Seminario

Simulación numérica en Ingeniería y Ciencias con MATLAB + COMSOL Multiphysics

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Máster Universitario
en Sistemas Inteligentes en Energía y Transporte
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ON THE MODELLING AND SIMULATION OF HIGH PRESSURE PROCESSES AND INACTIVATION OF ENZYMES IN FOOD ENGINEERING

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Collaborations:

Outlines

- **Introduction**
  -Industrial context
  -Description of HP device
  -Interesting problems

- **Inactivation of enzymes**
  -Kinetic equation
  -Inactivation rate

- **Heat and Mass Transfer Modelling**
  -System of equations
  -Physical parameters

- **Coupled model**
  -Sensitivity analysis
  -Incomplete models

- **Numerical experiments**
  -Considered experiments
  -Numerical Results

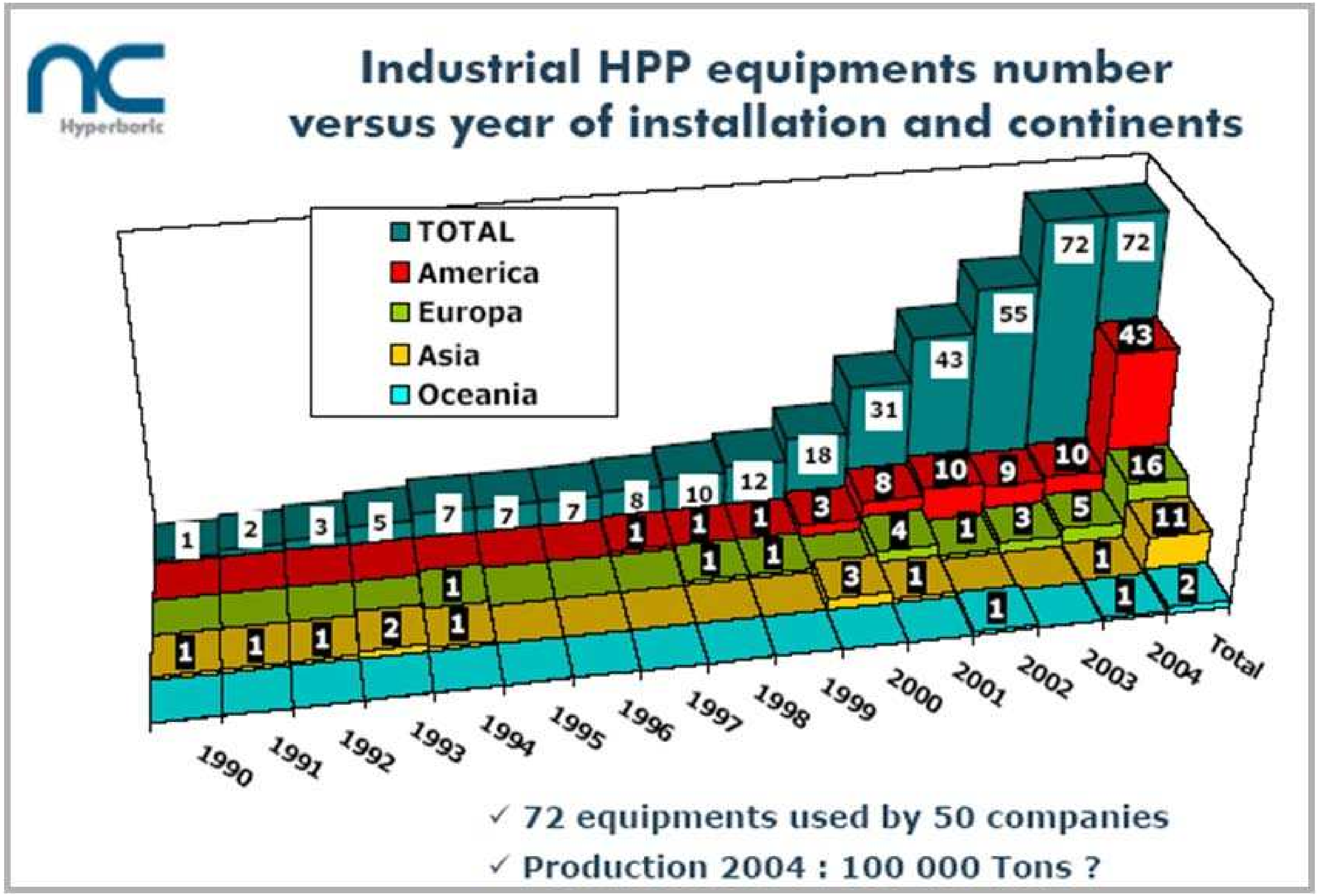
Part I: Introduction

HP in Food industry

- Industrial context: Increase of the demand of **safe and minimally processed food (liquid or solid)** prepared for immediate consumption: restaurants, collective dining rooms, domestic consumption, etc.
- Objective of the food treatments: Increase the shelf life of the food by inactivating some **biological entities**: bacteria, fungus, **enzymes** ...
- Most used treatments: Pasteurization (using high temperature), Freezing (Using low temperature), Chemical (using additives), UV treatment, HP treatment (using high pressures)... **Hybrid** treatments can be considered.
- Advantages of HP treatments:
  -Not based on the incorporation of additives
  -**Avoid treatments with low/high temperatures** which affect **nutritional** and **organoleptic** properties of the food.

