Universality in rheology of concentrated food biopolymers

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For applications of spray drying and plant protein extrusion, we are interested in the rheology of concentrated food biopolymers. We view that their rheology is similar to transient network, showing a master curve, with plateau zone, transient zone, and glassy regime. We present our first results concerning maltodextrins, which is relevant for spray drying applications, and starch, which is relevant for extrusion applications.

We show that the zero-shear viscosity of maltodextrins shows a similar behaviour as small carbohydrates, which scales with T/T_g, the temperature over the glass transition temperature (Sman,Mauer,2019). Note that, T_g incorporates the dependency with moisture. Subsequently, we have found that flow curves for maltodextrins and starch, showing viscosity as function of shear rate, can be mapped to a master curve, if viscosity is scaled by the zero-shear viscosity, and the shear rate by the inverse of the zero-shear viscosity (similar to Saito plots).

Finally, oscillatory rheology results of maltodextrins and starch can be mapped to a single master curve, via horizontal shifting. The shift-factor depends again on T/T_g. The master-curve can be described by the Marin and Graessley model, with a Maxwell-mode coupled to one or two Cole-Cole modes. All the modes have the same temperature dependence as the zero-shear viscosity.

Designing Superior Plant Based Food Emulsifiers: What Can a Theoretical Perspective Teach Us

Dr. Rammile Ettelaie, University of Leeds (UK)

Anyone involved in food related research would not have failed to notice the significant effort by food scientists and technologists in the past few years in attempting to replace animal derived food materials with equivalent plant based ones. Many important functional food ingredients are no exception to this trend, driven by issues of sustainability, health and environmental considerations. One important class of such functional ingredients are food grade emulsifiers. Currently most widely used emulsifiers and emulsion colloidal stabilisers used in food industry are animal derived proteins, particularly those obtained from milk and egg. Replacing these with plant-based proteins is a challenging task due to the low solubility, poor emulsifying capability and inferior surface adsorption properties associated with plant storage proteins. Nonetheless, several possible ways of improving their behaviour have been pursued in recent years, including electrostatic or covalently formed complexes of protein and polysaccharides, fragmentation of large proteins through selective enzymatic hydrolysis, or turning hydrophilic plant polysaccharides (e.g. starch) into amphiphilic macromolecules through attachment of a small number of hydrophobic groups.

The presentation examines some of the above mentioned techniques from a theoretical point of view. By applying the Self-Consistent-Field theory (SCF), barrowed from the field of polymer chemistry and physics, we attempt to predict the adsorption behaviour and the adopted confirmation of chains on surfaces. Similarly, the nature of colloidal inter-droplet forces, induced by adsorbed layers of such macromolecules, are studied. We discuss the implication of these results for improving the emulsifiers produced in relation to each of the above techniques, as well as limitations that such predictions place on what may and may not be achievable using each method. A comparison with selected preliminary experimental results from our own labs, will also be presented to better illustrate the role of such theoretical calculations in providing useful guidelines for the design of future superior plant protein-based emulsifiers.

In silico models for predicting food breakdown during the gastric process

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Highly processed foods tend to form weak structures which breakdown rapidly in the gastrointestinal (GI) tract, often causing negative effects on human metabolism and health. Developing healthier foods has been limited by the lack of understanding of how foods are digested. Through computational modelling we reveal mechanical gastric food breakdown phenomena and relate food mechanical properties with performance during critical initial digestion stages. Our model relies strictly on a viscoplastic-damage constitutive law, calibrated via rheological experiments on an artificial biscuit bolus and validated by simulating cutting tests. Simulations suggest that bolus separation during bolus backward extrusion and/or indentation by peristaltic waves, and, bolus agglomeration due to hydrostatic compression near the pylorus, are two competing phenomena that can influence the bolus free surface to volume ratio. This showcases the importance of including mechanical aspects of breakdown when designing foods for controlled chemo-mechanical breakdown and associated nutrient release rates.

Digital design and digital operation of food products and their manufacturing processes

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Food and beverage processing is very diverse, both in the unit operations applied and in the different feed and product streams that may be involved. Increasing understanding of these processes is highly desirable to the industry in order to improve process efficiency, ensure product quality and safety and to facilitate innovations. Physical experiments to develop understanding are often costly to run, and can even be impossible for most production facilities. The application of mechanistic, data-calibrated modelling is an approach to provide this insight which is increasing in use across the industry.

