A ROUTE TO CREAM CHEESE VIA GEOMETRIC MODELLING

August 14, 2012

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Intro for the layman

This project was done as part of a collaborative workspace named Design and development of REAlistic food Models with well-characterised micro- and macro-structure and composition (DREAM). The first challenge of DREAM is to integrate experimental and mathematical methods, so as to develop food models capable of predicting food behaviour. There are four areas of study: fruits and vegetables, dairy, meat and bakery products. Enhancing the understanding of the process-structure-property relations will impact industry , technology and science. Of importance to science is the understanding of the interactions involved in different scales, ranging from molecular to macroscopic.

Many difficulties arise when searching for models that allow for optimisation and control of food systems, namely: incomplete, piecewise available knowledge, spread out among different disciplines and contributors, scarcity, uncertainty and high cost of measured data, complexity of phenomena and intricacy of time and space scales. It is established that these problems require a nonlinear, dynamic, multi-physics and multi-scale approach, hence grounds for complex system science. Here there are newly developed techniques (modelled-based viability analysis, optimisation, Bayesian networks, etc.) which have been shown to be relevant and promising for complex food systems.[1]

The study reported here is relative to a subsection of dairy products: cream cheeses. These are emulsions of fat droplets, within and aqueous phase. On a smaller scale, one can find several types of milk proteins present which bind the system together.[2]
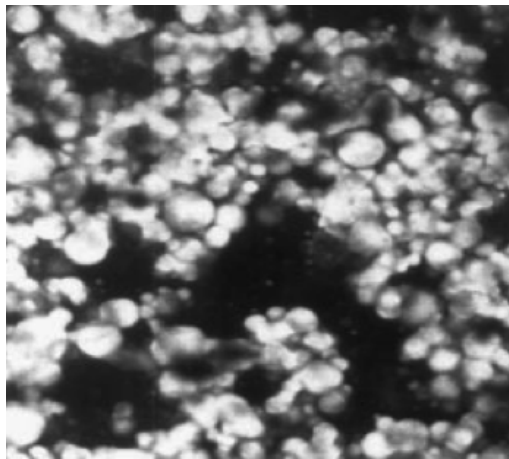

Figure 1: Confocal Laser Scanning Microscope micrograph of cream cheese structure [3].

This final structure is not just dependent on the components of the system, but also on the processing they went through. [3].

Abstract

Abstract

The complexity arising from the application of several unit processes with several control parameters leads to complicated relationship. Special focus is put upon the understanding of the structural implications of thermal treatment, homogenisation and acidification. Hence a geometrical model in a finite volume is studied; fat droplets adsorb native whey proteins and protein aggregates, these later aggregates glue the system together. As a first step to make an integrated model, focus is put upon the input parameters and predicted variables.

Contents

1 Manufacturing Process

The manufacturing process of cream cheese is not an unique process, however in order the protocols of manufacturing can be outlined. For this report the thermo-mechanical treatments are charted by the deliverable WP4 of the DREAM project.[2]

The ingredients involved in this process are: casein and whey protein powders, milk permeate, anhydrous milk fat, NaCl and lactococcus lactis starter suspension. Rehydration of the protein powders, milk permeate and salt takes place in a Stephan cutter, stirring at 360 rpm, with the water heated to 50°C for 15 min. After an emulsion is made by adding the fat to the mixture and agitated during 4h at the same temperature and rotation.

A first heat treatment is then applied to the mixture. The temperatures reached and maintained for around 20s may vary, however 72°C or 94°C where considered; this process takes place under pressure of 2.9 bars. After the emulsion is cooled down to the temperature of the next step, 30°C. It is important to understand the consequence of this step; previously the whey proteins were mainly native whey protein, however now there is a macroscopic amount of denaturated whey proteins. These denaturated whey proteins will coat the surface of the casein micelles.[4]

The preceding step is the acidification, where 0.00025% of a lactococcus lactis starter suspension prediluted at 1% is added to the emulsion. This process takes several hours to complete and is stopped when the desired acidification levels are reached. Structural changes take place in this step; the caseins, now with the new coating, aggregate together to form big clusters. [5] This acidification process is interrupted by a second thermal treatment, 80°C for 43s.