HP in Food industry

Evolution of the use of HP device:



HP in Food industry

Application of the HP-T treatments:

PRODUCTO	PAÍS	COMPAÑÍA	TRATAMIENTO
Productos de frutas	Japón	Meidi-Ya	400 MPa/10-30'/20ºC
Zumos de mandarina	Japón	Wakayama Food Int.	300-400 MPa/2-3'/20ºC
	Japón	Ehime	?
Zumos de frutas	Japón	Takansi	?
	Francia	Pampryl-Pernod Ricard	400 MPa/1'/20ºC
	USA	Frutmost-Avomex	?
	USA	Odwalla Inc.	?
Zumo de manzana y cítricos	Portugal	Frubaca	450 MPa/20-90"/12ºC
Zumos de naranja	Japón	Pon	?
	Reino Unido	Orchard House Foods Ltd.	500 MPa/20ºC
	Líbano	K-Sun	500 MPa
	Italia	Ortogel SpA	?
	México	Jumex	20"-1'
Frutas azucardas	Japón	Nisshin Fine Foods	50-200 MPa
Arroces	Japón	Echigo Seika	400-600 MPa/10'/45-70ºC
Sake	Japón	Chiyonosono	400 MPa/30'/15ºC
Guacamole y Salsas	USA	AvoClassic-Avomex	700 MPa/10-15'/20ºC
Hummus	USA	Hannah Internat. Foods	?
Jamón crudo	Japón	Fuji Chiku Mutterham	250 MPa/3 h/20ºC
Productos cárnicos	España	Esteban Espuña. S.A.	400-500 MPa/20ºC
	España	Campofrío Alimentación S.A.	500-600 MPa/10'/ 7ºC
	Italia	Vismara/Ferrarini	600 MPa/10'/ 7ºC
	Alemania	Gebr. Abraham GmbH	600 MPa/2'/ 5ºC
Productos cárnicos de cerdo cocidos, libres de nitritos: salchicas, jamón, bacón "Roast beef" loncheado	Japón	Ito Ham Foods Inc.	600 MPa/5'/ 5ºC
Productos precocinados "listos para consumir" de aves de corral	USA	Perdue Farms Inc.	600 MPa/2'
Pollo loncheado precocinado y Ternera para fajitas	USA	Menu Fresh-Avomex	600 MPa
Platos preparados de verdura "listos para consumir"	España	?	500 MPa
Jamón cocido loncheado, productos de cerdo y jamón de Parma	USA	Hormel Foods Corporation	600 MPa
Productos precocidos de pescado reconstituido: salmón y merluza	España	Campofrío Alimentación S.A.	500 MPa/ 5'
Elaborados de pescado	Japón	Yaizu Fisheries	400 MPa
Ostras	USA	Motivatit Seafoods, Inc. Nisbet Oyster Co. Joey Oyster Inc.	200-350 MPa/1-2'
Marisco	USA	Ocean Choice International	275 MPa/1'
Margarina	Japón	Kaneke Corp.	?

General description of the HP device

General description of the HP device

Considered HP device

We consider: **ACB GEC Alsthom – Instituto del Frío - CSIC**.

Interesting problems

We have studied two problems:

1- The control of the **food sample temperature** during a HP-T treatment: Increasing the pressure we also increase the temperature (can lead to **pasteurization**).

L. Otero, Á. M. Ramos, C. de Elvira, C. y P. D. Sanz: 'A Model to Design High-Pressure Processes Towards an Uniform Temperature Distribution'. Journal of Food Engineering (J. Food Eng.), Vol 78 (2007), 1463-1470

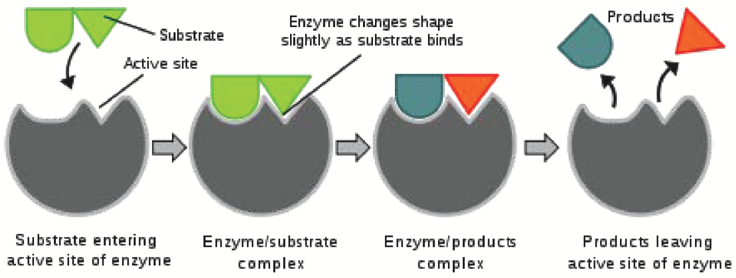
2- **Today we present:** The study of the **inactivation** of some **enzymes** in the food sample: useful in future works for **optimizing** a HP-T treatment.

J. A. Infante, B.Ivorra, Á. M. Ramos y J. M. Rey: 'On the Modelling and Simulation of High Pressure Processes and Inactivation of Enzymes in Food Engineering'. Mathematical Models and Methods in Applied Sciences, Vol. 19 (12) (2009), 2203-2229

Part II: Inactivation of enzymes

Enzyme

- What is an enzyme: Enzymes are molecules (essentially proteins) that **catalyze chemical reactions** essential for microorganisms.



- Interest of inactivating enzymes: block **chemical reactions** in order to **reduce the activity** of non-desired microorganism in food (producing fermentation, toxic...).

- Impact of the HP-T treatment on enzyme: Changing the pressure/temperature conditions, the enzyme progressively (in term of concentration) change form a **folded state** (active) to an **unfolded state** (inactive): thus the chemical reaction velocity decrease.

Kinetic equation

The **activity A of an enzyme** inside a food *'particle'* is defined by the considered **experimental protocol of measurement**. Mathematically, the time evolution of A can be described by the following first–order kinetic equation:

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

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}).

The solution at time t is obviously given by

$$A(t) = A(0) \exp\left(-\int_0^t \kappa(P(\sigma), T(\sigma))\, d\sigma\right).$$

Here $\kappa(P, T)$ is chosen, **depending on the considered enzyme**.

