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# A coupled numerical model for studying the thermal denaturation-aggregation of whey proteins

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**SCOPE**

When modeling the thermal denaturation-aggregation of whey proteins under continuous flow, a two-way dependence has to be considered. Firstly, fluid flow and heat transfer drive shear rate and temperature fields, which affect the product transformation. Secondly, the own transformation can modify the product properties (as its apparent viscosity). Inside a heat exchanger, the progressive occurrence of larger protein aggregates increases the product viscosity, slowing down the fluid parcels near heating walls and hence exposing them to additional heating and consequent transformation.

In this study we demonstrate the feasibility of modeling the thermal denaturation-aggregation of whey proteins under continuous flow through numerical simulations...

>>> by developing a computational fluid dynamics (CFD) model for solving the coupled problem of fluid flow, heat transfer, and thermal denaturation-aggregation of whey proteins, where the latter is represented with the help of a reaction kinetics of order 1.5; and

>>> by representing a laboratory processing unit (heater, holder and cooler) that effectively exists, with the help of a sequence of computational domains.

**METHODS (1): COMPUTATIONAL FLUID DYNAMICS**

Conservation equations for the liquid food product mass, momentum and energy are expressed as:

$$\nabla \cdot \mathbf{u} = 0 \quad \rho (\mathbf{u} \cdot \nabla) \mathbf{u} = \nabla \cdot (-p \mathbf{I} + \eta (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)) \quad \rho C_p (\mathbf{u} \cdot \nabla) T = \nabla \cdot (k \nabla T)$$

In the case of the concentration of native proteins, the following convection-diffusion equation is employed:

$$(\mathbf{u} \cdot \nabla) C_{nat} = dC_{nat} \{t\} / dt + \nabla \cdot (D \nabla C_{nat})$$

Coupled phenomena are solved for a sequence of two-dimensional axial-symmetric computational domains. They represent eight heating sections, a holder, and eight cooling sections. Computational domains have a radius of 4 mm, as in the experimental setup; their lengths were estimated from the actual volumes: about 0.4 m for heating and cooling sections and about 4 m for the holding section. Regular grids constituted of rectangular cells are employed.

At the inlet of the first heating section, a fully developed parabolic flow profile is assumed. Flow rate is 18.1 L/h, and mean velocity is about 0.100 m/s; Reynolds number is about 150. At the inlet of all the other (heating, holding and cooling) sections, uniform velocity profile is assumed.

**METHODS (2): KINETIC PARAMETERS**

A reaction kinetics of order 1.5 is assumed in representing the thermal unfolding and particle aggregation of the  $\beta$ -lacto-globulin present in the liquid food product of interest. Kinetic parameters were estimated after reconstructing the bulk thermal history of the liquid product. Such a history was based upon measurements of the product temperature at the exchangers' inlet and outlet. Three heat treatments were considered.

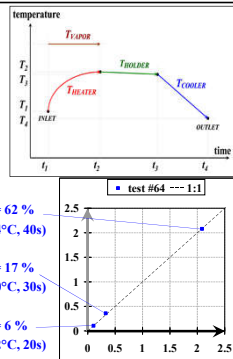
The integration over time along the exchangers gives:

$$\frac{dC_{nat} \{t\}}{dt} = -k_n C_{nat}^{1.5} \{t\}, \quad k_n = k_0 \exp\left(-\frac{E_A}{RT} \{t\}\right)$$

where  $\delta = 1 - C_{nat} \{t_{OUTLET}\} / C_0$  is the denaturation ratio.

$$2C_0^{0.5} (1 - (1 - \delta)^{0.5}) = -k_0 \int_{t_{inlet}}^{t_{outlet}} \exp\left(-\frac{E_A}{RT} \{t\}\right) dt$$

We obtained  $k_0 = 2.51 \times 10^{15}$  and  $E_A = 1.18 \times 10^5$  J/mol.



**METHODS (3): APPARENT VISCOSITY**

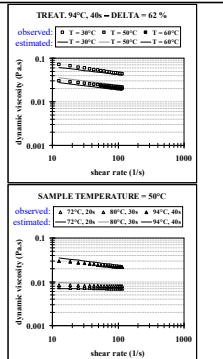
The liquid food product under consideration becomes progressively shear-thinning with the transformation. After a given heat treatment, apparent viscosity decreases with the temperature (upper figure). At a given temperature, apparent viscosity increases with the denaturation ratio (lower figure).