Homogenisation follows[6]. The mixture is pressurised and passed through a thin aperture. This has two main consequences; the emulsion is mixed homogeneously and the big structures are broken down. The fat is distributed as small fat droplets, to which the native whey proteins and protein aggregate adsorb to[7, 8]. Native whey protein are responsible for the stabilisation of surface tension, whilst the aggregate is liable for linking these droplets into structures. [3, 9, 10]

The cream cheese is then packaged and ready for consumption.

2 The Model

The complexity of the system arises from the application of a series of unit operations with a wide range of controls. Furthermore, experimental data is quite limited in terms of analysable variables; texture, concentrations and size distributions are possibly the few quantifiable qualities of the product. With this in mind a geometric model in finite volume was considered. The defining characteristics of the process (temperature, pressure and acidity) as well as component concentrations are tweaked at will, so they are taken as inputs to the model.
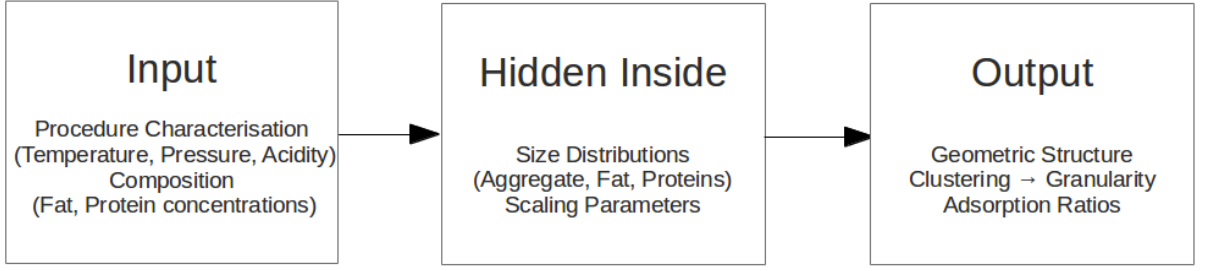
Figure 2: The data flow of the model.

2.1 Fat Droplets

It is possible to visualise the fat droplets using a Confocal Laser Scanning Microscope (CLSM). [9] Analysis of the diameter distribution of the fat droplets' diameter showed a lognormal distribution fitted the data best. The fitting was done by minimising the squares (done in Matlab and the file is provided).
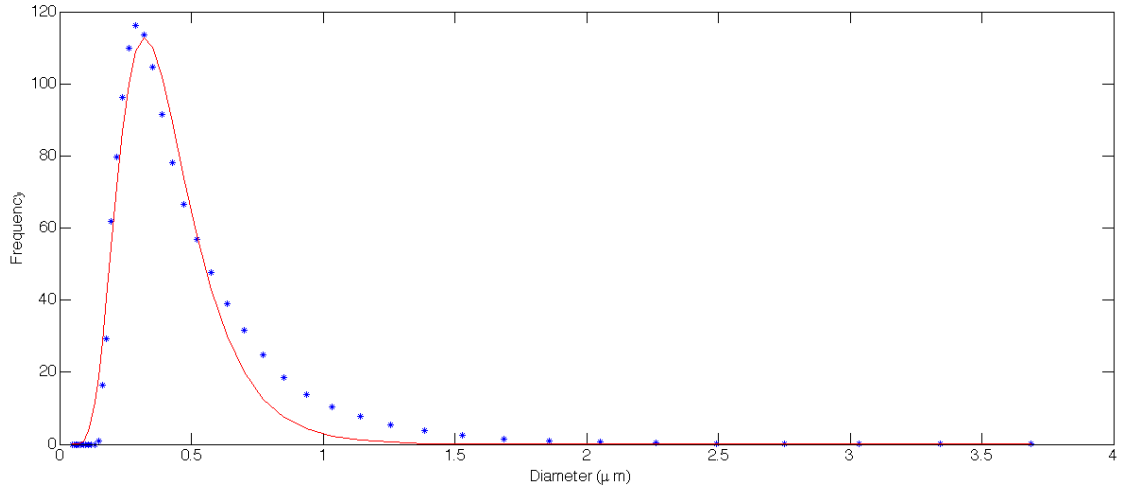

Figure 3: Fitting a Normal and a Lognormal distribution to the data of milk gels.