By using mathematical models built on physics and chemistry, properties gleaned from material characterization experiments can be used to predict performance of unit operations at scale. These models can be further validated, and then used as so-called digital twins of the physical process. A digital twin is in essence a collection of models that aim to describe aspects of a unit operation which are of interest for process performance in terms of product throughput, quality and safety. Digital twins can be applied for existing or conceptual processes. In the former case, the models could be used for optimizing process parameters and scheduling, while in the latter case the main use would be for technology transfer and process design evaluation. The overall advantage of digital twins is the general time efficiency gained from being able to evaluate a plethora of process options, which would take far longer or even be impossible to evaluate in practice. This methodology has been used to good effect already by companies in the food and beverage industries and beyond. The versatility and usability of such models is just as important as their fidelity, expanding their accessibility from highly trained engineers and scientists to operating technicians, process developers and others.

This presentation will go over several key process operations in food and beverage processing, such as membrane filtration, falling film evaporation and spray drying, and how digital twins can help improve R&D and operational approaches regarding these processes. The presentation will also discuss how an integrated experimentation and modelling approach is crucial to this success and the benefits this will provide to the food and beverage processing industry going forward. As an example, Figure 1 shows how a mechanistically-based membrane separation digital twin, built in gPROMS, was used to minimize fouling for a whey protein concentrate (WPC) application. The results enabled process control teams and site technologists to increase process run time before cleaning in both current and newly designed systems.

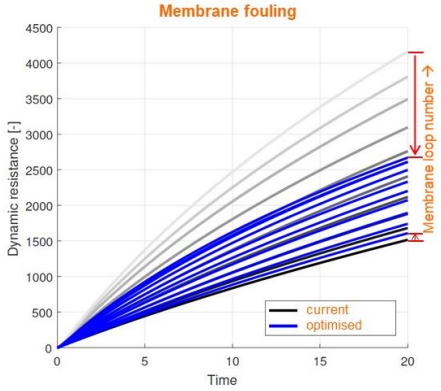

Figure 1: Current and optimised approaches to increase membrane separation run times through the use of a membrane separation digital twin

Chocolate Shell Formation & Strength

Edward Throp, Mondelēz (UK)

Testing new designs or changes to existing filled shell products is costly and time consuming. To enable virtual trials reducing the time and resources required to complete physical trials a simulation process has been developed. This applies both CFD and FEA modelling techniques to model the drainage of the chocolate from the mould cavity and the subsequent crushing of the formed shell to determine the chocolate strength. The CFD modelling process and challenges are outlines along with a summary of the FEA process along with discussion of the application of the model.

Simulation Democratization using PepsiCo's "Virtual Lab”

Stacie Tibos, PepsiCo (UK)

Democratization plays a pivotal role in PepsiCo's Digital Transformation. Maximising the number of associates able to leverage the power of modelling and simulation is the most effective way to generate business value from these tools. PepsiCo are building a "virtual lab" that utilises the COMSOL App platform. An overview of the first Apps within PepsiCo's "virtual lab" is presented and a brief roadmap of where PepsiCo are taking this capability is also shown.

Modelling Food Processing in a Solid-State Microwave/Convection Oven

Christopher Hopper, ITW (USA)

Utilizing solid-state RF generators in cooking ovens eliminates the need for stirrers, turntables, and duty-cycles often found in magnetron-based ovens to improve heating uniformity and overall food quality. Solid-state ovens can also read and interpret feedback from the oven cavity to adapt parameters such as frequency, phase, and output power to achieve specific cooking goals. Advances in simulation and numerical computation software allow for accurate prediction of the effects varying these, and other, parameters can have on the cooking results. This talk will discuss ways ITW engineers use simulation to design experiments, develop algorithms, and collaborate with customers through customized applications.

