ON THE APPROXIMATE SOLUTION FOR A FULLY COUPLED PARABOLIC-HYPERBOLIC PDES SYSTEM APPLIED IN THERMOMECHANICAL BEHAVIOUR OF HYDROGEL MATRIX USED IN DRUG DELIVERY

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ABSTRACT

This work deals with numerical methods for a fully coupled system of parabolic-hyperbolic partial differential equations modeling the thermo-mechanics of the hydrogel matrix of drug delivery devices. The model of hydrogel matrix is governed by heat conduction equation, wave equation and a thermodynamically admissible constitutive law. These equations are coupled by source terms. Transient analysis is assumed for the present study. Original numerical approach based on finite element formulation is developed to solve the problem. The model is developed to predict the reversible- irreversible entropy and heat production in the material to control drug delivery devices by following the temperature change. Experimentally, various situations are assumed in order to observe variations of entropy and temperature by using micro-calorimetric test for many frequency rates. Some numerical results in correlation with experimental measurements are presented in this work.

Keywords: finite element formulation, cyclic load, parabolic-hyperbolic equations, drug delivery.

1. INTRODUCTION

magneto-elasticity, and thermo-elasticity and for many other phenomena in science engineering, a coupled partial differential equation appears (Mohammed 2009; Jeffrey 2005; Xia 2010). In general, coupled system of parabolic and hyperbolic equations is obtained after deriving conservation equation (physical laws) of the system (Holzapfel 1995). And it is well known that in continuous media theory, the mechanics and the thermodynamics fields are coupled. Most theoretical foundations of such phenomenon were established by Duhamel, Coleman Noll (e.g. Rakotomanana 2009; Claire 2011). In this paper, we are in presence of thermomechanical process in the material. Then, the coupled partial differential equation are obtained by applying conservation law, first and second law of thermodynamics for heat conduction and linear momentum for the wave equation (e.g. Rakotomanana 2009; Betram 1990). The Hydrogel matrix has dissipation properties inducing temperature change under cyclic load (Mohandreza 2013; Philippe 2014). The mechanical loading is accompanied by a production of entropy and heat, which can influence the

temperature and the behavior of the material (Mahaman 2012). Material is mostly viscoelastic. First such phenomenon may be used to optimize drug delivery device induced by the temperature change, as in cartilage joint which is always under cyclic load (Mohandreza 2013; Philippe 2014; chi 2001). Elevation of the temperature) may induce defect in the material (prostheses) and may influence the formation of transfer film and contact at the interface between the biological tissues and the prosthesis (Chi 2001). So, we need to establish a predictive model to qualify and quantify the temperature effect in these materials and to determine the maximal temperature admitted for various situations.

Constitutive equation of some viscoelastic material, biological tissues, without temperature effect and undergoing large strain was previously established (Rakotomanana and Pioletti 2009). In order to include the material behavior, we introduce a new constitutive equation in strain gradient continuum taking into account the heat effect. Constitutive equation is first obtained by defining a Helmholtz free energy as in (Rakotomanana and Pioletti 2009) but taking into account an internal variable and temperature effect. We use classical Coleman and Noll approach for thermo-mechanical processes (Holzapfel 1995). To obtain numerical solutions of a thermo-mechanical problem, equations must be solved simultaneously.

Various papers exhibit some smooth solutions of the coupled parabolic-hyperbolic system. The uniqueness, local existence and asymptotic study of the solution were developed in (Hao, Maurizio, Songmu 2007; Yinghui 2013). Many assumptions are used to simplify the problem, some papers solve the problem for one or two dimensions (Shin and Seung 1999; Chi 2001; Kunish 2009), solves the problem by considering that the effect of stress with temperature production is small (in this case the problem is weakly coupled). The last method uses the Eulerian-Lagrangian method in order to obtain numerical solutions for this problem (Mohammed 2009). In this work, we assume that coupling term is not negligible, so the problem is fully coupled and reintroduce the internal variable and its evolution law in order to complete the behavior of the material.

Mechanical transformation is accompanied by production of entropy and heat, which can influence the

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temperature and the behavior of the material. For biological tissues, coupling is important. Indeed, some part of energy is converted into heat as dissipation, thus resulting in an irreversible temperature and entropy rise. In such a case, if temperature or entropy gradient is significant, mechanical coupling term cannot be neglected. We establish for the hydrogel the evolution law and then we study the response with a cyclic load.

This paper aim to develop a numerical approach for a fully coupled thermo-mechanical system under cyclically load and dynamical boundary conditions. First, we would like to better understand and quantify the influence of thermo-mechanical coupling on the material behavior and on the dynamic response of the viscoelastic biological tissues substitutes. Quantification is obtained by analyzing its effect on the dissipated energy and on the entropy production within the material for each cycle. We determine the behavior of artificial substitute by studying the correlation of the theoretical results with the experimental measurement. An artificial gel is used to substitute biological tissues, taking into account thermo-mechanical load in the material.

The first part of this paper illustrates the model for the thermo-mechanical coupling in the case of viscoelastic wires subject to a cyclically mechanical load. The numerical approach and the result are presented with the stability study on the evolution of the dissipated energy with the strain rate and on the influence of thermo-mechanical coupling. The second part presents briefly the experimental measurement and the correlation between results on the reversible and irreversible entropy. The thermo-mechanics approaches in this work are based on the Coleman and Noll based on the Clausis-Duhem inequality.

We assume that the Helmholtz's free energy and the equipresence theory by the Truesdell and Toupin to define the constitutive law of the material (Claire; Rakotomanana 2009; Holzapfel 1995). We introduce an internal variable in order to take into account the dependence of free energy, entropy and temperature gradient. These assumptions lead to consistent forms of the second principle of the thermo-mechanics and the Clausius-Duhem inequality. A new constitutive law is established for each internal variable.