It is characterised by random variables whose natural logarithm is normally distributed, $X \sim \ln \mathcal{N}(\mu, \sigma^2)$, and the Probability Density Function (PDF): [11]

$$\frac{1}{x\sqrt{2\pi\sigma^2}} exp\left(-\frac{1}{2}\left(\frac{lnx - \mu}{\sigma}\right)^2\right) \tag{1}$$

Sometimes the data is presented, not with a distribution of points, but by the mean and the variance. It is possible to relate between them.

$$mean = exp\left(\mu + \frac{\sigma^2}{2}\right) \tag{2}$$

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$$variance = \left(exp\left(\sigma^2\right) - 1\right) exp\left(2\mu + \sigma^2\right) \tag{3}$$

So to generate the diameter of the fat globules a Box-Muller method was used. [12] A set of uniformly distributed points is generated in a unitary circle, (y_1, y_2); after a Box-Muller transform is done to obtain two normally distributed (μ, σ^2) random variables (X_1, X_2):

$$X_1 = \sigma y_1 \sqrt{\frac{-2ln\left(y_1^2 + y_2^2\right)}{y_1^2 + y_2^2}} + \mu \tag{4}$$

$$X_2 = \sigma y_2 \sqrt{\frac{-2ln\left(y_1^2 + y_2^2\right)}{y_1^2 + y_2^2}} + \mu \tag{5}$$

To obtain the lognormal distribution the exponential of such random values was calculated. This method was chosen as it generates the random variables very quickly. Given the radii, we are now able to place and fix the fat droplets within a constrained volume.

Pressure (bar)	Temperature (^oC)	ph	μ	σ
0	94	5.2	-1.0231	0.6921
50	94	5.2	-1.4452	0.8523
200	94	5.2	-1.0766	0.4683
600	94	5.2	-2.0830	0.5958
0	72	4.9	-0.8492	0.7884
50	72	4.9	-0.6647	0.4414
200	72	4.9	-0.9574	0.4158
600	72	4.9	-2.1669	0.5434
0	72	5.2	-1.5546	0.8583
50	72	5.2	-1.8204	0.0020
200	72	5.2	-1.9833	0.6591
600	72	5.2	-2.2132	0.5114
0	94	4.9	-1.0424	0.7076
50	94	4.9	-0.7554	0.5261
200	94	4.9	-1.5601	0.7812
600	94	4.9	-2.2225	0.5052

Table 1: Lognormal fit to the fat droplet diameter; obtained for trials 56 and 57

2.2 Adsorption

Of great importance to the model is the adsorption of the aggregate and native whey proteins to the fat globules. This is a very fast process in very small scales, so it is not possible to visualise the underlying mechanics nor the size distributions of the particles involved, so they will be taken as having constant radii; aggregate 65nm and native whey protein 1.5nm. This difference in the size of the particles implies the two particles will need to be treated differently.

Aggregate particles are larger, hence much less numerous, hence it is possible to store more information about such particles. For our model, the place of adsorption within the fat globule for each protein aggregate is stored. Adsorption of such particles happens as such: a random place of a random droplet is chosen, then if there is enough area for the aggregate on the surface and there is no overlap between aggregates there is adsorption. As adsorption takes place, the aggregate expands instantaneously on the surface, expansion scaled by $k_{saggregate}$.

Native whey proteins are more numerous, hence the same process is not viable. Adsorption of these proteins only takes place if, on a random droplet, there is enough area. No exact place is considered. As before a variable is introduced in order to allow for these particles to expand on the surface k_{sNwp}.

Physically this makes sense. The larger and more massive aggregate particles once adsorbed are not subjected to an interaction strong enough that allows for their motion on the surface. However, the native whey proteins can be pushed around by the aggregate, so they will fill up the empty space left by the aggregate; no interaction is strong enough to remove particles from the surface.

Two other parameters are considered. The adsorption of each particles does not necessarily take place at the same rate for each particles; the rate of attempted adsorption is quatified by $fNwp$ (native whey proteins to aggregate proteins). The second parameter is a scaling of the actual surface area of the droplets; the radii are multiplied by a constant $k_{surface}$.