Kinetic Modelling of the Maillard Reaction

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The Maillard reaction is an incredibly important aspect of the thermal processing of food as it generates not only colour and flavour, but also process contaminants such as acrylamide. It is initiated by the reaction between reducing sugars and free amino groups (usually free amino acids) and after the formation of a series of semi-stable intermediates called the Amadori reaction products (ARP) it quickly escalates into a complex network of reactions occurring in series and in parallel. Understanding the detail of the formation pathways, the rate limiting steps and the competitive processes is critical for manipulating the reaction to optimize flavour formation and minimise the formation of undesirable process contaminants. One approach to test potential reaction pathways and identify critical control points is to use multireponse mathematical modelling of the kinetics based on the underlying chemistry.

In our group we have successfully modelled the formation of key aroma compounds and the formation of acrylamide. In the latter, we proposed two different chemical pathways for the formation of acrylamide. The detailed chemical pathways were converted into simplified kinetic pathways where only the rate limiting steps were incorporated, and by altering the precursors in the starting material, it was possible to monitor the reaction over a set of different time and temperature combinations under a range of different starting conditions. Heat and mass transfer were included in the model, to take account of the reaction occurring on the surface (and edges/corners) of the fries. Using this model we could demonstrate how the pathways changed depending on the ratio of the sugars and amino acids in the raw material.

In the latest project, we have used inorganic salts to mitigate formation of acrylamide in a biscuit model system, and are in the process of modelling precursors, intermediates, aroma and acrylamide. These preliminary data will be presented.

Product Design in Foods, the Digital Way

Michiel Gribnau, Unilever (Netherlands)

The Food related wishes and needs of consumers are changing continuously. This also relates to some major problems around such as obesity and hunger, food waste and climate change. A still very actual example are the changes created by the COVID pandemic with less people eating out of home and more people eating in home.

As a consequence Unilever needs to continously modify and optimise its product portfolio in order to match these changing needs and wishes. Traditionally this is a labour intensive process, but it can be greatly accelerated by the use of state of the art digital capabilities. Reliable models, either data driven or chemistry or physics based are essential to make this approach a success. Given the number of models required, Unilever is involved in setting up a system to conditionally share models between companies and organisations.

Estimating aroma losses from microwaved foods using a database approach

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Microwave heating has become a regular part of food preparation in domestic and commercial kitchens, where chilled or frozen meals are rapidly heated before consumption. In contrast to conventional oven heating, where heat transfer is mainly by conduction from the outside of the food to the interior, microwaves penetrate the food and cause more uniform heating. This mode of heating changes the way water is released from the food. With conduction, the outer food layers dry and the lowered water activity causes Maillard reactions that produces the typical brown colour and some aroma formation. With microwave heating, there is less of a temperature gradient, and the surface does not dry out, so surface browning is minimal. The other difference between the heating methods is that the wholesale heating by microwaves causes a significant flow of steam through the product, which can effectively remove aromas that are non-miscible with water, through the process of steam distillation.

To estimate which compounds could be lost through steam distillation, calculations were added to a database containing a list of around 2000 aroma compounds (and their physical properties) to estimate at what temperature each compound would distill using the Clausius-Clapeyron equation. The rules surrounding steam distillation were implemented using filters in the database to select non-miscible compounds using their water solubility data. Physical properties included the vapour pressure and boiling point of each aroma compound. Physical chemistry is not a common subject for many users of flavour, so the database was hosted on a general platform (Tibco Spotfire) so that results could be presented graphically. These visualisations made it easier for end-users to understand how steam distillation affected the aroma of their particular products after microwaving.

A live demonstration of how the database can be interrogated to adjust different scenarios will be part of the presentation.

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A micro-CFD study: modelling of macromolecules ultrafiltration fouling in food processing