2. EXPERIMENTAL METHODS

For measuring temperature change in substitute sample under cyclic load, deformation micro-calorimetric test was used. It consists to apply on a cylindrical sample of hydrogel matrix (4 [mm] and 6 [mm] of HEMA-EGDMA hydrogels) a cyclic load. For experimental measurements, various frequencies are tested to observe variations of entropy and temperature by using micro-calorimetric test. We assume that system is adiabatic.
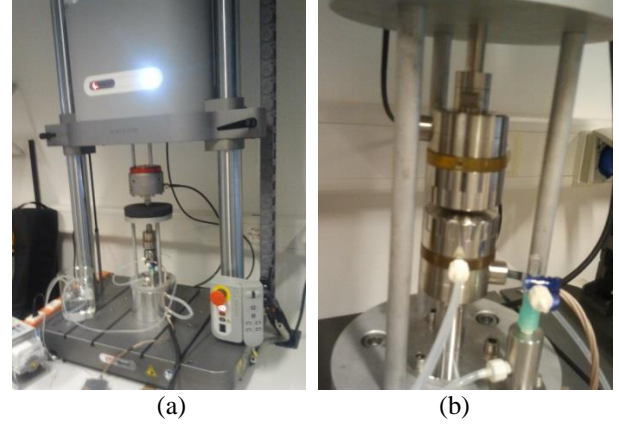

(a)   (b)
Figure 1: Deformation micro-calorimetric test.
The figure 1 illustrates the micro-calorimetric system: The left side (a) illustrates the global system. The right side (b) illustrates the sample (in middle of the two sensors). This system has a thermal insulation but no in the figure.

3. MATHEMATICAL MODEL

Let $\Omega \subset \mathbb{R}^d$ be a bounded domain in with smooth boundary $\partial\Omega \subset \mathbb{R}^{d-1}$ (it represents the sample in hydrogel matrix HEMA-EGDMA). For any time, mechanical and heat stress occupies this domain. Time is defined by scalar $t \in [0, T]$ with $t \subset \mathbb{R}_+$.

3.1. Constitutive equation

The constitutive equation is based on the thermodynamics potentials. The Helmholtz's free energy is given by

$$\psi(\mathbf{C}, \theta, \xi_i) = \psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i) \quad (1)$$

And the dissipation potential is given by

$$\chi(\mathbf{C}; \dot{\mathbf{C}}, \overline{\nabla\theta}, \overline{\nabla\xi_i}) = \chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_i}; \theta, \mathbf{C}) \quad (2)$$

The expressions of the invariant $\mathbb{J}_i$ are given in the appendix. In the equation (1) and (2) $\mathbf{C}$ denotes the Cauchy-Green strain tensor, given by:

$$\mathbf{C} = \frac{1}{2}(\nabla\mathbf{u} + \nabla^\mathbf{T}\mathbf{u} + \nabla^\mathbf{T}\mathbf{u}\nabla\mathbf{u}) \quad (3)$$

$$\dot{\mathbf{C}} = \frac{1}{2}(\nabla\dot{\mathbf{u}} + \nabla^\mathbf{T}\dot{\mathbf{u}} + \nabla^\mathbf{T}\dot{\mathbf{u}}\nabla\mathbf{u} + \nabla^\mathbf{T}\mathbf{u}\nabla\dot{\mathbf{u}}) \quad (4)$$

Where $\mathbf{u}$ denotes the displacement vector.

The second Piola-Kirchhoff stress tensor $\mathbf{S}$ is given by

$$\mathbf{S} = \mathbf{S^e} + \mathbf{S^v} \quad (5)$$

$$\mathbf{S^e}(\mathbf{C}, \theta, \xi_i) = 2\rho \frac{\partial}{\partial \mathbf{C}} \psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i) \quad (6)$$

$$\mathbf{S^v}(\mathbf{C}; \dot{\mathbf{C}}, \overline{\nabla\theta}, \overline{\nabla\xi_i}) = \frac{\partial}{\partial \dot{\mathbf{C}}} \chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_i}; \theta, \mathbf{C}) \quad (7)$$

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The potential $\psi(\mathbf{C}, \theta, \xi_i)$ and $\chi(\mathbf{C}; \dot{\mathbf{C}}, \overline{\nabla\theta}, \overline{\nabla\xi_i})$ are thermodynamically acceptable. They respect the entropy inequality and Clausius-Duhem inequality.

$$\rho\dot{e} + (\mathbf{S^e} + \mathbf{S^v}){:}\frac{\dot{\mathbf{C}}}{2} - \frac{\mathbf{Q}}{\theta}.\nabla\theta \geq 0, \forall\, \mathbf{C}, \dot{\mathbf{C}}$$

Then,

$$\rho\left[s\dot\theta + \dot\psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i)\right] + (\mathbf{S^e} + \mathbf{S^v}){:}\frac{\dot{\mathbf{C}}}{2}$$
$$-\frac{\mathbf{Q}}{\theta}.\overline{\nabla\theta} \geq 0, \forall\, \mathbf{C}, \dot{\mathbf{C}}$$

Where s denotes the entropy,
$s = s(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i)$

And then, the dissipation potential $\chi(\mathbf{C}; \dot{\mathbf{C}}, \overline{\nabla\theta}, \overline{\nabla\xi_i}) = \chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_i}; \theta, \mathbf{C})$ must be convex, positive and null and verify:

$$\frac{\partial}{\partial\dot{\mathbf{C}}}\chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_i}; \theta, \mathbf{C}){:}(\dot{\mathbf{C}} - \dot{\mathbf{C}}^*) +$$
$$\frac{\partial}{\partial\overline{\nabla\theta}}\chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_i}; \theta, \mathbf{C}){:}(\overline{\nabla\theta} - \overline{\nabla\theta}^*) +$$
$$\frac{\partial}{\partial\overline{\nabla\xi_i}}\chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_i}; \theta, \mathbf{C}){:}(\overline{\nabla\xi_i} -$$
$$,\overline{\nabla\xi_i}^*) \geq \chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_i}; \theta, \mathbf{C}) -$$
$$\chi(\mathbb{J}_1^*, \mathbb{J}_2^*, \mathbb{J}_3^*, \mathbb{J}_4^*, \mathbb{J}_5^*, \mathbb{J}_6^*, \mathbb{J}_7^*, \overline{\nabla\theta}^*, \overline{\nabla\xi_i}^*; \theta^*, \dot{\mathbf{C}}^*) \forall\, \mathbf{C}, \dot{\mathbf{C}}, \mathbf{C}^*, \dot{\mathbf{C}}^*$$