These parameters are introduced to the model as experts have pointed out that the competition between aggregate and native whey proteins for adsorption is very important. This implies the ratio between the particles in the fat droplet should not be the same as the ratio in the initial solution; the small scales of the particles involved make it very difficult for empirical analysis of this underlying competition. Another likely phenomenon that takes place is the overlap of two particles; indeed it feasible that the adsorbed native whey proteins coat the lipid droplet with a shell that is a few particles deep.

2.3 Linking

The fat globules are only allowed to link by connections of aggregate, the native whey proteins take no part in binding the structure. Introduce a constant k_{link} which scales the diameter into the maximum range of interaction; a value in this range is chosen uniformly and then all the possibilities of linkage are checked for that specific adsorbed aggregate. Final state of the model is represented below.

So, this model returns the exact position of both the lipid droplets and the protein aggregates; the number of adsorbed native whey proteins per droplet is also known. Via linking of the droplets by the aggregate the connected geometric structure is fully determined.
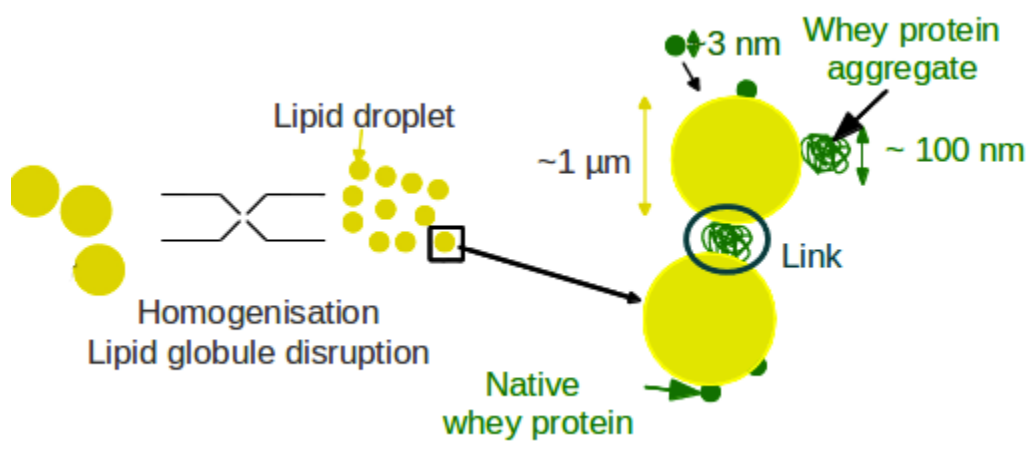
Figure 4: Schematic diagram of the homogenistation and of the adsorption of both native whey protein and aggregate to the fat globules.

3   Results

Aiming to describe the structure of cream cheese, rheological data was provided. It is the intent of this model to link the micro-structure to the consistency, observed in larger scale. So, the following behaviour was obtained:
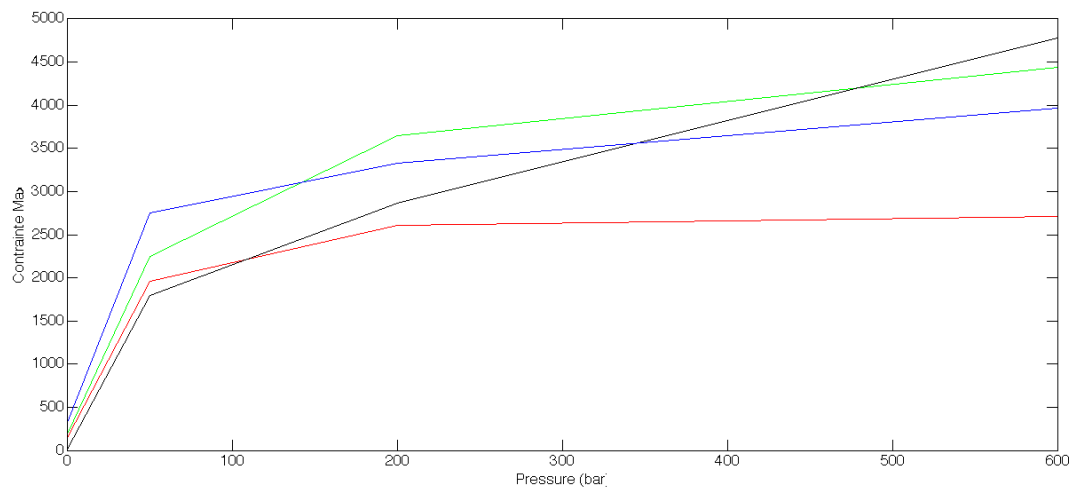