Inactivation rate

1- As a combination of **Arrhenius equation** (modelling the temperature dependence) and **Eyring equation** (modelling the pressure dependence):

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

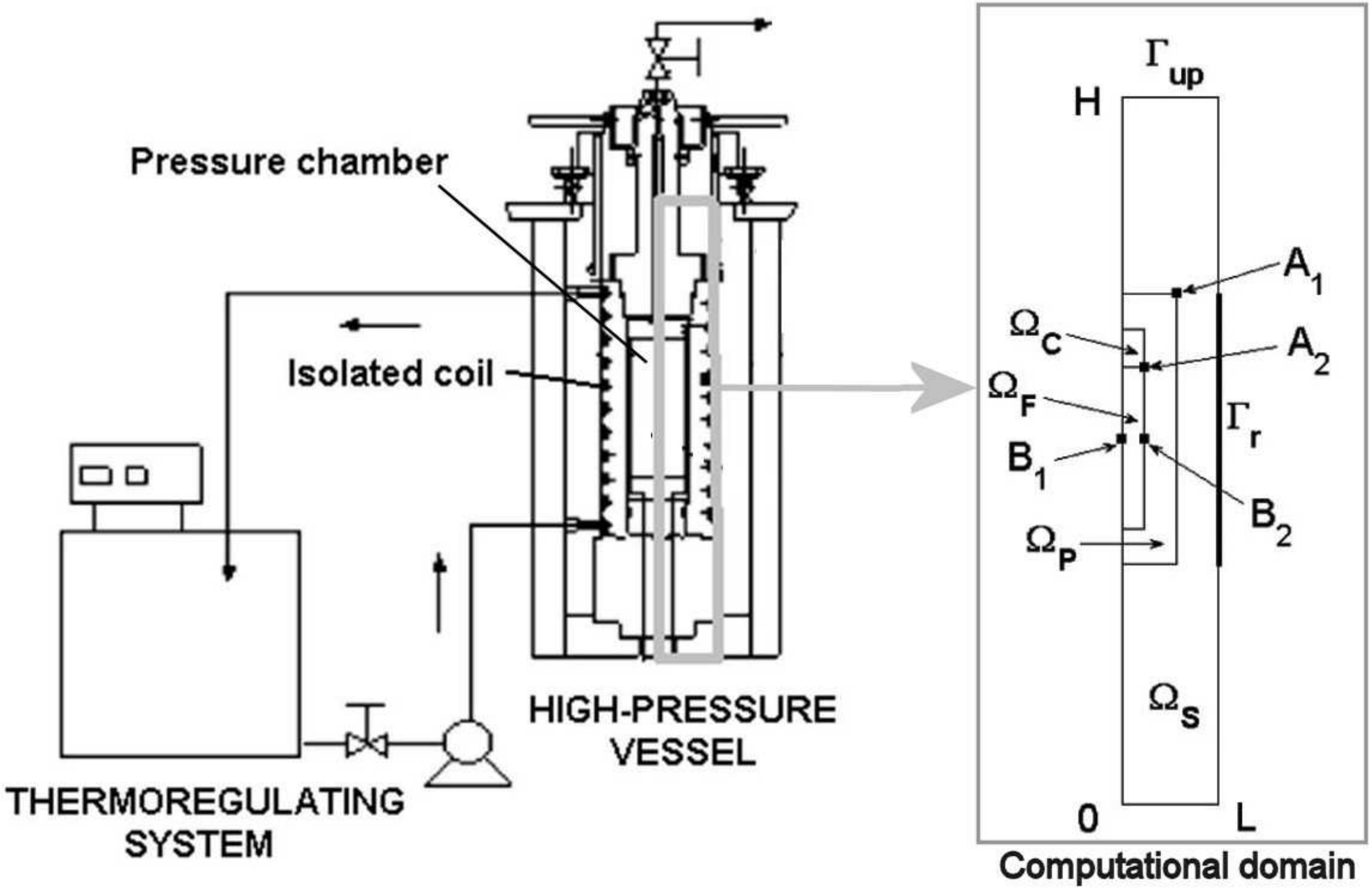
2- A model obtained by considering **Eyring's transition state theory**:

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

The parameters of the selected equation are estimated using **regression techniques** on experimental data.

Part III: Heat and Mass Transfer Modelling

Computational domain



Considered equations

The pressure evolution of the device is **given**.

In order to **determine the temperature evolution**, we consider the following model:

In the **full device**:

- Energy conservation $\longrightarrow$ **Conductive heat transfer Equation**.

In the **pressurized fluid and liquid food sample**:

- Momentum conservation $\longrightarrow$ **Navier-Stokes Equations**. We assume: Fluids are **compressible and Newtonian** (like water) $\longrightarrow$ **Stokes assumption**.

- Mass conservation $\longrightarrow$ **Continuity equation**.

Note: Those both equations can be **neglected** in the solid food sample case when food sample **filling ratio is high enough**.