Where $\chi(\mathbb{J}_1^*, \mathbb{J}_2^*, \mathbb{J}_3^*, \mathbb{J}_4^*, \mathbb{J}_5^*, \mathbb{J}_6^*, \mathbb{J}_7^*, \overline{\nabla\theta}^*, \overline{\nabla\xi_i}^*; \theta^*, \dot{\mathbf{C}}^*)$ denotes the dissipation potential in the dual base.

The state function in $\Omega \subset (\mathbb{R}^d \times \mathbb{R}_+)$ can be written as,

$$\begin{cases} \mathbf{S^e}(\mathbf{C}, \theta, \xi_i) = \dfrac{\partial}{\partial\mathbf{C}}\psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i) \\[2mm] \mathbf{S^v}(\mathbf{C}; \dot{\mathbf{C}}, \overline{\nabla\theta}, \overline{\nabla\xi_i}) = 2\rho\dfrac{\partial}{\partial\dot{\mathbf{C}}}\chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_i}; \theta, \mathbf{C}) \\[2mm] s(\mathbf{C}, \theta, \xi_i) = -\dfrac{\partial}{\partial\theta}\psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i) \\[2mm] \dfrac{\partial}{\partial\overline{\nabla\theta}}\psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i) = 0 \\[2mm] \dfrac{\partial}{\partial\overline{\nabla\theta}}\chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_i}; \theta, \mathbf{C}) = \dfrac{\mathbf{Q}}{\theta} \end{cases}$$

3.2. Governing equation

The governing equation in transient analysis is obtained as a parabolic-hyperbolic coupled system.

$$\begin{cases} \mathbf{Div}\,\mathbb{P} + \rho\mathbf{b} = \rho\dfrac{\partial^2\mathbf{u}}{\partial t^2}\ \text{in}\ \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \rho\dot{e} = \mathbf{S}{:}\dfrac{\dot{\mathbf{C}}}{2} - \mathbf{Div}\,\mathbf{Q} + \rho\mathbf{r}\ \text{in}\ \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \mathbf{Q} = -\kappa\theta\nabla\theta\ \text{in}\ \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \end{cases} \quad (8)$$

Where $\mathbf{f}$ and $\mathbf{r}$ denote respectively the force vector and the heat source in $\Omega \subset (\mathbb{R}^d \times \mathbb{R}_+)$.

The first Piola-Kirchhoff stress tensor $\mathbb{P}$ is given by $\mathbb{P} = \mathbb{F}\,\mathbf{S}$. Then, we have $\mathbb{P} = \mathbb{F}(\mathbf{S^e} + \mathbf{S^v})$.

$$\begin{cases} \mathbf{Div}\,[\,\mathbb{F}(\mathbf{S^e} + \mathbf{S^v})] + \rho\mathbf{b} = \rho\dfrac{\partial^2\mathbf{u}}{\partial t^2}\ \text{in}\ \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \rho\dot{e} = (\mathbf{S^e} + \mathbf{S^v}){:}\dfrac{\dot{\mathbf{C}}}{2} - \mathbf{Div}\,\mathbf{Q} + \rho\mathbf{r}\ \text{in}\ \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \mathbf{Q} = -\kappa\theta\nabla\theta\ \text{in}\ \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \end{cases}$$
$$(9)$$

Where $\mathbb{F}$ is the strain gradient, $\mathbb{F} = \nabla\varphi(\mathbf{x}, t)$, $\varphi(\mathbf{x}, t)$ denotes the holonomic transformation of the $\Omega \subset \mathbb{R}^d$. with the condition $\det\mathbb{F} > 0$. We have the relation

$\mathbf{C} = \mathbb{F}^\mathbf{T}\mathbb{F}$,

$\dot{\mathbf{C}} = \dot{\mathbb{F}}^\mathbf{T}\mathbb{F} + \mathbb{F}^\mathbf{T}\dot{\mathbb{F}}$,

The internal energy e is given by $e = s\theta + \psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i)$, and then we have

$\dot{e} = s\dot\theta + \dot{s}\theta + \dot\psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i)$,

The governing equation can be written as

$$\begin{cases} \mathbf{Div}\,[\,\mathbb{F}(\mathbf{S^e} + \mathbf{S^v})] + \rho\mathbf{b} = \rho\dfrac{\partial^2\mathbf{u}}{\partial t^2}\ \text{in}\ \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \rho[s\dot\theta + \dot{s}\theta + \dot\psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i)] = (\mathbf{S^e} + \mathbf{S^v}){:}\dfrac{\dot{\mathbf{C}}}{2} \\[1mm] \qquad -\mathbf{Div}\,\mathbf{Q} + \rho\mathbf{r}\ \text{in}\ \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[1mm] \qquad \mathbf{Q} = -\kappa\theta\nabla\theta\ \text{in}\ \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \end{cases}$$
$$(10)$$

