2nd Chemical and Physical Modelling of Food Conference

12 October 2021

Agenda – all times BST (GMT + 1)

Time	*Speaker*	*Presentation Title*
13:00 – 13:10	Mr. Robert Cordina – RSC Food Group Committee Chair	Welcome and Intro
Session 1 Chair: Mr John Bows – Food Physics Group Committee Chair		
13:10-13:30	Dr Yogesh Harshe Nestlé	A mechanistic model for infant-feeding via milk bottles
13:30-13:50	Dr John Melrose Consultant	Modelling molecular release in coffee brewing
13:50-14:10	Ms. Maria Victoria Caballero Technological University Dublin	Estimating pathogens grow in fermented food and smoked salmon through the interaction with background microflora
14:10-14:30	Dr José A. Piornos University of Reading	Multi-response kinetic modelling of the formation of five Strecker aldehydes during kilning of barley malt
14:30-15:00	Break	
Session 2 Chair: Dr Beccy Smith – Food Physics Group Committee Member		
15:00-15:20	Ms Kay Sun Mondelēz International	Physics-based comprehensive model for jelly candy stoving process
15:20-15:40	Dr Ben Coscia Schrödinger Materials	Exploring Flavour Molecule Binding and Encapsulation by Starch Using Molecular Dynamics Simulations
15:40-16:00	Dr Joe (Chao-Cheng) Shiau PepsiCo	Modelling hot fill process to predict food safety qualification of the bottle
16:00-16:20	Prof. Buddhapriya Chakrabarti University of Sheffield	Look out for drops, in lots, and lots of little drops
16:20-16:30	Dr Rim Harich RSSL	Modelling the effect of environmental changes on the flow properties of dairy powder

RSC INTEREST GROUP FOOD

IOP Institute of Physics
Food Physics Group

Abstracts

A mechanistic model for infant-feeding via milk bottles

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This work is a first attempt to model the milk flow out from a baby bottle under active suckling motion by a baby. The model results are compared with the experimental measurements obtained under controlled set of conditions with a breast pump connected to a milk bottle. The impact of applied suck pressure, bottle dimensions, tilt angle and bottle liquid filling level on the flow out from a bottle is evaluated. Based on the results obtained, relative importance of different parameters on the milk flow is discussed.

RESULTS

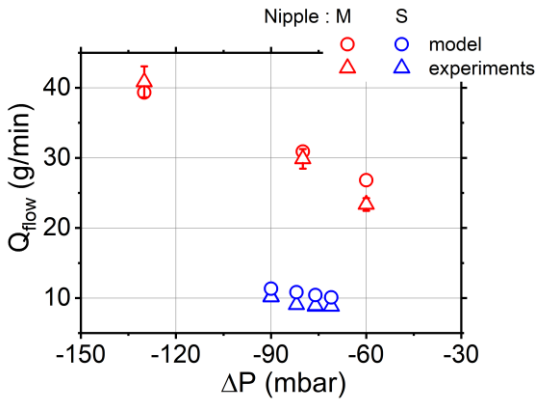

Figure 1: Model validation with experiments for flow of infant formula out of milk bottle two nipple openings S & M, respectively having 147 & 251 micron radius for different applied pressures

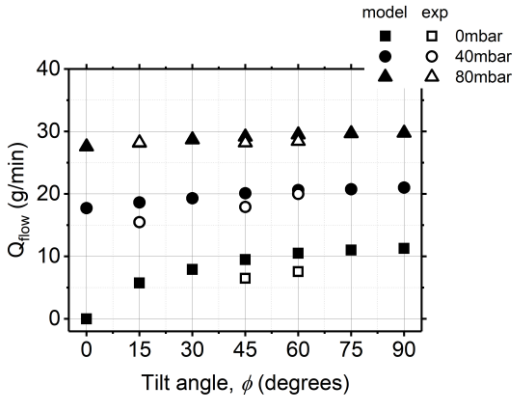

Figure 2: Impact of tilt angle on flowrate of water out of bottle with M nipple with and without applied pressure difference compared for model and experimental results

Modelling molecular release in coffee brewing

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RATIONALE
In recent years, there has been significant progress in the measurement of brew concentrations over time during coffee brewing from packed beds of coffee grinds. To understand this data, it is crucial to quantify those physical chemistry effects that occur internal to coffee grounds but which modulate the release out of the grounds.

METHODS
A multi-scale modelling tool is used to give insights into the underlying physical chemistry inside coffee grounds by fitting measured concentrations kinetics during both brewing and gas stripping (used in instant coffee production). The model includes source and sink terms internal to grounds to model adsorption and partitioning to phases within in grounds and models for hindered diffusion due to co-solute and grounds structure.