System of equations

$$
\left\{
\begin{array}{l}
\rho C_p \dfrac{\partial T}{\partial t} - \nabla \cdot (k \nabla T) + \rho C_p \mathbf{u} \cdot \nabla T = \alpha \dfrac{dP}{dt} T \text{ en } \Omega^* \times (0, t_{\mathrm{f}}), \\
\rho \dfrac{\partial \mathbf{u_F}}{\partial t} - \nabla \cdot \eta (\nabla \mathbf{u_F} + \nabla \mathbf{u_F^t}) + \rho (\mathbf{u_F} \cdot \nabla) \mathbf{u_F} \\
\qquad = -\nabla p - \dfrac{2}{3} \nabla (\eta \nabla \cdot \mathbf{u_F}) - \rho \mathbf{g} \text{ in } \Omega_{\mathrm{F}}^* \times (0, t_{\mathrm{f}}), \\
\rho \dfrac{\partial \mathbf{u_P}}{\partial t} - \nabla \cdot \eta (\nabla \mathbf{u_P} + \nabla \mathbf{u_P^t}) + \rho (\mathbf{u_P} \cdot \nabla) \mathbf{u_P} \\
\qquad = -\nabla p - \dfrac{2}{3} \nabla (\eta \nabla \cdot \mathbf{u_P}) - \rho \mathbf{g} \text{ in } \Omega_{\mathrm{P}}^* \times (0, t_{\mathrm{f}}), \\
\dfrac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u_F}) = 0 \text{ in } \Omega_{\mathrm{F}}^* \times (0, t_{\mathrm{f}}), \\
\dfrac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u_P}) = 0 \text{ in } \Omega_{\mathrm{P}}^* \times (0, t_{\mathrm{f}}).
\end{array}
\right.
$$

All physical parameters are assumed **P-T dependent**.

System of equations

We consider the following **boundary conditions**:

$$\begin{cases} k\dfrac{\partial T}{\partial \mathbf{n}} = 0 \ \text{ in } \ \Gamma^* \backslash (\Gamma_r^* \cup \Gamma_{\rm up}^*) \times (0, t_{\rm f}), \\ k\dfrac{\partial T}{\partial \mathbf{n}} = h(T_{\rm amb} - T) \ \text{ in } \ \Gamma_{\rm up}^* \times (0, t_{\rm f}), \\ T = T_{\rm ref} \ \text{ in } \ \Gamma_r^* \times (0, t_{\rm f}), \\ \mathbf{u_F} = 0 \ \text{ in } \ \Gamma_{\rm F}^* \times (0, t_{\rm f}), \\ \mathbf{u_P} = 0 \ \text{ in } \ \Gamma_{\rm P}^* \times (0, t_{\rm f}), \\ T = T_0 \ \text{ in } \ \Omega^*, \\ p = 10^5 \ \text{ in } \ A_1 \times (0, t_{\rm f}), \\ p = 10^5 \ \text{ in } \ A_2 \times (0, t_{\rm f}). \end{cases}$$

Numerical scheme

- Numerical tests computed in cylindrical coordinates using a **Finite Element Method**.
- Velocity and pressure spatial discretization is based on **P2–P1 Lagrange Finite Elements** satisfying the Ladyzhenskaya, Babuska and Brezzi (**LBB**) stability condition.
- The Time integration is performed using the Variable–Step–Variable–Order (**VSVO**) Backward Differentiation Formula (**BDF**)–based strategy.
- The nonlinear systems are solved with a **damped Newton method**.
- The algebraic linear systems are solved using Unsymmetric MultiFrontal Method for sparse linear systems(**UMFPACK**) combined with the stabilization technique Galerkin Least Squares (**GLS**).

Determination of physical parameters

- Solid food sample (Tylose): We have chosen **tylose** as an example of solid type food (**similar properties to meat**). The coefficients are obtained from literature for **atmospheric pressure**. A **rescaling procedure and a piecewise linear interpolation** have been applied for other values of pressure.

- Liquid medium: The physical parameters are supposed to be equal to those of **water**:
  - ρ, C_p and k are computed through a **shifting approach** (using phase diagram) from **atmospheric pressure**.
  - α we use a **known expression**.
  - η is computed by a **piecewise linear interpolation from given data**.

Part IV: Coupled model

Coupling models

In order to determine the **time and spatial** evolution of the activity in the food sample:

Solid case:

The particles of the food are **still**. The activity A of a particle located at the point $x \in \Omega_{\mathrm{F}}$ at time t:

$$A(x,t) = A(x,0)\exp\left(-\int_0^t \kappa\big(P(\sigma),T(x,\sigma)\big)\,d\sigma\right).$$

Liquid case:

Due to mass transfer, the particles **move** in the food domain Ω_{F}. In this case, for each point $x \in \Omega_{\mathrm{F}}$ we consider the trajectory X of a food particle that ends at point x.

$$A(x,t) = A(X(0),0)\exp\left(-\int_0^t \kappa\big(P(\sigma),T(X(\sigma),\sigma)\big)\,d\sigma\right).$$

Sensitivity analysis

In practice:

- The model coefficients are usually **approximated using experimental data** with a standard deviation lower than $\pm 5\%$.
- due to equipment limitations, some **experimental discrepancies** could occur during the process.

Objective: study the impact of these errors on the temperature and enzymatic activity evolutions.

We generate $N \in \mathbb{N}$ perturbed models from the original one, with coefficients perturbed randomly by $\pm 5\%$.

Then, we compute the **mean error** committed in the temperature and activity.

Incomplete models

Objective: **reduce the computational complexity** of the model.

We consider '**simplified models**', **cheaper** to evaluate and with results **close enough** to the full models:

- Solid food (**SCC**): We consider **constant coefficients**, by setting C_p, k, α, ρ and η to a mean value.
- Liquid food (**LCC**): As previously we consider **constant coefficients** except ρ.
- Liquid food (**LB**): **Boussinesq** approximation: considering the **incompressible** Navier-Stokes equations and **constant coefficients** except ρ when combined with the gravitational force.

