Enzymatic inactivation under high pressure processes:
Models, simulation and mathematical analysis

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Modelos Matemáticos en Ciencia y Tecnología

Introduction

- The demand of **safe and minimally processed food**, prepared for immediate consumption has increased significantly in order to give service to the needs of restaurants, collective dining rooms, domestic consumption, etc.
- One of the technologies that can be used for the processing of food is **high pressure**. These treatments have the great advantage of not being based on the incorporation of additives and they allow to **avoid treatments with high temperatures** which have adverse effects on some **nutritional** and **organoleptic** properties of the food.
- Here we focus on the **modelling** and **simulation** of the effect of the combination of **high pressure** with **thermal treatments** on food, considering the **inactivation** that may take place on certain **enzymes**, as well as on the **stability** of the model.
- Due to the high computational complexity needed for solving the full models, we also consider and study a **simplified version** of them.

Mathematical model for inactivation of enzymes

The evolution of the **activity A of an enzyme** can be described by a first–order kinetic equation of the following type:

$$\frac{dA(t)}{dt} = -\kappa(P(t),T(t))\,A(t), \tag{1}$$

where t is the time (min), $P(t)$ is the pressure (MPa) at time t, $T(t)$ is the temperature (K) at time t and $\kappa(P,T)$ is the **inactivation rate** (min^{-1}). Here $\kappa(P,T)$ is chosen, depending on the considered enzyme, among the following expressions:

1-

$$\kappa(P,T) = \kappa_{\text{r}} \exp\left(-B\left(\frac{1}{T}-\frac{1}{T_{\text{r}}}\right)\right)\exp\Big(-C(P-P_{\text{r}})\Big),$$

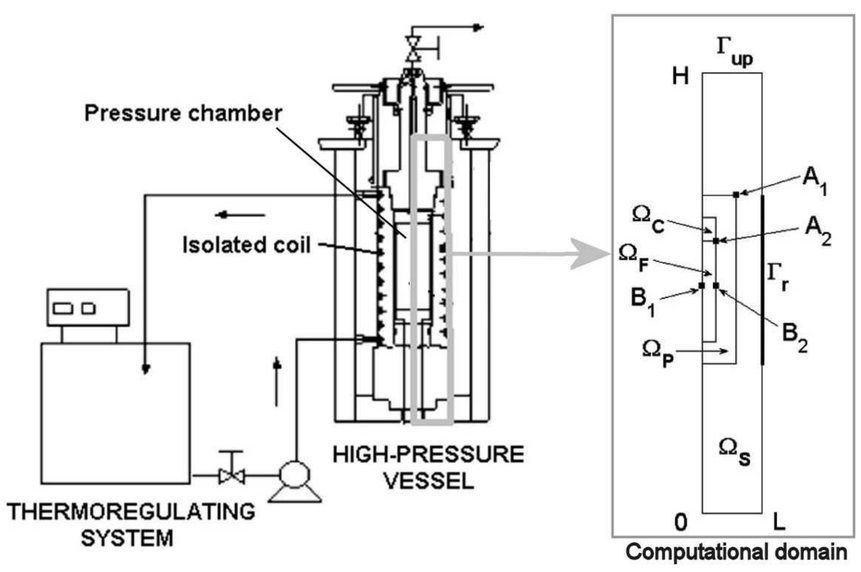
where T_{r} is a reference temperature (K), P_{r} is a reference pressure (MPa), κ_{r} is the inactivation rate at reference conditions (min^{-1}), B is the parameter (K) expressing the temperature dependence of κ and C is the parameter (MPa^{-1}) expressing the pressure dependence of κ.