We have,

$$\begin{cases} \mathbf{Div}\,[\,\mathbb{F}(\mathbf{S^e} + \mathbf{S^v})] + \rho\mathbf{b} = \rho\dfrac{\partial^2\mathbf{u}}{\partial t^2}\ \text{in}\ \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \rho c\dfrac{\partial\theta}{\partial t} - \rho\theta\dfrac{\partial^2\psi}{\partial\theta\partial\mathbf{C}}{:}\dot{\mathbf{C}} - \rho\left(\dfrac{\partial\psi}{\partial\xi_i} - \theta\dfrac{\partial^2\psi}{\partial\theta\partial\xi_i}\right){:}\dot{\xi_i} - \mathbf{Div}\,\mathbf{Q} \\[1mm] \qquad +\rho\mathbf{r} = 0\ \text{in}\ \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[1mm] \qquad \mathbf{Q} = -\kappa\theta\nabla\theta\ \text{in}\ \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \end{cases}$$
$$(11)$$

The boundary conditions are:

- Mechanical boundary condition

$$\begin{cases} \mathbb{F}(\mathbf{S^e} + \mathbf{S^v}).\mathbf{n} = T_M(\mathbf{n}, M) \\ \mathbf{u} = 0 \\ \mathbb{F}(\mathbf{S^e} + \mathbf{S^v}).\mathbf{n} = 0 \\ \mathbb{F}(\mathbf{S^e} + \mathbf{S^v}).\mathbf{n} = 0 \end{cases}$$

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Where $\mathbf{n}$ denote the outer unit vector, and $\boldsymbol{T}_M(\mathbf{n}, \boldsymbol{M})$ is the external body force applied in some part of Ω.

- Thermal boundary condition

$$\begin{cases} -\kappa\theta\nabla\theta.\,\mathbf{n} = 0 \\ -\kappa\theta\nabla\theta.\,\mathbf{n} = 0 \\ \theta = \theta_0 \\ -\kappa\theta\nabla\theta.\,\mathbf{n} = k_c(\theta - \theta_f) \end{cases}$$

Where k_c denotes the convection coefficient, θ_f denote the reference temperature.

Finally, we have:

$$\begin{cases} \mathbf{Div}\,[\,\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v})] + \rho\mathbf{b} = \rho\frac{\partial^2\mathbf{u}}{\partial t^2} \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \mathbf{S^e} = 2\rho\frac{\partial}{\partial\mathbf{C}}\,\psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i) \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \mathbf{S^v} = \frac{\partial}{\partial\dot{\mathbf{C}}}\,\chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_i}; \theta, \mathbf{C}) \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \rho c\frac{\partial\theta}{\partial t} - \rho\theta\frac{\partial^2\psi}{\partial\theta\partial\mathbf{C}}:\dot{\mathbf{C}} - \rho\left(\frac{\partial\psi}{\partial\xi_i} - \theta\frac{\partial^2\psi}{\partial\theta\partial\xi_i}\right):\dot{\xi_\iota} - \mathbf{Div}\,\mathbf{Q} \\[2mm] \qquad + \rho\mathbf{r} = 0 \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \qquad \mathbf{Q} = -\kappa\theta\nabla\theta \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \end{cases}$$

We consider two cases:

- We consider that the effect of the heat produced by the internal variable ξ_i is equal to zero, $\rho\left(\frac{\partial\psi}{\partial\xi_i} - \theta\frac{\partial^2\psi}{\partial\theta\partial\xi_i}\right):\dot{\xi_\iota} = 0$.

In this case the governing equation is given by:

$$\begin{cases} \mathbf{Div}\,[\,\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v})] + \rho\mathbf{b} = \rho\frac{\partial^2\mathbf{u}}{\partial t^2} \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \mathbf{S^e} = 2\rho\frac{\partial}{\partial\mathbf{C}}\,\psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i) \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \mathbf{S^v} = \frac{\partial}{\partial\dot{\mathbf{C}}}\,\chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_i}; \theta, \mathbf{C}) \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \rho c\frac{\partial\theta}{\partial t} - \rho\theta\frac{\partial^2\psi}{\partial\theta\partial\mathbf{C}}:\dot{\mathbf{C}} - \mathbf{Div}\,\mathbf{Q} + \rho\mathbf{r} = 0 \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \qquad \mathbf{Q} = -\kappa\theta\nabla\theta \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \end{cases}$$

- We consider that the effect of the heat produced by the internal variable ξ_i is equal to zero, $\rho\left(\frac{\partial\psi}{\partial\xi_i} - \theta\frac{\partial^2\psi}{\partial\theta\partial\xi_i}\right):\dot{\xi_\iota} \neq 0$.

In this case the governing equation is given by:

$$\begin{cases} \mathbf{Div}\,[\,\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v})] + \rho\mathbf{b} = \rho\frac{\partial^2\mathbf{u}}{\partial t^2} \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \mathbf{S^e} = 2\rho\frac{\partial}{\partial\mathbf{C}}\,\psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i) \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \mathbf{S^v} = \frac{\partial}{\partial\dot{\mathbf{C}}}\,\chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_i}; \theta, \mathbf{C}) \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \rho c\frac{\partial\theta}{\partial t} - \rho\theta\frac{\partial^2\psi}{\partial\theta\partial\mathbf{C}}:\dot{\mathbf{C}} - \rho\left(\frac{\partial\psi}{\partial\xi_i} - \theta\frac{\partial^2\psi}{\partial\theta\partial\xi_i}\right):\dot{\xi_\iota} - \mathbf{Div}\,\mathbf{Q} \\[2mm] \qquad + \rho\mathbf{r} = 0 \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \qquad \mathbf{Q} = -\kappa\theta\nabla\theta \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \end{cases}$$

For the soft biological tissue and for the sample HEMA-EGDMA, we propose the thermodynamics potential in $\Omega \subset (\mathbb{R}^d \times \mathbb{R}_+)$.

$$\begin{cases} \psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i) = \frac{\lambda}{2}\exp[\mu(\mathbb{I}_1 - 3)] - \frac{\lambda\mu}{4} \\ (\mathbb{I}_2 - 3) - (\lambda + 2\mu)(\mathbb{I}_3 - 1) - (3\lambda + 2\mu)\kappa(\theta - \theta_0)\mathbb{I}_3 \\ \qquad\qquad - \frac{c}{2\theta_0}(\theta - \theta_0)^2 \\ \chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_\iota}; \theta, \mathbf{C}) = \frac{\eta}{2}\mathbb{J}_2(\mathbb{I}_1 - 3) \\ \qquad\qquad + \frac{1}{2}\kappa \parallel \overline{\nabla\theta} \parallel^2 + \mathbb{i}(\dot{\xi_\iota}) \end{cases}$$

Where $\mathbb{i}(\dot{\xi_\iota})$ denotes an indicative function, we assume that the Lamé's constants $\lambda = \lambda(\xi_i)$ and $\mu = \mu(\xi_i)$.