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Ultrafiltration (UF) has been extensively applied in food processing industry for the last thirty years due to its advantages, namely gentle product treatment, high selectivity, low energy consumption, over conventional separation processes. Nonetheless, membrane fouling compromises the benefits of ultrafiltration as fouling, resulting from the accumulation of the rejected species on the membrane surface, drastically reduces the performance and hence increases the cost of UF. The aim of this work was the fundamental characterization of cake formation occurring during proteins ultrafiltration. A twisted Monte-Carlo (MC)/Computational-Fluid-Dynamic (CFD) approach was developed to obtain a set of macroscopic fluid-dynamic proprieties. Different fluid-dynamic simulations, performed on the basis of the knowledge acquired by a MC analysis, which resulted in a set of boxes of aggregated molecules, were performed. Thanks to the MC techniques, various 3D structures were developed and characterized. These structures represented the deposit layers, which formed at different distances from the membrane. By means of a number of well-assessed computer-aided tools, these geometries were imported in a CFD simulation environment and several meshes were created to perform micro-fluid dynamic calculations (m-FD). From these simulations, a set of valuable macroscopic parameters was calculated. The resistance to flow of deposit layers accumulated during membrane operation, $Radd$, generally estimated by experimental methods, was computed starting from the ab-initio knowledge acquired at sub-nanoscopic scale, without exploiting any empirical macroscopic coefficient, which is usually introduced to characterize the UF process. The developed computational platform, since based on the actual knowledge of proteins characteristics as acquired at sub-nanoscopic scale, represents a powerful and versatile predictive tool that allows attaining a deeper understanding of deposited layers structure. As shown in a typical case in Fig. 1, it is possible to predict the actual velocity profile developing in the cake under different process conditions. Finally, a fully dynamic coupling of microscale and macroscale simulation models was also implemented to estimate the dynamic extent of membrane fouling occurring in a variety of membrane processes of interest to the food industry.

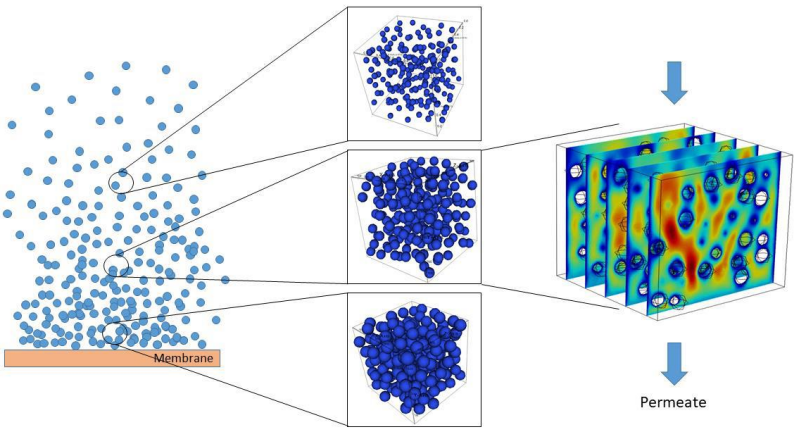

Fig. 1 - micro-CFD approach to develop a complete fluid dynamic study on the deposited cake layers during membrane filtration. The number of MC-CFD simulations depends on the computational resources

Starch granule swelling and suspension rheology: DEM simulations and Experiments

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Starch is the predominant food reserve in plants and provides 70-80% of the calories consumed by humans worldwide in various forms of food products. Starch is found as dense granules which is its native form in a variety of grains and tubers. The phenomena of starch gelatinization where granules swell, i.e. their diameter increases while they become soft and deformable particles have been of an active area of research for some time now. During this phenomena, granule volume fraction in a suspension grows rapidly and eventually swollen granules occupy almost the entire volume. Such a feature is fundamental from the industrial perspective because the product transformation (starch swelling) has consequences on the product properties (starch viscosity) and then on the flow behaviour of the product throughout the processing unit. Thus understanding the material properties and transformations of starch are quintessential for designing differentiated products, process design and control. There are recent efforts reported in the literature to decipher the origin of shear-thinning in non-brownian suspensions[1,2,3,4] and chemically modified maize starch suspension is one such model system. In this work, we discuss briefly a kinetic model for starch gelatinization at the granule scale for chemically modified maize starch which in future could be coupled with a DEM or DEM-CFD model. We further present preliminary results of DEM shear flow simulations with lubrication forces of fully swollen starch granules with relevant material properties to predict the suspension rheology. The DEM results are compared with experimental rheology and possible explanations for the discrepancy between the same are discussed along with possible leads for future research in this area.

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Modelling acoustic propagation in suspensions – micro-rheology and rheology

Megan J Povey, University of Leeds (UK)

Acoustic propagation in suspensions cannot be approached as a straightforward combination of the properties of the suspending and suspended phases. The interfacial region always contributes; generally, in the form of scattering in which sound is both redirected and thermally dissipated.

