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ABSTRACT SUBMISSION TEMPLATE

Title (Calibri 12 font)

Modeling competition phenomena in a dairy oil-in-water emulsion using hybrid kinetic Monte Carlo simulations

Authors & Affiliations (Calibri 10 font, using the below layout)

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Introduction

The design of models for dairy products raises a series of difficult issues. For instance, considering dairy oil in water emulsions stabilized with milk proteins, texture depends in a non-trivial manner on the initial concentration and type of proteins, nature of heat treatment and type of homogenisation. Those emulsions, involving competitive adsorption of mixed particles in a turbulent way at the oil/water interface, are not thermodynamically controlled. Classical models like the Langmuir one are thus not able to predict its behaviour with precision (Dickinson, 2011). Hybrid models (Descamps, 2014) have been recently proved to be promising for dealing with those complex phenomena. We present an extension of this approach, using an individual-based framework whose implementation is based on a kinetic Monte Carlo approach (MC) combined with a mean field model. MC schemes are widely used in chemical science to deal with discrete events (Gillespie, 75). Individual-based models (also known as agent-based) are convenient for representing local rules at the nano/micro scale, with macroscopic properties appearing as a consequence of an emergence process. Individual-based frames, however, often rely on stochastic simulations and require time-consuming computations to yield a robust estimation for the emergent quantities. In the proposed methodology, computational efficiency is provided by performing appropriate simplifications along the simulation process thanks to an ODE-based continuous mean field formulation.

Materials & methods

The considered system is a continuous phase made of a mixture of milk proteins, caseins and native whey proteins, dissolved in permeate, and a dispersed phase made of saturated lipids: anhydrous milk fat heated to become liquid. The emulsion is then obtained by homogenization. In order to evaluate the impact of the initial conditions, heating temperatures of the protein solution and homogenisation process on the structure and texture of the emulsion, experiments were carried out with various initial conditions yielding two databases (Surel, 2014), used as learning and test set, respectively. The following measurements were collected to characterise the emulsions at a micro/nano-scale: diameters and size distribution of lipid droplets (d32, d43), of whey protein aggregates, interfacial concentration and percentage of adsorbed caseins.

Modeling

The hybrid model has been designed to represent concurrent complex phenomena: on one hand the competition between adsorption and coalescence, and on the other hand, the competition at the lipid droplet interface between several protein-based surfactants, with different sizes and properties. Physical laws are inspired from a model developed by (Håkansson, 2013) using ODE to simulate a continuous size distribution.

The flowchart of the proposed model is presented in figure 1. The individual-based system is represented as follows: Each droplet is an individual, immersed in a common volume that contains all particles. Four events can occur, shared into two categories, discrete or continuous. The adsorption of native whey proteins is considered as a continuous process governed by a set of differential equations, while coalescence of two droplets, whey protein aggregates and casein micelles adsorption are considered as discrete events. The selection of one of these three latter events is

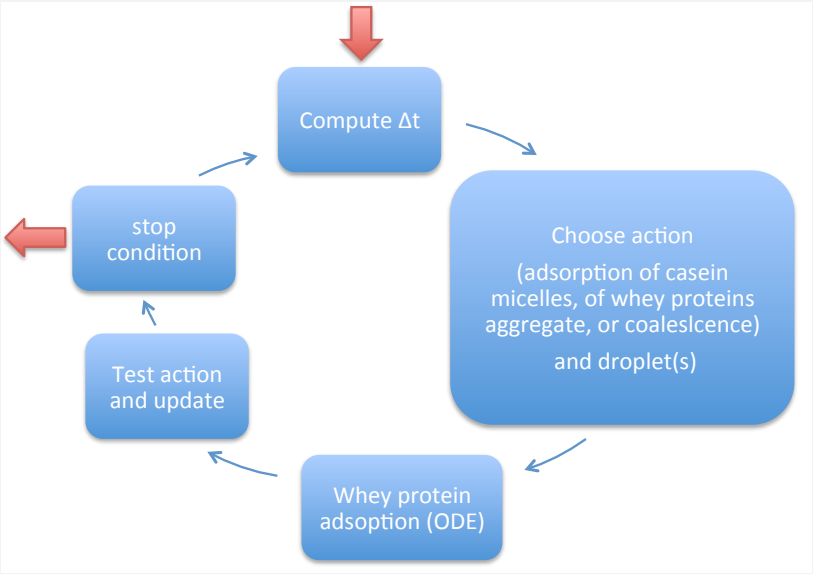

Fig 1. Flowchart of the simulation algorithm

stochastic and depends on physical parameters described in the literature.

The simulation loop first computes a Δt corresponding to the expected time of the next action of the system knowing the various kernels of the discrete events in competition. An action is then chosen, the continuous whey proteins adsorption process is simulated for the duration Δt, before updating. This process is repeated until the system stabilises (stop condition).

Results & discussions

An experimental analysis of this model shows that it is versatile enough to predict the composition of the interface of a homogenized oil-in-water emulsion in various conditions, approaching real-world measurements (figure 2). Experiments are conducted with a system initialised with 10^5 to 10^6 droplets, to get 10^2 to 10^3 droplets after coalescence, and having between 10^3 and 10^4 aggregates and casein micelles, and up to 10^8 native whey proteins. Thanks to a convenient algorithmic structure for combining the three components (continuous ODE, event-driven MC simulation, individual-based approach) simulations of the model remain computationally affordable, in particular for learning unknown parameters on experimental data. This latter step is formulated as an inverse problem, and solved using an evolutionary optimisation algorithm that requires a large number of simulations.

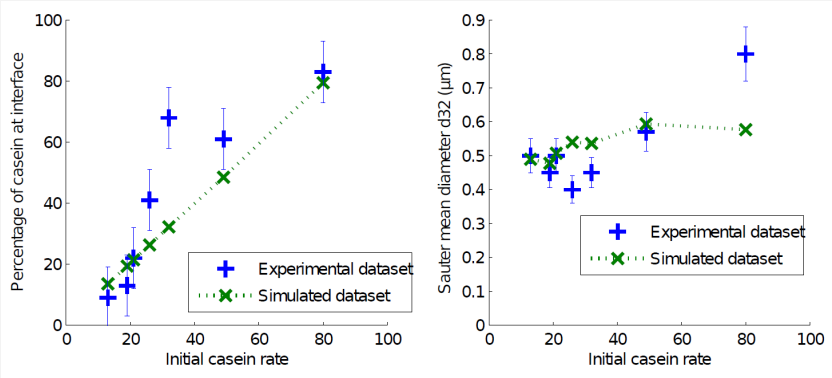

Figure 2 Simulation results versus experimental data for the protein solution heated at 80°C (See (Surel, 2014) for details about experimental conditions).

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