We propose the governing equation of the internal variable ξ_i: We assume that we have one internal variable, and his evolution law is given by:

$$\begin{cases} \mathbb{i}(\dot{\xi_\iota}) + \frac{\partial\psi}{\partial\xi_i} \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm] \mathbb{i}(0) = \mathbf{I} \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \end{cases}$$

4. NUMERICAL METHODS

The numerical method used to solve the problem is based on finite element formulation (FEM). We use the software Comsol Multiphysics to solve the governing equation in $\Omega \subset (\mathbb{R}^d \times \mathbb{R}_+)$.

So we introduce the variational principle and the finite element discretization. For the two cases we consider respectively $\delta\mathbf{u}$, $\delta\theta$ and $\delta\xi_i$ the virtual displacement, temperature and the internal variable.

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- **Case 1:**

$$\begin{cases}
\text{Div}\,[\,\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v})] + \rho\mathbf{b} = \rho\dfrac{\partial^2 \mathbf{u}}{\partial t^2} \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm]
\mathbf{S^e} = 2\rho\dfrac{\partial}{\partial \mathbf{C}}\,\psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i) \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm]
\mathbf{S^v} = \dfrac{\partial}{\partial \dot{\mathbf{C}}}\,\chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_i}; \theta, \mathbf{C}) \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm]
\quad\begin{cases}
\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v}).\,\mathbf{n} = T_M(\mathbf{n}, \boldsymbol{M}) \\
\mathbf{u} = 0 \\
\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v}).\,\mathbf{n} = 0 \\
\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v}).\,\mathbf{n} = 0
\end{cases} \\[8mm]
\rho c\dfrac{\partial \theta}{\partial t} - \rho\theta\dfrac{\partial^2 \psi}{\partial \theta \partial \mathbf{C}}:\dot{\mathbf{C}} - \text{Div}\,\mathbf{Q} + \rho r = 0 \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm]
\mathbf{Q} = -\kappa\theta\nabla\theta \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm]
\quad\begin{cases}
-\kappa\theta\nabla\theta.\,\mathbf{n} = 0 \\
-\kappa\theta\nabla\theta.\,\mathbf{n} = 0 \\
\theta = \theta_0 \\
-\kappa\theta\nabla\theta.\,\mathbf{n} = k_c(\theta - \theta_f)
\end{cases} \\[8mm]
\hat{\mathbb{I}}(\dot{\xi}_\iota) + \dfrac{\partial \psi}{\partial \xi_i} \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm]
\hat{\mathbb{I}}(0) = \mathbf{I} \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+)
\end{cases}$$

Using the Galerkin's Method the weak formulation of t case 1 is given by:

$$\begin{cases}
\displaystyle\int_\Omega \text{Div}\,[\,\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v})]\delta\mathbf{u}\,d\Omega + \int_\Omega \rho\mathbf{b}\delta\mathbf{u}d\Omega = \rho\int_\Omega \dfrac{\partial^2 \mathbf{u}}{\partial t^2}\delta\mathbf{u}d\Omega \\[4mm]
\displaystyle\int_\Omega \rho c\dfrac{\partial\theta}{\partial t}\delta\theta d\Omega - \int_\Omega \rho\theta\dfrac{\partial^2 \psi}{\partial\theta\partial\mathbf{C}}:\dot{\mathbf{C}}\,\delta\theta d\Omega - \int_\Omega \text{Div}\,\mathbf{Q}\,\delta\theta d\Omega \\[4mm]
\qquad\qquad + \displaystyle\int_\Omega \rho r\,\delta\theta d\Omega = 0 \\[4mm]
\displaystyle\int_\Omega \hat{\mathbb{I}}(\dot{\xi}_\iota)\delta\xi_i\,d\Omega + \int_\Omega \dfrac{\partial\psi}{\partial\xi_i}\delta\xi_i\,d\Omega = 0
\end{cases}$$

We have,

$$\begin{cases}
-\displaystyle\int_\Omega [\,\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v})]:\nabla\delta\mathbf{u}\,d\Omega + \int_{\partial\Omega} \hat{\sigma}.\,\delta\mathbf{u}.\,\mathbf{n}\,d(\partial\Omega) \\[4mm]
\qquad + \displaystyle\int_\Omega \rho\mathbf{b}\delta\mathbf{u}d\Omega = \rho\int_\Omega \dfrac{\partial^2 \mathbf{u}}{\partial t^2}\delta\mathbf{u}d\Omega \\[4mm]
\displaystyle\int_\Omega \rho c\dfrac{\partial\theta}{\partial t}\delta\theta d\Omega - \int_\Omega \rho\theta\dfrac{\partial^2 \psi}{\partial\theta\partial\mathbf{C}}:\dot{\mathbf{C}}\,\delta\theta d\Omega - \int_\Omega \mathbf{Q}.\nabla\delta\theta d\Omega \\[4mm]
\qquad - \displaystyle\int_{\partial\Omega} \mathbf{Q}.\,\delta\theta.\,\mathbf{n}\,d(\partial\Omega) + \int_\Omega \rho r\,\delta\theta d\Omega = 0 \\[4mm]
\displaystyle\int_\Omega \hat{\mathbb{I}}(\dot{\xi}_\iota)\delta\xi_i\,d\Omega + \int_\Omega \dfrac{\partial\psi}{\partial\xi_i}\delta\xi_i\,d\Omega = 0
\end{cases}$$

The weak formulation is computed with Comsol multiphysics of the problem and their constitutive law.