2-

$$\kappa(P,T) = \kappa_{\text{r}} \exp\Big[\left(\frac{-\Delta V_{\text{r}}}{RT}(P-P_{\text{r}})\right)+\left(\frac{\Delta S_{\text{r}}}{RT}(T-T_{\text{r}})\right)+\left(\frac{\Delta\nu}{2RT}(P-P_{\text{r}})^2\right)+\left(\frac{-2\Delta\zeta}{RT}(P-P_{\text{r}})(T-T_{\text{r}})\right)+\left(\frac{\Delta C_p}{RT}\left(T(\ln\frac{T}{T_{\text{r}}}-1)+T_{\text{r}}\right)\right)\Big]$$

where $R = 8.314$ ($\text{J mol}^{-1}\,\text{K}^{-1}$) is the universal gas constant, ΔV_{r} is the volume change at reference conditions ($\text{cm}^3\,\text{mol}^{-1}$), ΔS_{r} is the entropy change at reference conditions ($\text{J mol}^{-1}\,\text{K}^{-1}$), ΔC_p is the heat capacity change ($\text{J mol}^{-1}\,\text{K}^{-1}$), $\Delta\zeta$ is the thermal expansibility factor ($\text{cm}^3\,\text{mol}^{-1}\,\text{K}^{-1}$) and $\Delta\nu$ is is the compressibility factor ($\text{cm}^6\,\text{J}^{-1}\,\text{mol}^{-1}$).

Considered high pressure device



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Heat and mass transfer modelling

Considering a liquid food sample in Ω_{F}^*, the **governing equations** inside the whole domain Ω^* are:

$$\begin{cases}
\rho C_p\dfrac{\partial T}{\partial t} - \nabla\cdot(k\nabla T) + \rho C_p\mathbf{u}\cdot\nabla T = \alpha\dfrac{dP}{dt}T & \text{in } \Omega^*\times(0,t_{\text{f}}),\\
\rho\dfrac{\partial \mathbf{u_F}}{\partial t} - \nabla\cdot\eta(\nabla\mathbf{u_F}+\nabla\mathbf{u_F^t}) + \rho(\mathbf{u_F}\cdot\nabla)\mathbf{u_F} = -\nabla p - \dfrac{2}{3}\nabla\left(\eta(\nabla\cdot\mathbf{u})\right) + \rho\mathbf{g} & \text{in } \Omega_{\text{F}}^*\times(0,t_{\text{f}}),\\
\rho\dfrac{\partial \mathbf{u_P}}{\partial t} - \nabla\cdot\eta(\nabla\mathbf{u_P}+\nabla\mathbf{u_P^t}) + \rho(\mathbf{u_P}\cdot\nabla)\mathbf{u_P} = -\nabla p - \dfrac{2}{3}\nabla\left(\eta(\nabla\cdot\mathbf{u})\right) + \rho\mathbf{g} & \text{in } \Omega_{\text{P}}^*\times(0,t_{\text{f}}),\\
\dfrac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u_F}) = 0 & \text{in } \Omega_{\text{F}}^*\times(0,t_{\text{f}}),\\
\dfrac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{u_P}) = 0 & \text{in } \Omega_{\text{P}}^*\times(0,t_{\text{f}}),\\
+\text{ points, boundary and initial conditions,}
\end{cases} \tag{2}$$