In all cases, we compute the **error** committed in the temperature and activity.

Part V: Numerical experiments

Considered enzymes

- Bacillus Subtilis α–Amylase (**BSAA**): It is an enzyme produced by a bacteria called Bacillus Subtilis. This bacteria, present in the ground, can contaminate food and in rare occasions cause **intoxications**. This enzyme catalyzes the hydrolysis of starch, generating sugars (as maltose) that can **modify the taste of the aliment**.

- Lipoxygenase (**LOX**): This enzyme is present in various plants and vegetables such as green beans and green peas. It is responsible of the appearance of **undesirable aromas** in those products.

- Carrot Pectin Methyl–Esterase (**CPE**): Common in most vegetables. It can be present in vegetable juices producing low–methoxyl pectin. This process **reduces juice viscosity and generates cloud loss** (affecting juice flavor, color, texture and aroma).

Considered treatments

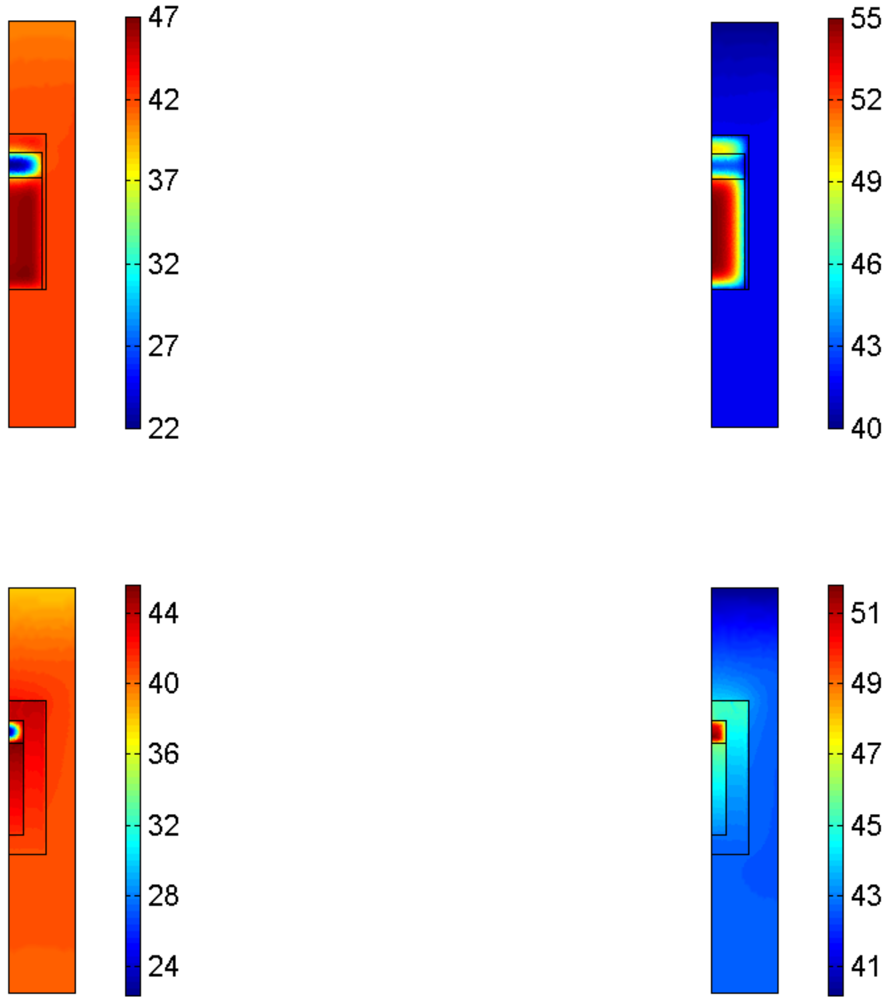
We consider a **big solid and a small liquid** food sample submitted to one of the following treatment:

- Process P1: The initial temperature is $T_0 = 40°$C in the device and 22°C in the food sample and the pressure is linearly increased during the first 305 seconds until reaching 600 MPa.

- Process P2: The initial temperature is $T_0 = 40°$C in the whole domain Ω and the pressure is linearly increased (with the same slope as before) during the first 183 seconds until reaching 360 MPa.