- **Case 2:**

$$\begin{cases}
\text{Div}\,[\,\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v})] + \rho\mathbf{b} = \rho\dfrac{\partial^2 \mathbf{u}}{\partial t^2} \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm]
\mathbf{S^e} = 2\rho\dfrac{\partial}{\partial \mathbf{C}}\,\psi(\mathbb{I}_1(\mathbf{C}), \mathbb{I}_2(\mathbf{C}), \mathbb{I}_3(\mathbf{C}), \theta, \xi_i) \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm]
\mathbf{S^v} = \dfrac{\partial}{\partial \dot{\mathbf{C}}}\,\chi(\mathbb{J}_1, \mathbb{J}_2, \mathbb{J}_3, \mathbb{J}_4, \mathbb{J}_5, \mathbb{J}_6, \mathbb{J}_7, \overline{\nabla\theta}, \overline{\nabla\xi_i}; \theta, \mathbf{C}) \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm]
\quad\begin{cases}
\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v}).\,\mathbf{n} = T_M(\mathbf{n}, \boldsymbol{M}) \\
\mathbf{u} = 0 \\
\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v}).\,\mathbf{n} = 0 \\
\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v}).\,\mathbf{n} = 0
\end{cases} \\[8mm]
\rho c\dfrac{\partial \theta}{\partial t} - \rho\theta\dfrac{\partial^2 \psi}{\partial \theta \partial \mathbf{C}}:\dot{\mathbf{C}} - \rho\left(\dfrac{\partial\psi}{\partial\xi_i} - \theta\dfrac{\partial^2 \psi}{\partial\theta\partial\xi_i}\right):\dot{\xi}_\iota - \text{Div}\,\mathbf{Q} \\[2mm]
\qquad + \rho r = 0 \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm]
\mathbf{Q} = -\kappa\theta\nabla\theta \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm]
\quad\begin{cases}
-\kappa\theta\nabla\theta.\,\mathbf{n} = 0 \\
-\kappa\theta\nabla\theta.\,\mathbf{n} = 0 \\
\theta = \theta_0 \\
-\kappa\theta\nabla\theta.\,\mathbf{n} = k_c(\theta - \theta_f)
\end{cases} \\[8mm]
\hat{\mathbb{I}}(\dot{\xi}_\iota) + \dfrac{\partial \psi}{\partial \xi_i} \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+) \\[2mm]
\hat{\mathbb{I}}(0) = \mathbf{I} \text{ in } \Omega \subset (\mathbb{R}^d \times \mathbb{R}_+)
\end{cases}$$

The weak formulation can be written as:

$$\int_\Omega \text{Div}\,[\,\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v})]\delta\mathbf{u}\,d\Omega + \int_\Omega \rho\mathbf{b}\delta\mathbf{u}d\Omega = \rho\int_\Omega \dfrac{\partial^2 \mathbf{u}}{\partial t^2}\delta\mathbf{u}d\Omega$$

$$\int_\Omega \rho c\dfrac{\partial\theta}{\partial t}\delta\theta d\Omega - \int_\Omega \rho\theta\dfrac{\partial^2 \psi}{\partial\theta\partial\mathbf{C}}:\dot{\mathbf{C}}\,\delta\theta d\Omega - \int_\Omega \text{Div}\,\mathbf{Q}\,\delta\theta d\Omega$$

$$-\rho\int_\Omega \left(\dfrac{\partial\psi}{\partial\xi_i} - \theta\dfrac{\partial^2 \psi}{\partial\theta\partial\xi_i}\right):\dot{\xi}_i\delta\theta d\Omega + \int_\Omega \rho r\,\delta\theta d\Omega = 0$$

$$\int_\Omega \hat{\mathbb{I}}(\dot{\xi}_\iota)\delta\xi_i\,d\Omega + \int_\Omega \dfrac{\partial\psi}{\partial\xi_i}\delta\xi_i\,d\Omega = 0$$

Then,

$$-\int_\Omega [\,\mathbb{F}\,(\mathbf{S^e} + \mathbf{S^v})]:\nabla\delta\mathbf{u}\,d\Omega + \int_\Omega \rho\mathbf{b}\delta\mathbf{u}d\Omega = \rho\int_\Omega \dfrac{\partial^2 \mathbf{u}}{\partial t^2}\delta\mathbf{u}d\Omega$$

$$\int_\Omega \rho c\dfrac{\partial\theta}{\partial t}\delta\theta d\Omega - \int_\Omega \rho\theta\dfrac{\partial^2 \psi}{\partial\theta\partial\mathbf{C}}:\dot{\mathbf{C}}\,\delta\theta d\Omega - \int_\Omega \mathbf{Q}.\nabla\,\delta\theta d\Omega$$

$$-\int_{\partial\Omega} \mathbf{Q}.\,\delta\theta.\,\mathbf{n}\,d(\partial\Omega) = 0$$

$$-\rho\int_\Omega \dfrac{\partial\psi}{\partial\xi_i}:\dot{\xi}_i\delta\theta d\Omega - \rho\int_\Omega \theta\dfrac{\partial^2 \psi}{\partial\theta\partial\xi_i}:\dot{\xi}_i\delta\theta d\Omega + \int_\Omega \rho r\,\delta\theta d\Omega$$

$$\int_\Omega \hat{\mathbb{I}}(\dot{\xi}_\iota)\delta\xi_i\,d\Omega + \int_\Omega \dfrac{\partial\psi}{\partial\xi_i}\delta\xi_i\,d\Omega = 0$$

The weak formulation is computed with Comsol multiphysics of the problem and their constitutive law.