The influence of shear rate  $\dot{\gamma}$ , denaturation ratio  $\delta$  and temperature T on the apparent viscosity  $\eta$  associated with the liquid food product is represented as:

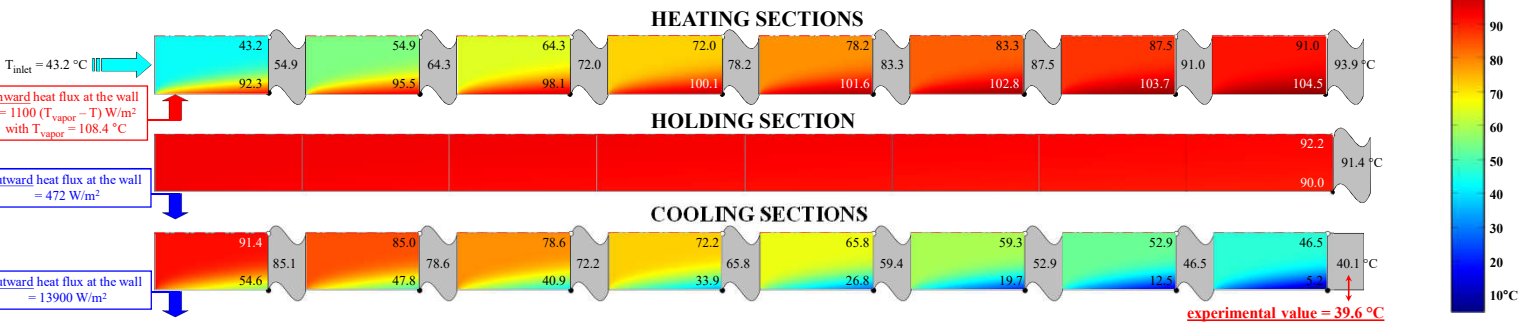
$$\eta(\dot{\gamma}, \delta, T) = A \dot{\gamma}^B \delta^C \exp(C / (RT)) \exp(D \delta)$$

Parameters A, B, C and D were estimated through the least squares method from measurements conducted at 30, 50, and 60°C, taking into account the liquid product transformed according to three heat treatments (72°C during 20s; 80°C during 30s; and 94°C during 40s).

We obtained  $A = 1.39 \cdot 10^{-6}$ ,  $B = -0.298$ ,  $C = 2.24 \cdot 10^4$  and  $D = 3.64$ .

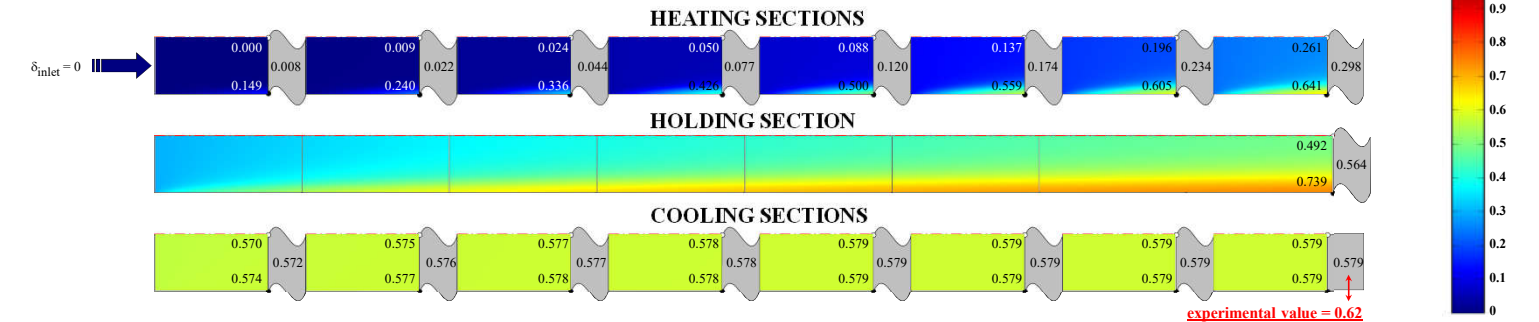


**TEMPERATURE**



Bulk values (T and  $\delta$ ) are evaluated at the outlet of each domain; they are later assumed as boundary conditions at the inlet of the following domain. Such an approach help us to represent the occurrence of mixing along the corners which connect two successive sections.

**DENATURATION RATIO**



**SUMMARY**

The model represents the evolution of the liquid food product along the exchangers; the radial distribution of temperature and denaturation ratio is put in evidence. The model reproduces reasonably well the bulk values of temperature and denaturation ratio at the cooler outlet when we assume the operating conditions under which the kinetic parameters and the viscosity approximation parameters were estimated. Consistent results have been obtained under other operating conditions of interest.

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