Non-invasive acoustic techniques are a valuable way of measuring the viscosity of fluids during processing, however, interpretation of the data (velocity and attenuation spectra) is generally not simple and models based on scattering theory such as the well-known Epstein-Carhart-Allegra-Hawley (ECAH[1,2]) theory are needed.

Extraction of rheological data from acoustic data requires a good understanding of the nature of the acoustic propagation in the system of interest on one hand and knowledge of the thermo-acoustic properties of the different phases of which the system is comprised on the other. For example, is the propagation a bulk compressional wave, is it a surface wave or is it a rapidly decaying shear wave at an interface, is the wavelength longer, shorter or of the same order as the size of the dispersed phase? So, choice of excitation method, frequency and pulse length are all significant.

Solution of scattering theory equations is possible numerically but requires knowledge of at least 13 different physical parameters. In this talk I will present an approach based on analytic solutions of the scattering equations in different asymptotic regimes which permit extraction of rheological data such as bulk viscosity and shear viscosity from frequency dependent attenuation data.

Depending on the scattering regime, these rheological data may pertain to the properties of a small region surrounding the dispersed phase (micro-rheology) rather than the bulk rheology measured by conventional means. However, if the wavelength of sound (acoustic or ultrasonic) is long in comparison to the size of the dispersed phase and its mean separation, the determined rheological parameters will be those of the bulk at the measurement frequency.

The concept of longitudinal viscosity will be introduced and examples of both micro-rheological and bulk viscosity determinations using ultrasound spectroscopy will be given.

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Neutron Scattering and Quantitative Modelling of Curd Formation in Commercial Milk

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Roughly 25% of world bovine milk production is dedicated to cheese manufacture as the fundamental material in the process of cheese curd preparation. Casein micelles are a primary constituent of those curds. Aggregation and gel formation occurs as a result of enzymes hydrolysing surface proteins of the micelles, primarily kappa casein. We have developed a two-step model to describe the aggregation process in detail. First, short strands of hydrolysed micelles are formed. We model these strands as cylinders with binding sites at the ends. Monte Carlo simulations show that these basic units combine to form a larger branched fractal structure. A calculation of the resulting structure function gives an approximate mass fractal dimension of 2. The measured fractal dimension and the results of computer simulation suggest that the aggregates are analogous to swollen randomly branched polymers. After including polydispersity, this model gives an excellent description of our own neutron scattering data on coagulants resulting from bovine and fungal rennet added to commercial skim and whole milk. These simulations and measurements provide an important foundation for continuing study of the structure of commercial cheese.

Physics-based modelling of the GI tract

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Physics-based (PB) models can combine the mathematics of fluid dynamics, solid mechanics, chemistry and biomechanics to simulate the body's functions from first principles. The benefits of building PB models include:

- The ability to test hypotheses of how in-body processes occur with specific control over all variables,
- The identification of experimental characterisations that have not been performed (but should be), and
- A cheap and scalable framework for scenario (or what-if?) testing.

PB models must be comprehensive in terms of the types of physical processes included, well calibrated, and sufficiently validated. Depending on the application, the model may also need to be personalised to an individual or population subgroup. This talk will outline the efforts by the group at CSIRO aimed at fulfilling these requirements for models of mastication, gastric mixing and emptying, and intestinal flow.

Combinations of biomechanical (B) models of anatomical structures, smoothed particle hydrodynamics (SPH) representations of continua (fluid and solids) and discrete element modelling (DEM) representations of particulates are used to represent different components of the GI tract. For the mouth a coupled B-SPH model is used to investigate food breakdown, interactions between solid and liquid foods, softening of solid foods from saliva, tastant release, and melting. A coupled B-SPH-DEM (discrete element method) model of gastric fluid and particulate flow is presented, which includes mixing and emptying functions.

A coupled B-SPH-DEM model of intestinal flow is presented which incorporates muscle motor patterns, flow, nutrient transport and densification. Early efforts at inclusion of models of microbiological growth and decay are described which incorporate flow characteristics and species competition. The simulation framework is currently being extended to include the connecting features of the individual models. This end-to-end GI tract model with the ability for personalisation will used to address larger scientific questions than the individual components on their own.