5. SOME RESULTS AND DISCUSSIONS

We assume two cases of cyclic mechanical loads. For each test, we change the frequency of the load in order to study the material response. We particularly analyze the sensitivity of the material in low frequency. The application of the cyclic load is done in three steps. The

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first step is the pre-loading, the second is the loading with the cyclic load and the third step is the unloading. For the first case we use the magnitude and the second case take into account of the magnitude change. Two cyclic mechanical loads were studied. For each test, we change the load frequency. Figures report entropy production during cyclic loading.
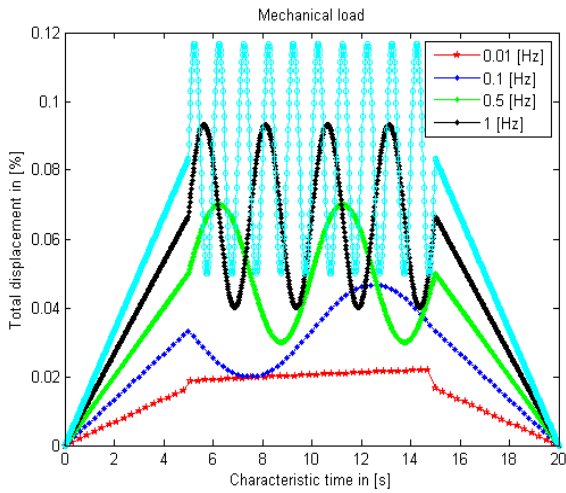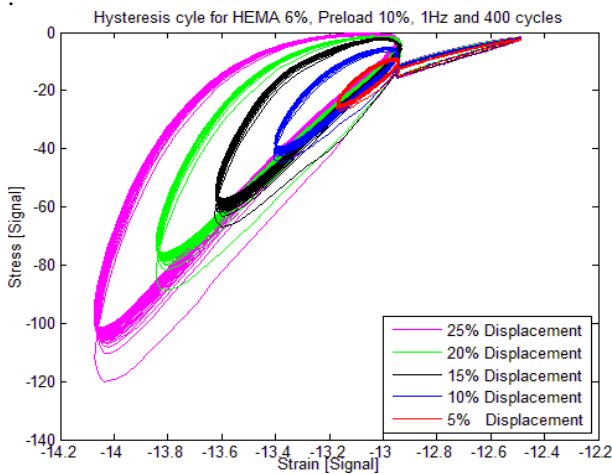

Figure 2: Mechanical load vs. time
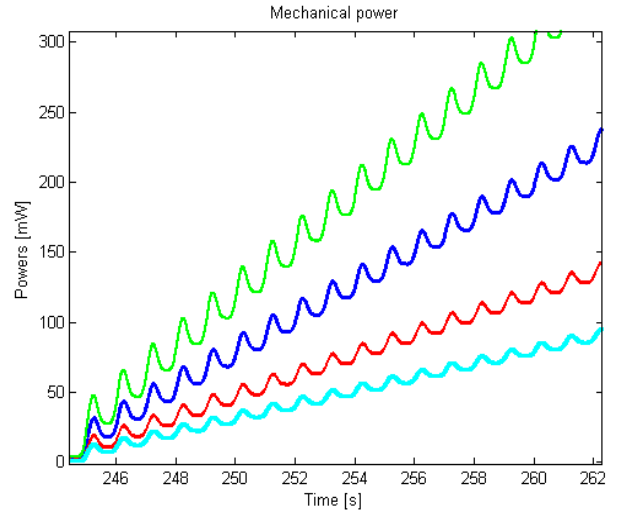
.

Figure 3: Hysteresis curves of the material

Figure 4: Mechanical Power vs. time

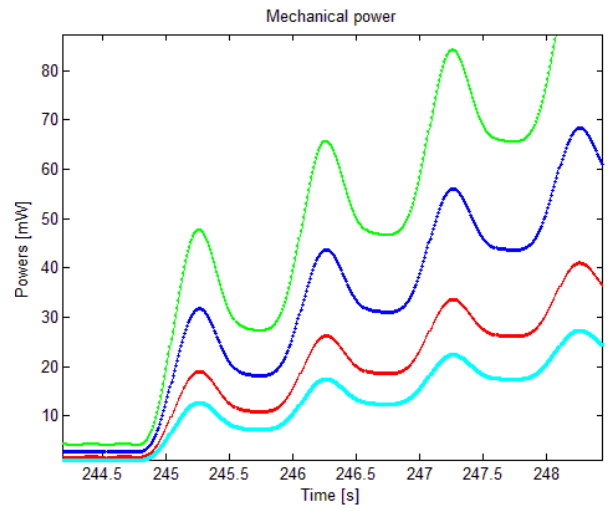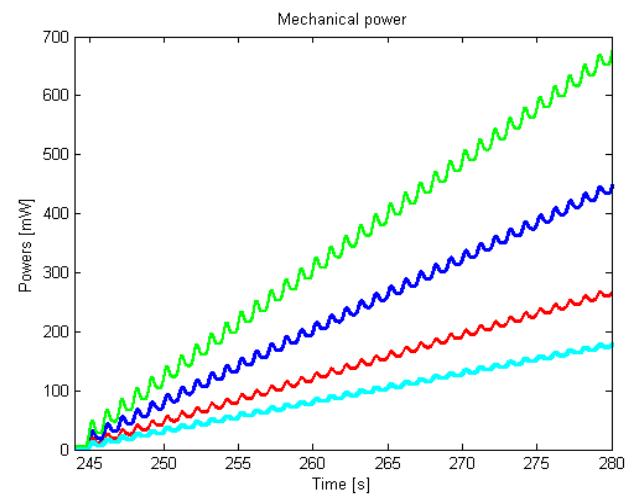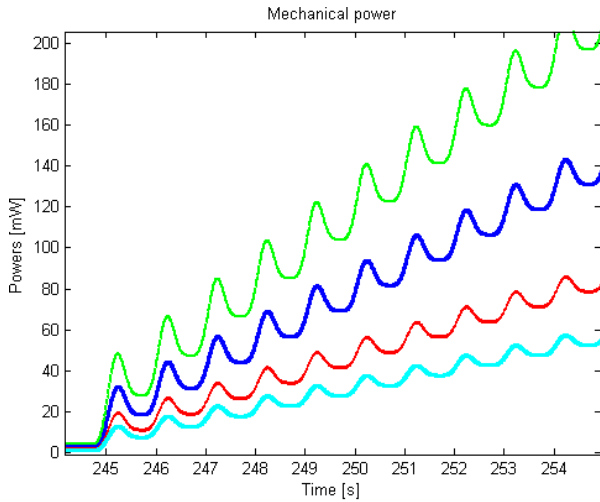Figure 5: Mechanical Power vs. time, obtained by zooming the figure 4.in order to show the behavior in small time