Figure 5: Rheological data provided by experiments. The red line is the data relates to the $94^{o}C$ and ph 5.2, the green line $72^{o}C$ and ph 4.9, the black line $72^{o}C$ and ph 5.2 and finally the blue line $94^{o}C$ and ph 4.9.

The following data was modelled for a $6.4 \times 10^{11} nm^3$ volume; for each data point presented 20 trials were made, with the exception of the case of 600 bars, where only to runs were made (on average the fat droplet size is smaller and the run time is significantly larger). The lipid mass percentage was 35.9%, of the proteins 88% were casein, the fat globule size was truncated between $0.025\mu m$ and $7.5\mu m$. The denaturation rate was determined experimentally.

Pressure (bar)	Temperature(^oC)	ph	Denaturation rate (%)
0	94	5.2	59.57
50	94	5.2	62.39
200	94	5.2	70.85
600	94	5.2	74.61
0	72	4.9	19.13
50	72	4.9	25.71
200	72	4.9	49.22
600	72	4.9	68.97
0	72	5.2	19.13
50	72	5.2	25.71
200	72	5.2	49.22
600	72	5.2	68.97
0	94	4.9	59.57
50	94	4.9	62.39
200	94	4.9	70.85
600	94	4.9	74.61

Table 2: Denaturation rate obtained experimentally. Note that it increases with temperature. It also increases with pressure, which can be explained by the relationship between pressure and temperature; if the pressure increases so will the temperature.

So, a first approach to analysing the structure is to look at the number of links; there should be a relationship between the linking cohesion and rheology.
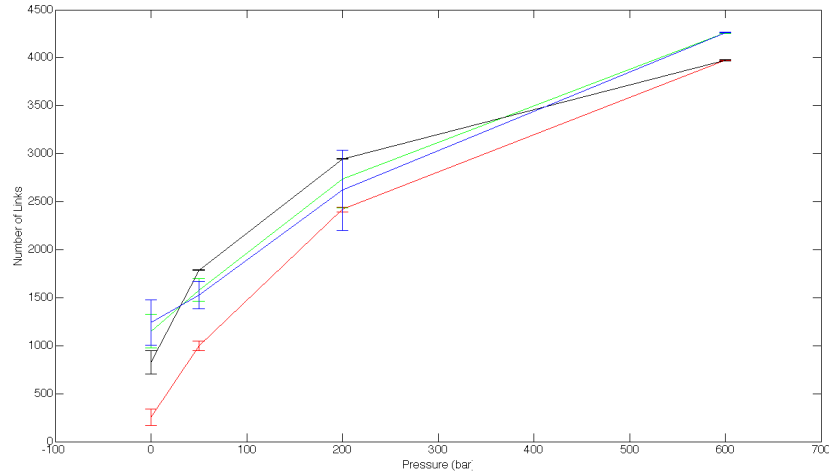

Figure 6: Modelled data. The red line corresponds to experimetal temperature 94^oC and ph 5.2, the green line 72^oC and ph 4.9, the black line 72^oC and ph 5.2 and finally the blue line 94^oC and ph 4.9. The k_{link} was set to 5, and the rest of the parameters were set to 1 ($fNwp$, $k_{surface}$, $k_{saggregate}$ and k_{sNwp})

