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COUPLING FLUID FLOW, HEAT TRANSFER, AND DENATURATION-AGGREGATION OF BETA-LACTOGLOBULIN:

RELATIVE IMPORTANCE OF PERIKINETIC AND ORTHOKINETIC TERMS OF THE AGGREGATION KERNEL

Artemio Plana-Fattori[1,2,3 #], Nicolas Erabit[4], Graciela Alvarez[4], Denis Flick[1,2,3]

1 – AgroParisTech, UMR1145 Ingénierie Procédés Aliments, F-91300 Massy, France

2 – INRA, UMR1145 Ingénierie Procédés Aliments, F-91300 Massy, France

3 – Le Cnam, UMR1145 Ingénierie Procédés Aliments, F-91300 Massy, France

4 – IRSTEA, F-92761 Antony, France

e-mail: artemio.planafattori@agroparistech.fr, nicolas.erabit@irstea.fr , denis.flick@agroparistech.fr

corresponding author address: Artemio Plana Fattori, AgroParisTech – MMIP, 16 rue Claude Bernard, 75231 Paris CEDEX 5, France

ABSTRACT

Modeling of thermal denaturation-aggregation of whey proteins can provide assistance in developing dairy products as well as in understanding the mechanisms which drive the formation of fouling deposits. Aggregation of whey proteins depends on temperature (perikinetic contribution, due to Brownian motion) and shear (orthokinetic contribution). Under realistic conditions, different temperature and shear histories are associated with fluid parcels which progress more or less quickly, far or close to the heating wall, inside the processing unit. A numerical approach is proposed for evaluating the thermal denaturation-aggregation of whey proteins, combining computational fluid dynamics and the population balance equation. Fluid flow and heat transfer are solved through the finite-element-method in the Eulerian frame, while product transformation is evaluated along representative Lagrangian trajectories. Therefore, no assumptions are performed regarding dynamical and thermal histories. The approach is illustrated by the evolution of a suspension of beta-lactoglobulin, along the first section of a tubular heating exchanger (length 0.4 m, radius 0.004 m, flow rate 20 L/h, inward heat flux 13500 W/m²); at its inlet, the suspension contains 6 % of beta-lactoglobulin at 60 °C. Particle breakage is avoided (shear rate values below 125 s⁻¹). Simulations are performed with and without the orthokinetic term of the aggregation kernel. Results put in evidence that the perikinetic and orthokinetic terms exhibit dominant role for particles sizes below and above about 1 µm, respectively.

PROBLEM

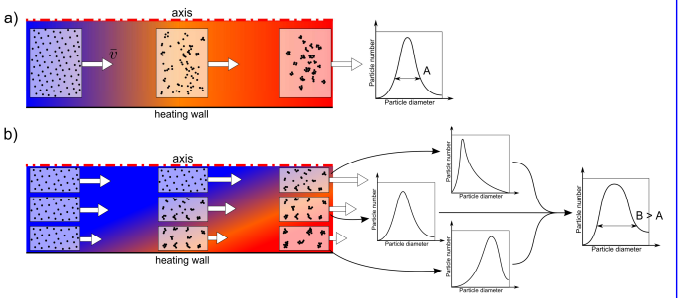


FIGURE 1. Evolution of a suspension of beta-lactoglobulin under continuous heat treatment: a) simple 1D approach; b) coupled 2D approach (from Chantoiseau *et al.*, *Journal of Food Engineering*, in press).

APPROACH

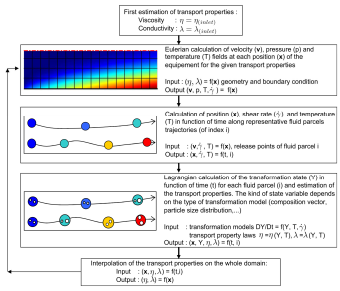


FIGURE 2. Schematic diagram of the Eulerian-Lagrangian approach for coupling of fluid flow, heat transfer and liquid food product transformation.

METHODS

▪ Eulerian mesh (fluid flow and heat transfer): 80 rectangles along the domain's radius and 800 rectangles along the length

▪ Lagrangian sampling (product transformation): 80 trajectories with 8000 positions each; release positions are uniformly distributed along the domain inlet

▪ relative viscosity as a function of the volume fraction that is occupied by the particles (Φ) – We retained the model proposed by Thomas (1966, *Journal of Colloid Science*, 20: 267-277):

$$\frac{\eta}{\eta_w} = \eta_R = 1 + 2.5\,\Phi + 10.05\,\Phi^2 + 0.00273\,\exp(16.6\,\Phi)$$

▪ particle aggregation – The evolution of the number of particles containing k monomers (N_k) is expressed as:

$$\frac{dN_1\{t\}}{dt} = k_{LS}\,C_{sat}^{LS}\{t\}\,N_A - N_1\{t\}\sum_{i=1}^{M} Q_{1,i}\,N_i\{t\}$$

$$\frac{dN_k\{t\}}{dt} = \frac{1}{2}\sum_{i=1}^{k-1} Q_{k-i,i}\,N_i\{t\}N_{k-i}\{t\} - N_k\{t\}\sum_{i=1}^{M} Q_{k,i}\,N_i\{t\}$$

in the cases $k = 1$ and $k > 1$, respectively, where $N_i\{t\}$ is the number of unfolded monomers at time t, M the maximum number of monomers in an aggregate and N_A the Avogadro number.