RESULTS
Good fits to literature data will be reported for total yield, Caffeine, Acetaldehyde, Acetic acid and a range of molecules with varying polarity (data from Khun et al 2017, Mateus et al 2007, Mestdagh et al 2014 resp.). From the total yield data, a bi-modal distribution of release rates was found. For the individual molecules, the modelling quantifies: the relative roles of hindered diffusion within coffee particles due to structure and co-solutes; the neutralisation effect of coffee bases on organic acids; and, for non-polar molecules, the effect on brew extraction rates of partitioning between water and oil phases internal to coffee grounds. Co-solutes have a strong effect on hindrance in the case of gas stripping from wet grounds.

CONCLUSIONS AND PERSPECTIVES
Most parameters in the model are taken from physical chemistry data sets (e.g. partition coefficients) for the individual molecules and coffee brews. The main fit parameters are structural hinderance and choice of representative grain size from the measured PSD, however a good degree of accuracy can be achieved using a combination of independently measured parameters and some fit – the latter however have expected values. This opens the route for combining modelling and experiment to systematically explore and manipulate effects within grounds which modulate brew composition.

References

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Estimating pathogens grow in fermented food and smoked salmon through the interaction with background microflora

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Fermentation processes are used to produce many different foods. Since foodborne disease outbreaks were first reported caused by pathogenic bacteria, food safety issues have attracted worldwide attention[1,2]. The natural food microflora may include lactic acid species (LAB) and pathogenic bacteria. Interactions between bacterial populations may have consequences for food safety and suppression of pathogens by benign species is of particular interest[3]. Mathematical models are useful tools to predict and describe this behavior[4].

The aim of our study was to model the interactions between *Listeria monocytogenes* and lactic acid bacteria (LAB) in smoked salmon. Twelve mathematical models from the scientific literature were investigated. The secondary models proposed by Gimenez et al. were used[5]. Simulations were made considering a standard error of 0.5 log CFU/g for the same scenario for each model. Then, interaction parameters were fitted by using the simulated data to assess the models.

The model performance was asssessed using the bias and accuracy factors according to Ross[6], modified by Baranyi, Pin, and Ross[7]. A dataset for validation was created by randomly combining the outputs of the simulations. The model proposed by Fujikawa et al.[8] had the best bias factor for LAB (1,0046) and the worst bias factor for *L. monocytogenes* (0,7766). The best accuracy factors were given by the models of Jia et al.[9] for LAB (1,1297) and Valik et al. for *L. monocytogenes* (1,1621).

The models of Valik, L. et al. [10] and Poschet, F. et al.[11] were also testedbecause, although the model proposed by Fujikawa et al.[8] had the best bias factor for LAB, bias and accuracy for *L. monocytogenes* were the worst. The Valik L. et al.[10] model has the second best bias value for *L. monocytogenes*. The model from Poschet, F. et al.[11] had the second best bias and accuracy for LAB (1,0497 and 1,1869 respectively).

The influence of environmental factors against the interaction terms was evaluated by a sensitivity analysis: aw, temperature, pH, concentration of nitrate, concentration of phenols, and concentration of sodium lactate. The studied range was that of the normal industrial parameters in smoked salmon production, namely 0.91 to 0.97 for aw; 4 to 20°C for temperature; 4.9 to 6.3 for pH; 0 to 150 ppm of nitrate; 0 to 18 ppm of phenols and 0 to 5% of sodium lactate.

In the model of Valik, L et al.[10] the factor with the biggest influences for *L. monocytogenes* was temperature, followed by a_w and concentration of nitrates. For LAB, a_w had the greatest influence in the growth simulation. Phenol, nitrate concentration and pH showed no sensitivity for this species. Interaction terms showed significant sensibility to the predictions. The Poschet, F. et al.[11] model showed significant effects only for temperature and aw. For LAB this was only for a_w.

This study shows that pathogen-microflora interaction can be observed in normal experiments and that it may be a significant interaction parameter that will influence the potential growth of pathogens.

References

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Multi-response kinetic modelling of the formation of five Strecker aldehydes during kilning of barley malt

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Strecker aldehydes are responsible for the characteristic aroma of malts, but also important aroma compounds in beer. In malt, they are formed during the curing stage of kilning. The formation of five Strecker aldehydes (2-methylpropanal, 2-methylbutanal, 3-methybutanal, phenylacetaldehyde and methional) during this process was studied at pilot scale. Green malts were dried and cured at different temperatures (65, 78 and 90 °C) isothermally for 8.4 h. Multi-response kinetic modelling was used to develop a mathematical model based on precursors concentration, Amadori rearrangement products (ARP), Strecker aldehydes, temperature and time. This model demonstrated that the formation of Strecker aldehydes in malt was controlled from the formation of two intermediates: ARP and short chain dicarbonyls. The kinetic model proposed in this study will help maltsters and researchers understand and manipulate the formation of these compounds in malt and the organoleptic quality of the beers brewed from them.