Figure 6: Mechanical Power vs. time

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Figure 7: Mechanical Power vs. time, obtained by zooming the figure 6, in order to show the behavior in small time.
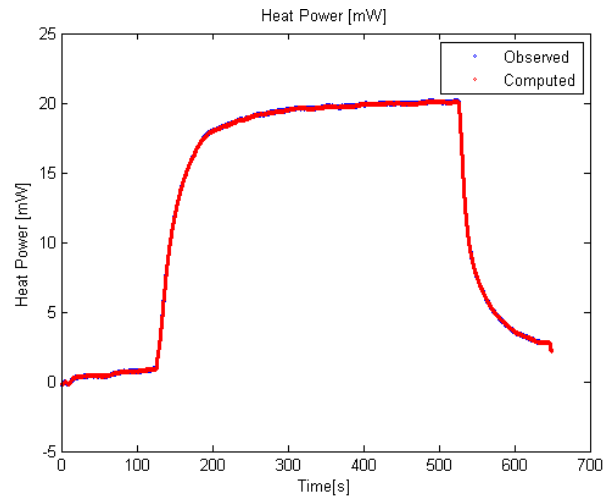

Figure 8: Mechanical Power vs. time

6. CONCLUDING REMARKS

Theoretical model was successfully developed in the present work to analyze the thermo-mechanical behavior of hydrogel matrix HEMA-EGDMA. New constitutive equation is proposed in thermo-viscoelasticity by assuming an adiabatic system.

Then, two new thermodynamics potentials and the energy conservation for this material were proposed. The thermo-mechanical of the coupled and transient system was solved by using simplified geometry. Fundamental and general trends can be clearly illustrated with validation with the help of the experimental measurement. New numerical approach to solve the coupled partial differential equation (governing equation) based on finite element method has been developed.

Reciprocal interaction between mechanical and thermal energy has been performed by this approach. This approach has revealed detailed information to qualify the temperature change and characterize the entropy production in the hydrogel matrix under cyclic loads. These results were shown that the heat effects to the dissipation energy were significant and may exploited to control the drug delivery device driven by the temperature.

ACKNOWLEDGMENTS

APPENDIX
A- Notations
We introduce several notations which will be throughout this work. Let us:

h_0 : Henry constant
ρ: Density
$\rho\mathbf{b}$: Volumic force
$\mathbf{u}$: Displacement
$\mathbf{r}$: Heat source
$\mathbf{P}$: Piola-Kirchhoff's first stress tensor
$\mathbb{F}$: Strain gradient
$\mathbf{S}$: Piola-Kirchhoff's second stress tensor
$\mathbf{S^e}$: Elastic Piola-Kirchhoff's second stress tensor
$\mathbf{S^v}$: Viscous Piola-Kirchhoff's second stress tensor
$\mathbf{E}$: Green-Lagrange's strain tensor
$\mathbf{C}$: Cauchy-Green's strain tensor
$\mathbf{I}$: Identity matrix
s: Entropy
ρ: Density
e: Internal energy
σ: Cauchy's stress tensor
θ: Temperature
θ_f: Reference temperature
θ_0: Prescribed temperature
k_c : Convection coefficient
ψ: Helmholtz free energy
χ: Dissipation potential
ξ_i: Internal variable
κ: Conduction coefficient of the hydrogel
$\mathbf{Q}^{rev}$: Reversible heat
$\mathbf{Q}^{irr}$: Irreversible heat
$\mathbf{n}$: Outer unit normal vector
Ω_s : Polymer domain

B- Operators
$\nabla.$: Divergence operator
∇: Gradient operator
$\cdot$: Scalar product
$\times$: Vector product
$\otimes$: Tensor product
$\dot{x}$: Temporal derivative operator of the variable x
$\mathbf{det}(...)$: Determinant
$\mathbf{Tr}(...)$: Trace

C- Tensor Invariant
$\mathbb{I}_1$: First invariant of the stress tensor
$\mathbb{I}_2$: Second invariant stress tensor
$\mathbb{I}_3$: Third stress tensor

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$$\mathbb{J}_1 = \mathbf{Tr\dot{C}},$$
$$\mathbb{J}_2 = \mathbf{Tr\dot{C}^2},$$
$$\mathbb{J}_3 = \mathbf{Tr\dot{C}^3},$$
$$\mathbb{J}_4 = \mathbf{Tr(C\dot{C})},$$
$$\mathbb{J}_5 = \mathbf{Tr(C^2\dot{C})},$$
$$\mathbb{J}_6 = \mathbf{Tr(C\dot{C}^2)},$$
$$\mathbb{J}_7 = \mathbf{Tr(C^2\dot{C}^2)}.$$

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