▪ particle aggregation – The kernel of aggregation $Q_{k,l}$ depends on the local temperature, on the continuous phase viscosity (η_w), on the shear rate ($\dot{\gamma}$), and finally on the radii a_k and a_l of the aggregates under consideration:

$$Q_{k,l} = \frac{2}{3}\frac{k_B}{W}\frac{T}{\eta_w}\frac{(a_k + a_l)^2}{a_k\,a_l} + \frac{4}{3}\frac{\dot{\gamma}}{W}(a_k + a_l)^3$$

where k_B is the Boltzmann constant and W the Fuchs stability factor. Fuchs stability factors were identified for this specific model fluid.

▪ model fluid – solution with 6% of purified β-lactoglobulin powder rehydrated at 40°C with addition of 5 mM of calcium chloride

▪ unfolding of the monomers –The proportion α of unfolded monomers is defined by :

$$\ln \alpha = c_\alpha \left[\frac{1}{T_{trans}} - \frac{1}{T}\right]$$

where c_α is the unfolding coefficient and T_{trans} the temperature of transition between unfolding-limiting area and aggregation-limiting area

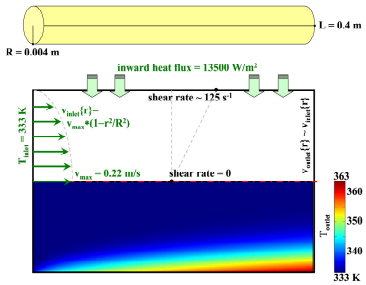


FIGURE 3. Schematic view of the computational domain under consideration, where the dotted red line indicates the axis of symmetry of the cylindrical section. **Boundary conditions (green symbols) and relevant values are indicated in the upper part.** The velocity field at the domain outlet is quite similar to that at the inlet because the relatively weak degree of transformation of the liquid food product. The resulting temperature field is displayed in the lower part (see color bar).

RESULTS

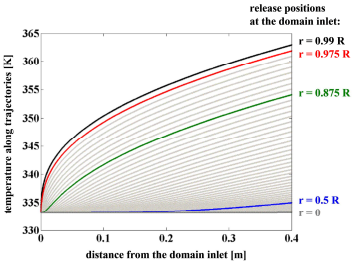


FIGURE 4. Temperature evolution from the domain inlet (z = 0) to the outlet (z = 0.4 m) along selected trajectories. The latter are indicated by their release position at the domain inlet: r = 0, 0.5*R, 0.875*R, 0.975*R and 0.99*R. Because the (relatively) weak degree of the product transformation and corresponding influence on the suspension viscosity, the trajectories (not shown) are roughly parallel to each other.

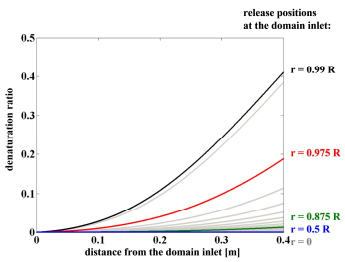


FIGURE 5. As in FIGURE 4, but displaying the denaturation ratio. At a given position of the computational domain, such a ratio can be evaluated as the number of unfolded monomers (aggregated or not), divided by the number of native (folded) monomers at the domain inlet.

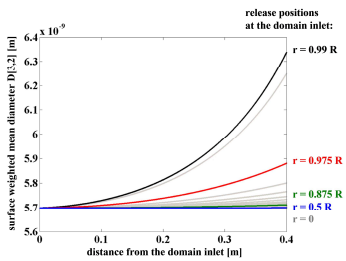


FIGURE 6. As in FIGURE 4, but displaying the surface weighted mean diameter associated with the whole particle size distribution (D[3,2]), also known as Sauter diameter.

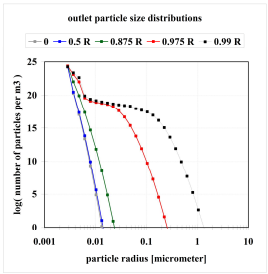


FIGURE 7. Outlet particle size distribution associated with the trajectories followed by fluid parcels released at the positions r = 0, 0.5*R, 0.875*R, 0.975*R and 0.99*R at the domain inlet.

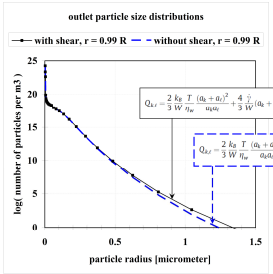


FIGURE 8. Outlet particle size distribution associated with the trajectory followed by fluid parcels released at the position 0.99*R at the domain inlet, as in FIGURE 7 (black symbols) and after neglecting the role played by the shear rate in the aggregation kernel (dotted blue line) (see boxes).

CONCLUSIONS

- A realistic population balance model can be used to estimate the aggregation of whey proteins, after splitting the fluid flow and heat transfer from the determination of the degree of transformation associated with the liquid food product.
- Our approach puts in evidence the diversity of the output product properties depending on the time, temperature, and shear rate histories of different flow parts.
- Aggregation of whey proteins is driven by the Brownian motion for particles smaller than 1 µm, whereas the contribution due to the shear rate is progressively important for larger sizes.