Physics-based comprehensive model for jelly candy stoving process

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Jelly candies or gummies are a popular snack product. They are made mostly of corn syrup, sucrose, gelatin, starch and water with small amounts of colouring, flavour and acids. The starch, gelatin, pectin and other gelling agents are used to give the candy its unique chewy/bouncy texture, which is a key driver of consumer preference. In commercial manufacturing, jelly candies are often deposited into starch moulds to give the shape, and then dried to the final moisture in a large oven. This oven drying process is called stoving, which is energy intensive and time-consuming, often the bottleneck of the process.

The traditional approach to product development requires lab-scale testing, then physical trials to scale up and to confirm new product concepts. The long development timeline motivates us to move from physical to virtual trials. In this work, we present a physics-based comprehensive model for this jelly candy stoving process with three interconnected submodules: heat transfer, moisture diffusion and sucrose inversion reaction kinetics; to simulate and predict the physical chemical transformation during this process. The model has been validated against Mondelēz International products and provides predictive power for product and process developers to virtually design new products and optimize process time and conditions.

Exploring flavour molecule binding and encapsulation by starch using molecular dynamics simulations

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Amylose, a major component of starch, is capable of forming non-covalent helical inclusion complexes with small molecules such as volatile flavour molecules. Encapsulation of these compounds aids in flavour retention and can help protect against oxidation. The kinetics and mechanisms of flavour molecule binding and release impact the flavour quality of the product. While experimental techniques are able to indirectly measure the uptake of flavour molecules by amylose, and even characterize the helical conformation of crystallized inclusion complexes, we lack lucid explanations of binding and release mechanisms that could accelerate progress in the field. In this work we develop a molecular model that helps us begin to generate these explanations both quantitatively and qualitatively. Our approach aims to broaden the usage of techniques typically used to probe protein-ligand interactions in drug discovery, adapting them to more flexible host molecules like amylose. Specifically, we adapt the theory of Markov state models in order to characterize the behaviour and transitions between different dynamic states in a dilute solution of amylose and flavour compounds. With knowledge of the rates of transition between dynamical states, it is straightforward to estimate the equilibrium dissociation constants for inclusion complexes, as well as binding free energy. We validate our approach by comparison to experimental literature. Overall, this work lays the groundwork to study more complex and novel systems.

Modelling hot fill process to predict food safety qualification of the bottle

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In the beverage industry, hot fill process refers to filling the heated product into the package and then inverted to allow the heat to sterilize the package as well as the closure. This process has been applied in different PepsiCo's beverage brands including Gatorade, Pureleaf, and Tropicana. A tool that can be used to evaluate this hot fill process for product, package and closure iterations to meet the business need represents tremendous value. This study developed a model to simulate the hot fill process of the beverage processing using the Computational Fluid Dynamics (CFD) tool. The model's target application is to provide temperature profile for log kill prediction under different line conditions and package/closure iterations. In addition, the predicted temperature profile can also be used as an input condition for structural analysis to evaluate the impact of the process on the bottle shape.

An unsteady three-dimensional two-phase (liquid/air) laminar flow model with conjugated heat transfer is developed. The Volume of Fluid (VOF) method is applied to capture the interphase between air and liquid as fill level tracking. Evaporation/condensation at the interface is included to accurately model the cap temperature throughout the process. For the model validation, the predicted log kill from the model generated temperature history of specific process parameter is found to match physical results gathered through consumer feedback of the product procured from specific production lines. Alternate methods for physical validation are currently under development.

The virtual food safety qualification from this model allows quick individual line process and quality assessment, which can serve as a guardrail for new hot fill process and provide improvement guidance when process/package iteration happens.

This study was funded by PepsiCo. The views expressed in this abstract are those of the authors and do not necessarily reflect the position or policy of PepsiCo, Inc.

Look out for drops, in lots, and lots of little drops

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I will discuss our recent work on the thermodynamics of binary mixtures with the volume fraction of the minority component less than the amount required to form a flat interface. In this situation surface tension dominates the equilibrium phase behaviour of the mixture resulting in a macroscopic droplet. Elastic interactions in gel-polymer mixtures stabilize a micro-droplet phase. Using a thermodynamic model we compute the droplet size as a function of the interfacial tension, Flory parameter, and elastic moduli of the gel. Our results illustrate the role of elastic interactions in dictating the phase behaviour of synthetic and biopolymers undergoing liquid-liquid phase separation.

Our work sheds light on the connection between coarsening phenomena and network elasticity that cuts across several disciplines, including biological regulation of cellular function, tailoring mechanical properties of materials, controlling morphology, size of precipitates in food products, and even growth of methane bubbles in aquatic sediments.

References

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Modelling the effect of environmental changes on the flow properties of dairy powder

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The transport and handling of powder materials is notoriously challenging due to the varied nature of materials and associated flow properties. This is particularly relevant in food manufacturing where raw ingredients, semifinished and finished products are prone to physicochemical changes when exposed to the environment. For example, changes in temperature and sorption of atmospheric moisture can significantly affect the flowability of a powder material, potentially leading to poor discharges from hopper and silos, blockages or caking.

Here, we look into how the effect of environmental conditions on the flow of dairy powders can be modelled.

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