DEVELOPING A CFD MODEL FOR STUDYING WHEY PROTEIN DENATURATION-AGGREGATION

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SCOPE AND GOALS

▪ The modeling of thermal treatment of a liquid food product under continuous flow is a challenging problem. Fluid flow and heat transfer determine the temperature field, which can influence product transformation; in turn, the transformation can modify the product transport properties (as its viscosity). Such a two-way dependence has to be considered when modeling coupled processes such as thermal denaturation-aggregation of whey proteins.

▪ Our goal is to demonstrate the feasibility of modeling, through numerical simulation, the thermal denaturation-aggregation of whey proteins under continuous flow:

- ▪ 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

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

$$\nabla.\mathbf{u} = 0$$

$$\rho\,(\mathbf{u}.\nabla)\mathbf{u} = \nabla.(-p\,\mathbf{I} + \eta\,(\nabla\mathbf{u} + (\nabla\mathbf{u})^T))$$

$$\rho\,C_p\,(\mathbf{u}.\nabla)T = \nabla.(k\,\nabla T)$$

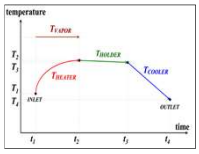
In the case of the concentration of native proteins, the following convection-diffusion equation is employed:

$$(\mathbf{u}.\nabla)C_{nat} = R + \nabla.(D\,\nabla C_{nat})$$

▪ Coupled phenomena are solved for a sequence of two-dimensional axial-symmetric computational domains. They represent eight heating sections, a holder, and a cooling section. 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 each heating section and about 4 m for the holding and cooling sections. Regular grids constituted of rectangular cells are employed for all the domains.

▪ Selected boundary conditions are presented below.

▪ Protein unfolding and particle aggregation are represented with the help of a kinetics of order 1.5. Parameters are estimated after reconstructing the bulk thermal history of the liquid food product.



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

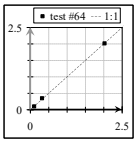
The integration over time along the exchangers gives:

$$\left[2C_0^{-0.5}\left(1-(1-\delta)^{-0.5}\right)\right] = \left[-k_0\int_{t_{INLET}}^{t_{OUTLET}}\exp\left(-E_A/RT\{t\}\right)dt\right]$$

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

treatment	test #64
72°C, 20s	δ = 6 %
80°C, 30s	δ = 17 %
94°C, 40s	δ = 62 %

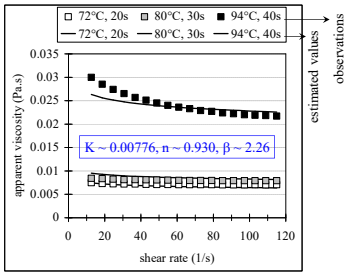
$k_0 \sim 2.51\ 10^{15}$, $E_A \sim 1.18\ 10^5$ J/mol



▪ The influence of shear rate $\dot{\gamma}$ and denaturation ratio δ on the apparent viscosity η associated with the liquid food product was approximated through the expression:

$$\eta = K\,\dot{\gamma}^{\,n-1}\exp(\beta\,\delta)\ .$$

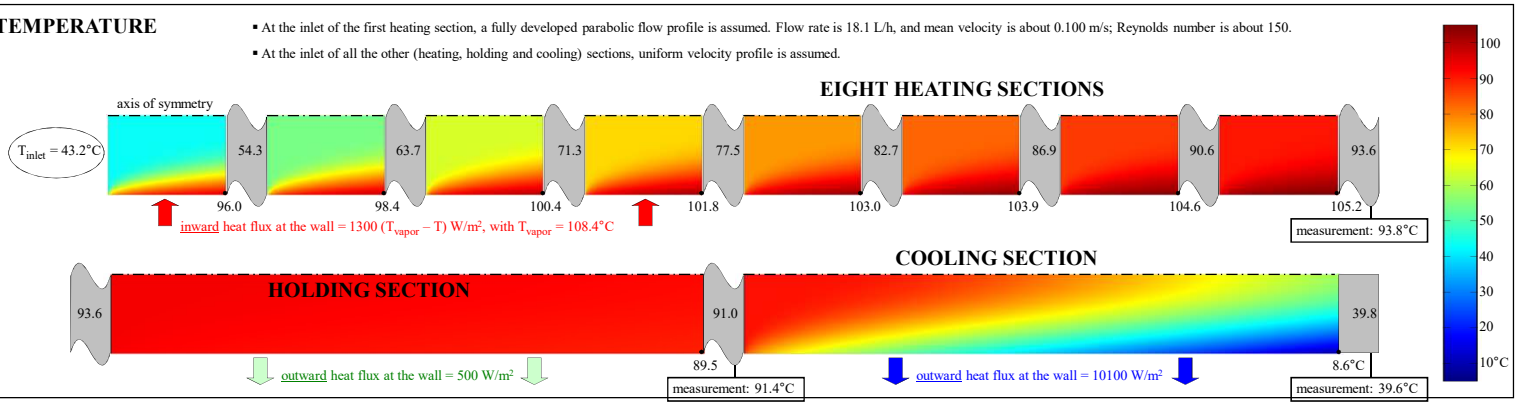
Parameters K, n, and β were estimated through least squares method, from measurements performed at 50°C after three heat treatments of the liquid food product.



TEMPERATURE

▪ 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.

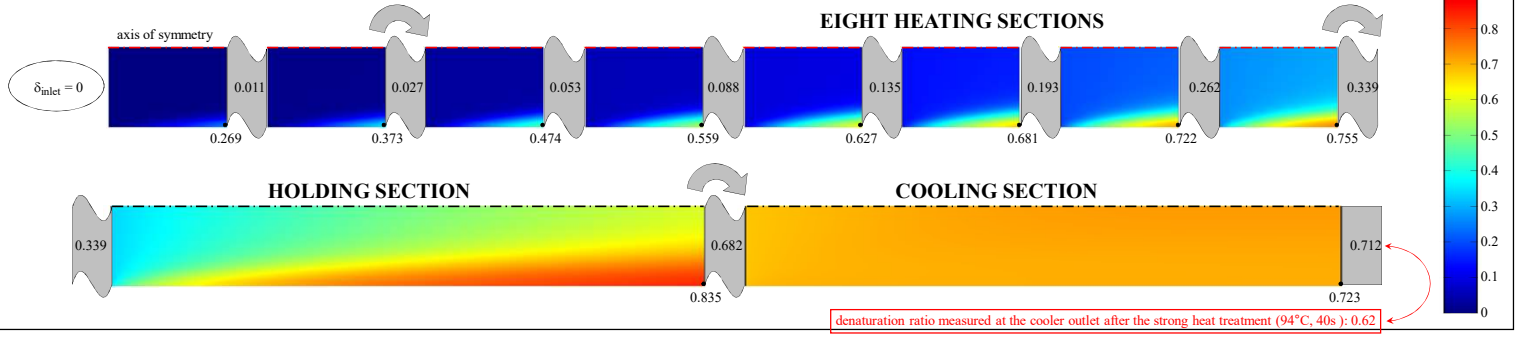
▪ At the inlet of all the other (heating, holding and cooling) sections, uniform velocity profile is assumed.



DENATURATION RATIO

▪ Bulk values of temperature and concentration are evaluated at the outlet of each computational 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.



CONCLUSIONS AND FUTURE WORK

▪ We demonstrate the feasibility of modeling the thermal denaturation-aggregation of whey proteins under continuous flow through numerical simulations. COMSOL Multiphysics was employed, and no reasons forbid the application of other commercial or in-house modeling software.

▪ The development of a CFD model for representing a liquid food product transformation requires reliable information about the product properties (like its viscosity) as well as about the transformation model itself. Satisfying results were obtained in the case of the thermal denaturation-aggregation of whey proteins by assuming a reaction kinetics.

▪ The reconstruction of bulk thermal history experienced by the liquid food product along the experimental setup allowed us to estimate the parameters of a reaction kinetics of order 1.5. Future work may consider an ensemble of test cases under similar operating conditions, in order to improve the robustness of our approach. Efforts remain to be accomplished regarding the influence of the temperature on the apparent viscosity associated with the liquid food product.

▪ Future work has to consider sensitivity tests regarding the influence of key modeling issues, including the mesh resolution.

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