Further analysis was done on the unknown parameters. The first one considered was k_{link}. Changing this parameter changes the range that the aggregate proteins can stretch to for links.
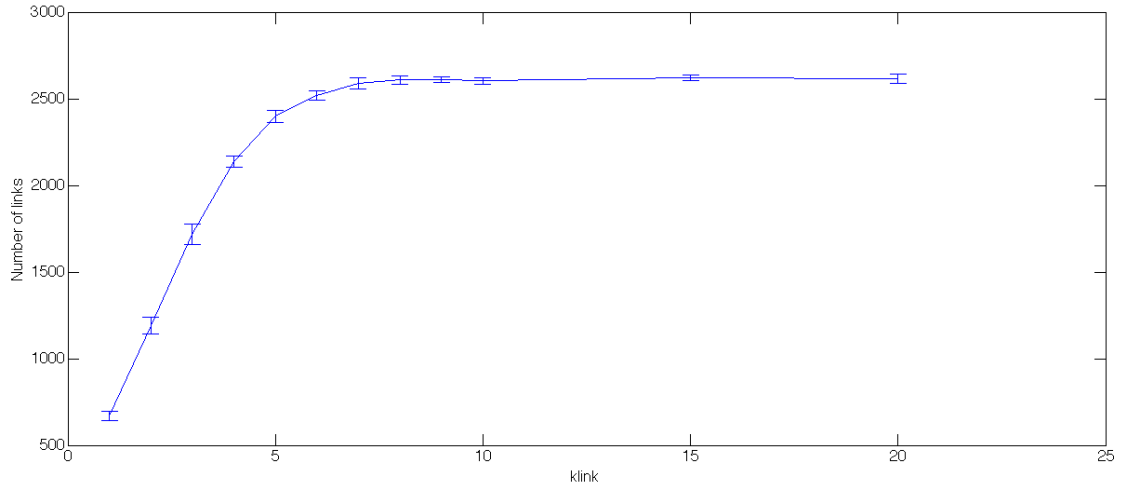
Figure 7: Modelled data for a varying k_{link}. The droplets correspond to the experimental temperature 72^oC, pressure of 200 bars and ph 4.9, and the rest of the parameters were set to 1 ($fNwp$, $k_{surface}$, $k_{saggregate}$ and k_{sNwp})

After the $k_{saggregate}$ and k_{sNwp} parameters were altered; these should increase the occupied area by each particle and hence limit the number of adsorbed particles when adsorbed.
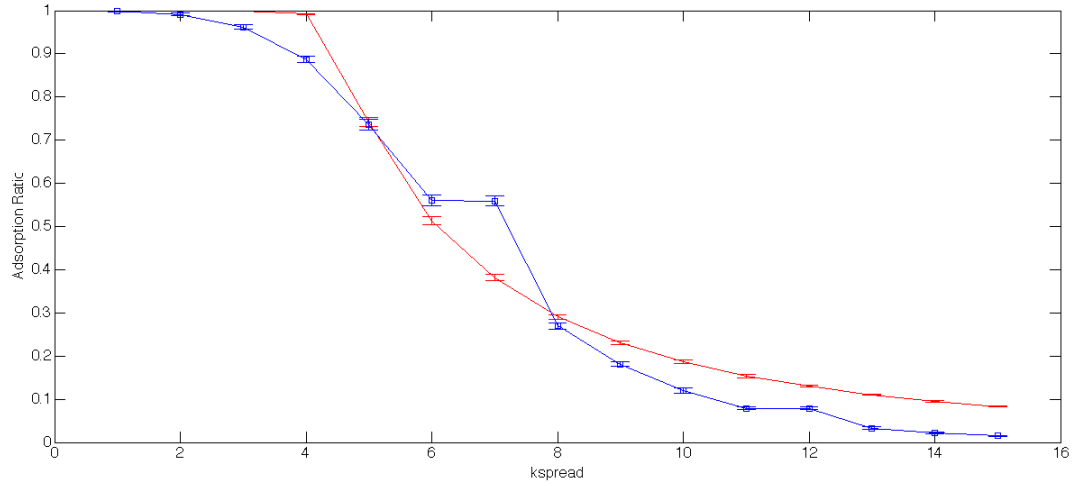

Figure 8: Modelled data for a varying $k_{saggregate}$ and k_{sNwp}; the red line is for the native whey proteins and the blue line for the aggregate. The adsorption ratio is the number of adsorbed particles divided by the total number of particles of a given kind. The droplets correspond to the experimental temperature 72^oC, pressure of 200 bars and ph 4.9, k_{link} was set to 5 and the rest of the parameters were set to 1 ($fNwp$ and $k_{surface}$)