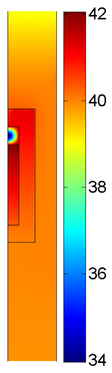
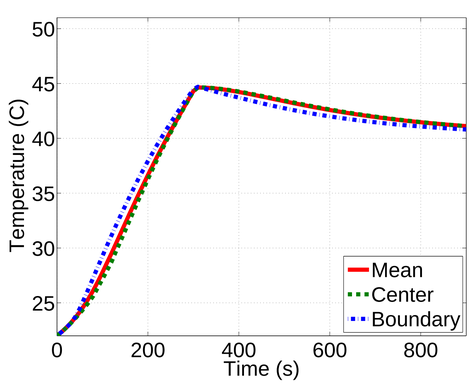
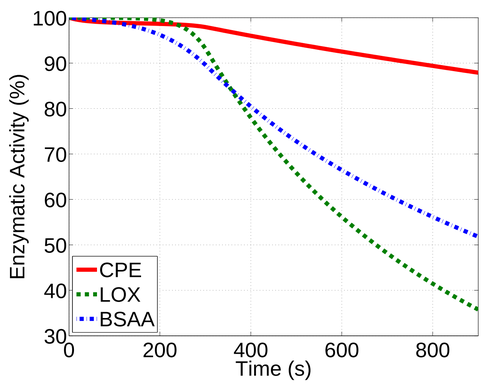
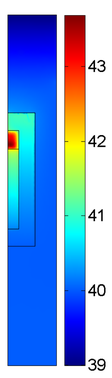
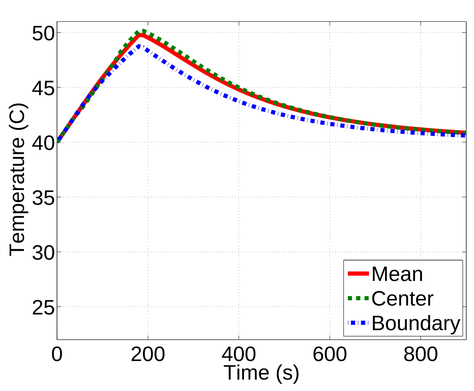
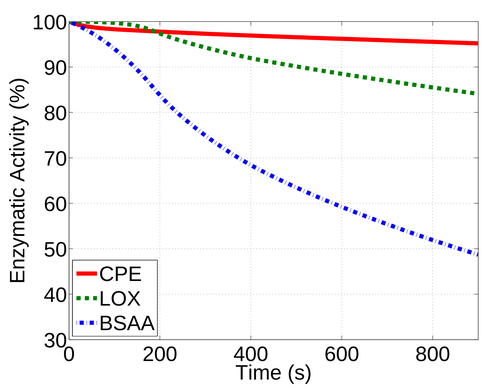
where $\mathbf{u_F}$ is the food velocity field, $\mathbf{u_P}$ is the pressurizing fluid velocity field, ρ is the density (kg m^{-3}), C_p is the heat capacity ($\text{J kg}^{-1}\,\text{K}$), k is the thermal conductivity ($\text{W m}^{-1}\,\text{K}^{-1}$), t_{f} (min) is the final time, $\mathbf{g}$ is the gravity vector (m min^{-2}), η is the dynamic viscosity (Pa min), P is the pressure (Pa) applied by the equipment, p is the pressure (Pa) generated by the mass transfer inside the fluid and α is the thermal expansion coefficient (K^{-1}). * means 3D-domains obtained by **rotating** around the (0,H)–axis.

We also consider a simplified version of previous model considering the **Boussinesq approximation** (i.e. considering the incompressible Navier-Stokes equations and constant model coefficients). This approximation allows to **reduce the computational time by 3**.

Numerical tests

- **Processes:** We consider two 15–minute processes:
  - **Process P_A**: For initial temperature T_0=40°C in Ω_{S} and 22°C in $\Omega\backslash\Omega_{\text{S}}$, a constant pressure increase in the first 305 seconds until reaching 600 MPa is considered.
  - **Process P_B**: Considering initial temperature $T_0 = 40$°C in the whole domain Ω and applying the same constant pressure increase in the first 183 seconds until reaching 360 MPa.
- **Numerical Models:** The **axial symmetry** of the model allows us to work in a **2D–domain**. The heat and mass transfer model (2) is **coupled** with the kinetic equation (1). Velocity and pressure spacial discretization is based on P2–P1 **lagrange finite elements** satisfying the LBB stability condition.
- **Enzymes:** We study the impact of the two processes P_A and P_B on the inactivation of three different enzymes: **Bacillus Subtilis α–Amylase** (BSAA), **Lipoxygenase** (LOX) and **Carrot Pectin Methyl–Esterase** (CPE).
- **Sensitivity analisis:** In practice, the model coefficients are usually **approximated using experimental data**. Furthermore, due to equipment limitations, some **experimental discrepancies** could occur during the process. In order to study the impact of these errors on the enzymatic activity evolutions, we perform a **sensitivity study** of the models considering a standard deviation less than ±5% of the parameters.

Numerical results

Proc.	Final Temperature	Temperature evolution (C)	Enzymatic Activity Evolution (%)	Activity Reduction
$\mathbf{P}_\text{A}$				Model / Enzyme: BSAA LOX CPE Full model: 49% 64% 12% Boussinesq: 51% 66% 12% **Sensitivity analisis** Minimum: 41% 50% 9% Maximum: 54% 77% 18%
$\mathbf{P}_\text{B}$				Model / Enzyme: BSAA LOX CPE Full model: 52% 16% 5% Boussinesq: 53% 17% 5% **Sensitivity analisis** Minimum: 44% 11% 4% Maximum: 60% 23% 5%