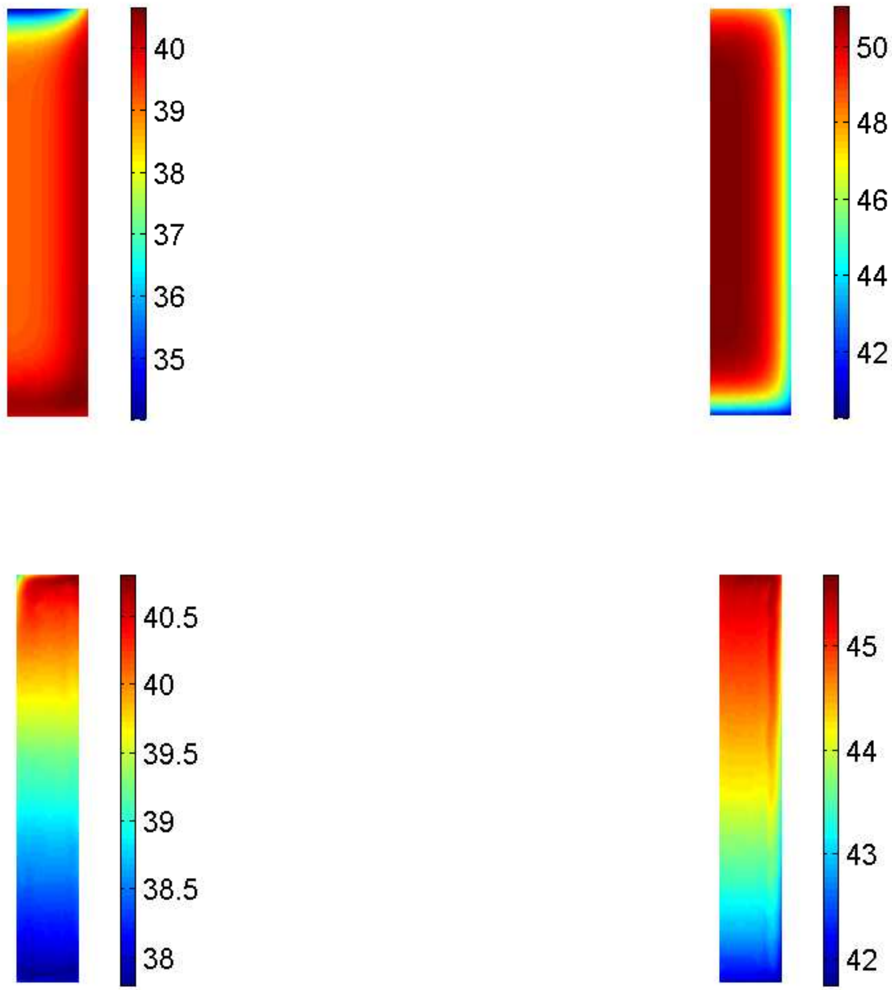
Temperature analysis

Final temperature distribution in the whole domain:



Temperature analysis

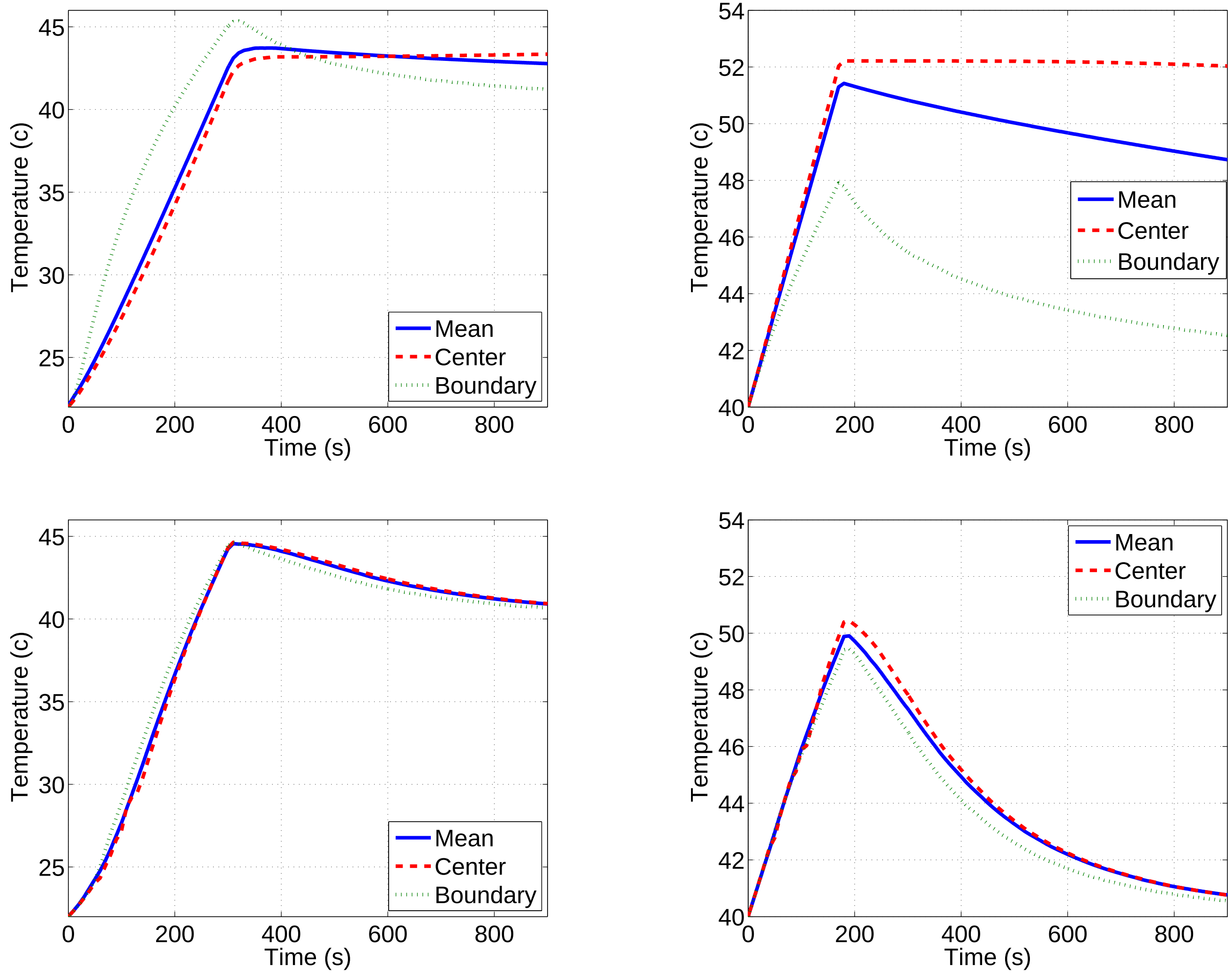
Final temperature distribution in the food sample:



Example of temperature distribution (liquid-P1):

Temperature analysis

Mean temperature evo:



Temperature analysis

Sensitivity analysis: **Mean Relative Temperature Error** (in %)

Process	Food	Whole domain	Sample
P1	Solid	2.74	3.34
P2	Solid	2.75	2.93
P1	Liquid	2.68	2.70
P2	Liquid	2.83	2.67

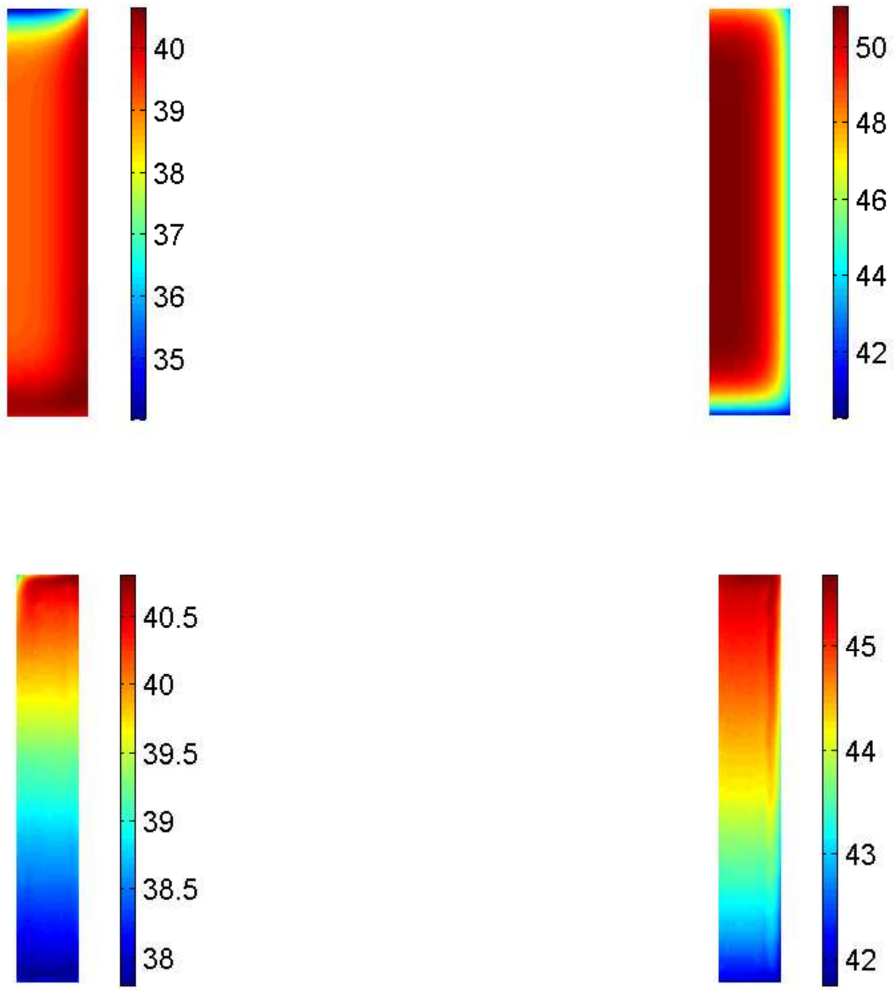
Temperature analysis

Incomplete models: **Relative Temperature Error** (in %)

Process	Model	Whole domain	Sample	Comp. Time (s)
P1	SFull	—	—	53
P2	SFull	—	—	51
P1	SCC	0.77	4.77	4
P2	SCC	0.10	0.52	4
P1	LFull	—	—	3135
P2	LFull	—	—	4141
P1	LCC	0.41	2.07	2459
P2	LCC	0.06	0.20	2877
P1	LB	0.37	1.96	2196
P2	LB	0.08	0.22	2475

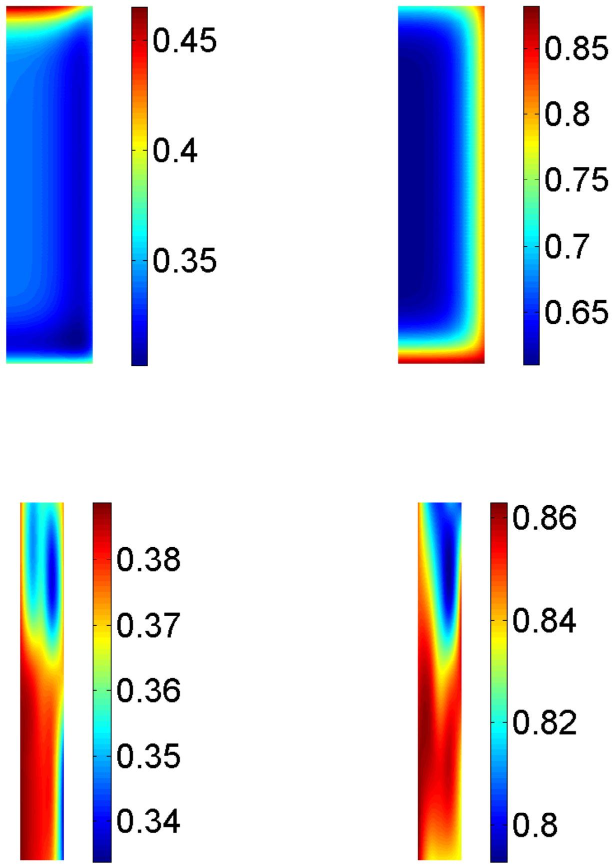
Enzymatic analysis

Final temperature distribution in the food sample:



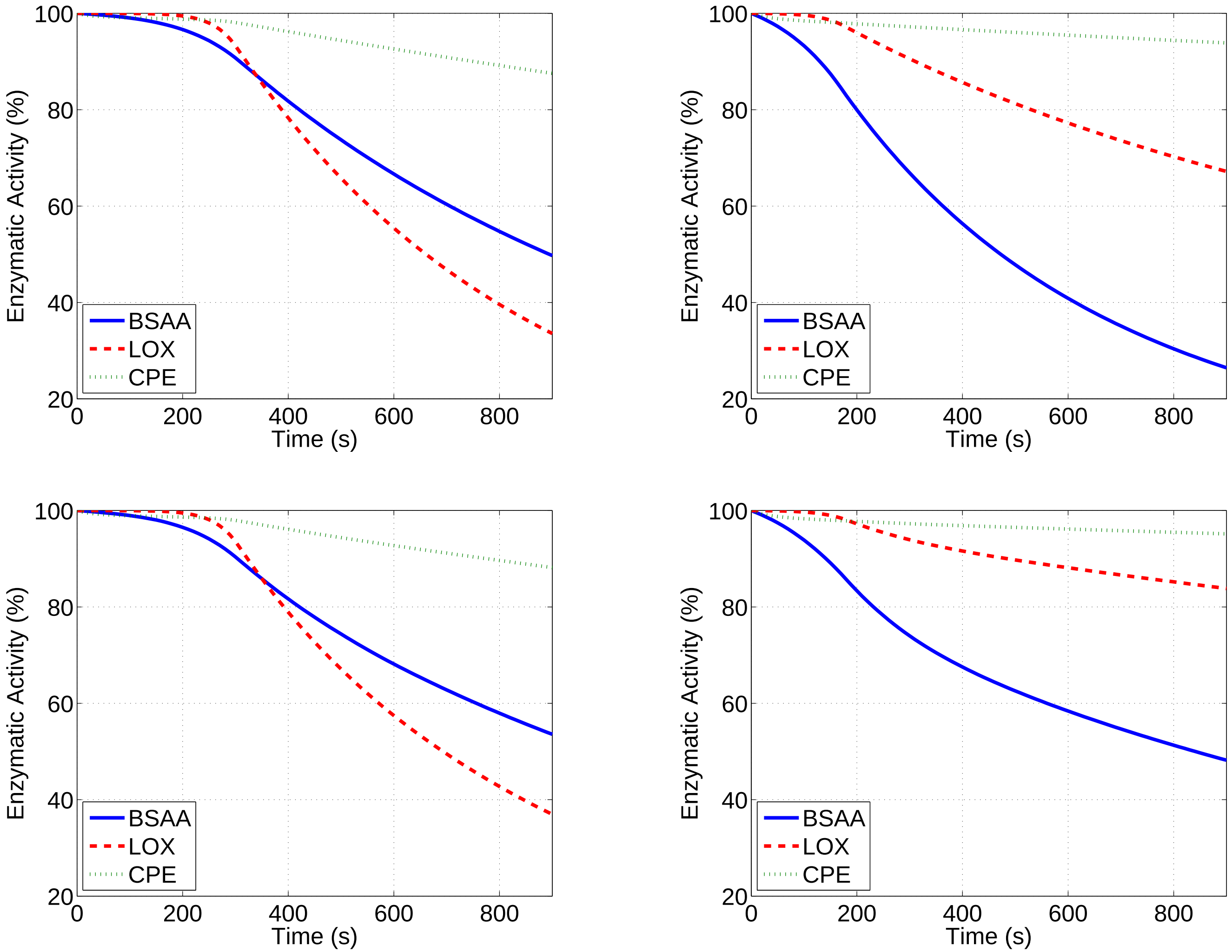
Enzymatic analysis

LOX final activity distribution in the food sample:



Enzymatic analysis

LOX Mean Activity evolution:



Example of temperature and LOX activity distribution (Solid-P1):

Enzymatic analysis

Sensitivity analysis: **Mean Activity Error** (in %)

Process	Food	BSAA	LOX	CPE
P1	Solid	4.60	6.81	2.28
P2	Solid	5.01	6.43	0.52
P1	Liquid	4.02	7.45	2.40
P2	Liquid	3.97	2.51	0.28

Incomplete models: **Activity Error** (in %)

Process	Model	BSAA	LOX	CPE
P1	SCC	7.44	5.20	1.33
P2	SCC	0.96	1.11	0.10
P1	LCC	2.81	1.75	0.40
P2	LCC	1.14	0.65	0.06
P1	LB	3.04	2.00	0.45
P2	LB	2.23	1.31	0.12

Conclusions and perspectives

Conclusion and perspectives

- The mathematical models described in this paper provide a **useful design tool**.
- The model is **robust**.
- Several simplified versions of the full models are proposed and are **suitable** for optimization procedures.

Future work:

- **New model** for enzymatic inactivation.
- **Identify** the most important enzymes to be inactivated and the organoleptic properties to be preserved.
- Perform optimization techniques in order to **reduce the enzymatic activities and preserve organoleptic properties of the food**, without using high temperatures.

Conclusion and perspectives

!!! Thank You !!!