Finally the $fNwp$ parameter was varied. Logarithmic x-axis was chosen so there would be some symmetry around 0.
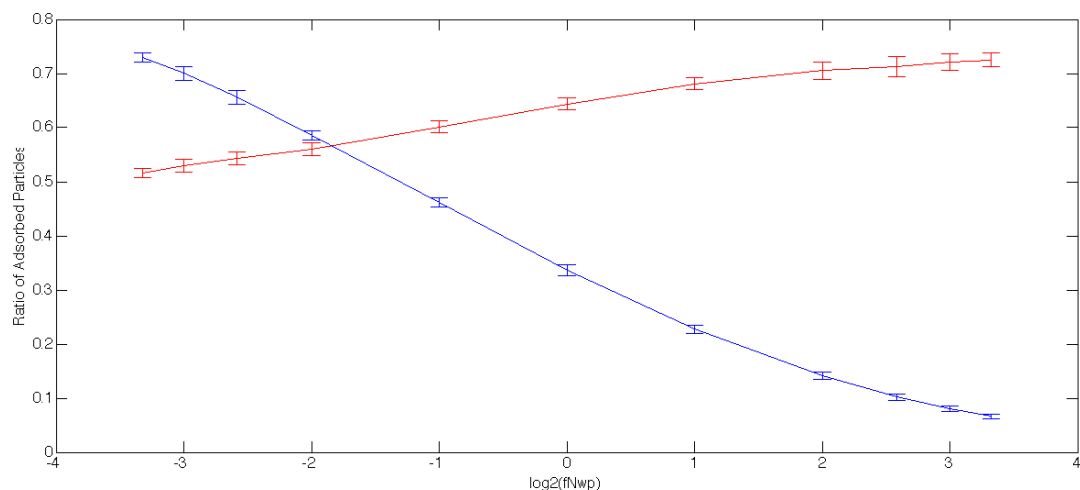
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Figure 9: Modelled data for a varying $fnwp$; the red line is for the native whey proteins and the blue line for the aggregate. The adsorption ratio is the number of adsorbed particles divided by the total number of particles of a given kind. The droplets correspond to the experimental temperature 72^oC, pressure of 200 bars and ph 4.9, k_{link}, $k_{saggregate}$ and k_{sNwp}) were set to 5 and the $k_{surface}$ was set to 1.

4 Conclusion

Looking at the fitting of the fat droplet distribution, the d_{32} is smaller than what is expected. When talking with Julie it was suggested that the procedure is not fully calibrated; this means there is a shift in the fat droplet sizes. To be able to shift the distribution scale another parameter was introduced, k_{d32}; the fitted pdf is multiplied by this constant, mitigating the intrinsic shift.

Generating the fat droplet sizes from a lognormal distribution is very fast and allows there to be a stronger relationship between the experiments and the model; modelling homogenisation within the system and maintaining a dependence upon the experimental conditions (pressure and temperature). There is no clear relation between the parameters and the conditions, so at the moment they need to be fitted every time, however with more data one can hope to attain the μ and σ parameters simply by having the temperature and pressure.

The higher the pressure the more linked the structure is, figure 6; analysis has shown two main reasons for this. Firstly, as one increases the pressure, the temperature will rise accordingly, there will be a larger denaturation rate; this means there is more glue for the system to bind together. Secondly, higher pressure yield smaller fat droplets; this leads to an increase in the likelihood of a give adsorbed protein aggregate, hence more linking on average. This ties in with was is observed empirically, figure 5, even though total number of links is a naive quantification to the texture.

A change in the k_{link} parameter alters the cohesion of the cream cheese, figure 7; this should be intuitive as a higher value makes adsorbed protein aggregates reach a bigger range of possible links. A plateau is reached close to a k_{link} of 8, where most of the

aggregate is now linking. Actual ranges of link has not been obtained experimentally, so it is not easy to choose an adequate value for the parameter.

The following two figures, 8 and 9, address the competition between the two particles. Indeed, on figure 8 as the area occupied by each particle increases, $k_{saggregate}$ and k_{sNwp}), a threshold is reached, where the fat droplets no longer have available area; from that threshold onward the competition matters, as some particles will be left in the solution. The by changing $fnWp$ competition can be imposed, as seen in figure 9. By increasing the occupied surfaces above the threshold, not every particle will be able to adsorb, which is what is observed computationally.

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