range of viscoelastic gel systems were developed using Xanthan gum and/or Whey protein, and were rheologically characterised. Stationary phase *Listeria* was grown in these systems, with/without a sublethal concentration of nisin, and then treated with ultrasound at a range of frequencies. The viscosity/structure of the system was shown to affect the efficacy of ultrasonic treatment, with different effects at the different frequencies. The presence of nisin also affected post-treatment survival.

Conclusions: A clear impact of system structure on the efficacy of minimal food processing techniques is observed. We highlight the importance of accounting for bacterial stress adaptation in solid(like) systems when designing novel decontamination processes for use in the food industry.

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P4. Biotransformation of wastes of agrifood industries for animal feeding

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In Morocco, the halieutic sector has an important role in the national economy, but it can generate a lot of waste. Due to lack of funds oran absence of binding legislation, these wastes are usually rejected into the environment without any treatment [1].

In order to reach sustainable production and consumption with respect to the environment, the goal is to develop industrial processes that are sustainable and focus on three strategies: prevention, recovery and recycling.

The technological biotransformation theory suggests that in order to get an interesting product, the elemental composition of starting mixtures (source of carbon, nitrogen, phosphorus) must be balanced and must be optimized and the conditions necessary for growth and microbial activity must be ensured. It is therefore essential to distinguish what optimal configuration that will ensure that this biotransformation is directed toward the generation of a product with high added value [2-3].

The objective of this study is to use statistical approach to design and analysis of mixture experiments containing covariate(s) that will yield a better understanding and study biotransformation of ternary mixture of industrials wastes: fish waste, molasses and yeasts in order to produce an interesting poultry food with a best quality. This methodology was chosen for its simplicity and its opportunity to offer good information, reducing number of tests, time and cost incurred.

This study shows that it is possible to realize easily in optimal time and at low cost, a poultry food rich in protein, fat and carbon-based sardine waste, 12% of molasses and 18 % of yeast. This product also has good hygienic properties. The performance tests as a well poultry feed have shown that our products are more interesting than some commercially available products.

Key words: Biotransformation, Agrifood industry, Fish waste, Mixture experiments, Poultry food.

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P5. Lay's shapes has created exciting products to deliver Lay's branded snacks to consumers in emerging markets, via soft matter physics & material science tools

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A soft matter physics approach was applied to the development of new snack products for consumers in emerging markets (India, Thailand, Indonesia to date) unlocking significant cost reductions (sales price of £0.05 per bag) and a reduced reliance on raw materials imported from Europe.

Complex Disperse System modelling was used to interpret multiple physical analyses and generate insights into the specific functionalities of various constituents within the product formulation, resulting in replacement of high-cost imported ingredients with low-cost local alternatives.

Lay's is the world's largest food brand and is aspirational to consumers everywhere seeking a global brand as an assurance of safety and quality. Based on physics principles, this breakthrough provided a new route to delivering Lay's-branded quality snacks to consumers in emerging market. Sales 2 years after launch are at 120% of the Volume plan, and are highly incremental to Lay's potato chips.

P6. Effect of melt temperature on cocoa butter lipolysis

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Cocoa butter (CB) is a fat of plant origin that forms the continuous phase in chocolate. It consists of a number of triacylglycerols (TAGs), and when tempered into its βv polymorphic form, that which is required in chocolate, has an average melting point (MP) of ~34 °C. Nevertheless, some of its component TAGs have MPs of 40 °C and above, thus, the ability of pancreatic lipase to perform hydrolysis on these microcrystalline forms is unclear when the process is executed at 37 °C (body temperature -Tbody-)(1, 2).

Therefore, the aim of this study was to elucidate the proportion of lipolysis that occurs when CB is melted at Tbody and above. For this, a static in vitro digestion model was used to evaluate the percentage of free fatty acids (FFAs) released from CB first melted at the different temperatures: 37, 50 and 80 °C, then intestinal digestion performed at 37 °C. Experimental results show that the initial melting temperature of CB does have an effect on the degree of lipid hydrolysis (DHlipid), with the 80 oC melt outperforming the 37 and 50 °C melts in terms of overall FFA release. This result suggests that the microcrystalline TAG structures present at human body temperature are not easily digested during transport through the small intestine.

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P7. Modelling moisture loss in roasting coffee beans

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A model (1) is developed to give insight into the evolution of the profiles of temperature and moisture (liquid and vapour phases and transition between) internal to a roasting bean. Modified evaporation rates and chemical reaction groups improve existing mathematical models (2). We model the phase change from liquid to vapour water within the bean during roasting using first-order Arrhenius-like global reactions. For other components of the bean, we consider a three-component solid phase model for organic compounds which allows for porosity of the solid matrix to vary during the roasting process. Simulations are compare against data for the overall moisture loss data of roasting of whole beans and chopped beans. It is found that the multiphase model with global water reactions and three-component solid phase reactions agree with experimental data for the average moisture content in whole beans and chopped bean, but that the data allows for a range to possible parameter values. It is discussed what experimental data might be collected to more firmly determine the parameters.

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P8. The modelling of coffee bew yield

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Models of coffee brewing have been developed recently (1,2). A key question is how to parameterise such models against controlled experiments allowing predictions to be made on a wide set of brew conditions. Brew experiments were performed on a range of grind sizes from 200 to 1000) in both dilute batch conditions and flow through a packed bed for a range of flow rates in conditions similar to that of espresso brewing (3). nUsing a model based on diffusion out of particles (1), the yield vs time data can be fit using a single particle length scale and two diffusion constants. In reality, however, coffee grinds are bi-modal in particle size with fine and coarse distributions. Furthermore, diffusive release from fines and the outer rim of coarse particles can be expected to be with bulk solution diffusion constants whilst that from the core of coarse particles to with be hindered (lower) values. A bi-modal model with fine and coarse particles was also used to fit the data set, with hindered diffusion constants in the range expected, however, the distribution of hindered diffusion constants was itself bi-modal.

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P9. An in vitro study of the effect of lubrication on swallowing

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Understanding the formation of the post swallow residues is instrumental to modulate and enhance aroma release and to manage swallowing disorders.

In this study, the in vitro experiment originally developed by de Loubens et al. was improved to assess the im pact of bolus viscosity and salivary flow rate on the thickness of the bolus coated on soft surfaces inspired by the pharyngeal mucosa. The time required for complete bolus clearance was observed to depend on the rheological properties of the lubricant layer, providing a tool to investigate the role of changes of salivary properties (e.g. xerostomia) on swallowing.

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