

A numerical study on the heat transfer generated by a piezoelectric transducer in a microfluidic system

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Abstract. The present work describes the modelling of heat transfer produced by the acoustic streaming phenomenon, generated through a piezoelectric transducer in a microagitator. Besides the fluids mixing, this phenomenon also promotes the fluids heating. The numerical approach used in this work comprises three main groups of equations: the piezoelectric, the compressible Navier-Stokes, and the heat transfer equations. It was concluded that the heat transfer due to the acoustic wave propagation, without other external heat sources, is not sufficient to increase significantly the fluid temperature.

1. Introduction

A new generation of miniaturized diagnostic systems, with immediate, low-cost and reliable results, has been developed, in order to face the healthcare sector challenges [1], [2]. These microfluidic devices tend to be used for point-of-care applications, for the detection and quantitative evaluation of several biomolecules in biological fluids, since they feature small size, low power consumption, high analytical performance and potential for system integration, high sensitivity and precision [3]. The small dimension of those devices leads to a difficulty in driving and mixing the fluids, which are key requirements for the success of the device. The resultant flow is laminar, due to the low Reynolds number (typically less than 1), which limits the movement of fluids and impedes the formation of vortices [4] – [6]. Thus, molecular diffusion becomes the basic mixing mechanism, resulting in a slow mixing process, in particular for large biomolecules with low diffusivity [7].

The microagitation generated by a piezoelectric transducer can be a solution to accelerate the fluids mixing and overcome the slow diffusion times [8] – [10]. This phenomenon, called acoustic streaming, was initially studied by Rayleigh [11], and is based on the absorption and propagation of acoustic waves by the fluids, resulting in a force in the direction of propagation and acoustic attenuation, thereby promoting pressure gradients that generate the flows [12] – [14]. The harmonic oscillation of the solid boundary near the fluid, generated by the piezoelectric effect, causes the propagation of the acoustic waves in the fluid and a steady mean flow field. The streaming effects result from the non-linearity of the Navier-Stokes equations, when combined with viscosity [13].

The poly(vinylidene fluoride) – PVDF piezoelectric polymer, in its β phase, can be used as the transducer material for the generation of acoustic waves and, consequently, for improving the

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microagitation process [15], [16], since it has the largest piezoelectric response among the polymers, as well as low acoustic and mechanical impedance, which are important for the generation and propagation of acoustic waves in the fluids [17]. Furthermore, β -PVDF features some interesting properties for incorporation in microfluidic devices [4], [16], [17]. The acoustic streaming phenomenon at microscale for promoting fluid flows, as well as the viability of using PVDF in its β phase as transducer, are already being studied, numerically and experimentally, by our research team [16], [18]. Besides the kinetic energy, the acoustic energy is also converted into thermal energy, through the effects of viscous dissipation and heat conduction and convection [19]. Since the acoustic microagitation is characterized by the referred production of heat, as the acoustic waves propagate through the fluid [14] this phenomenon becomes advantageous for the majority of the biological fluids analysis, which should be performed at an optimal temperature of 37° C.

Therefore, the main objective of this article is the study of the heating effect generated by the acoustic microagitation. The presented work comprises the modelling and simulation of the heat transfer phenomenon during acoustic streaming, implemented in COMSOL Multiphysics software.

2. Background

The numerical model of the problem comprises a separated analysis of the piezoelectric effect, the compressible fluid flow and the heating in the microfluidic domain.

2.1. Piezoelectricity

Piezoelectricity is a property exhibited by certain materials which produce an electric polarization, when exposed to a mechanical strain in suitable directions. When the material is subjected to a strain, the molecular structure of the material is deformed, and the electrical charge distribution on the surface of the material is changed. As a consequence, an electric potential is generated between two electrodes placed on opposite faces of the material (direct piezoelectric effect). The inverse piezoelectric effect occurs when a mechanical strain is produced in response to an external electric field [20], [21] and presents linearity between the electrical field and the resultant displacement [22], [23]. This linear phenomenon is described by the constitutive equations (1) and (2), where d^T and d^E are piezoelectric coefficients, T the mechanical stress, E the electric field, S the mechanical strain, D the electrical displacement, ε the dielectric permittivity and s^E the elastic coefficient [21]. The study of the piezoelectric effect took into account the Rayleigh damping, which depends on the transducer quality factor and on the resonance frequency, and affects the s^E value [23].

$$S = s^E T + d^T E \quad (1)$$

$$D = \varepsilon^T E + d^E T \quad (2)$$

The constitutive equation (1) establishes a relation between the stress tensor T and the strain tensor S , given by $S = (\nabla \mathbf{u} + (\nabla \mathbf{u})^T)/2$, through the Hooke's law, where \mathbf{u} is the mechanical displacement of a piezoelectric material [24]. Equation (2) is an analogy of the Hooke's law applied to the electric displacement. Besides the constitutive relations, the piezoelectric effect model also solves a set of equations for the balance of momentum and electric field [24]. The mechanical displacement \mathbf{u} of a piezoelectric material is given by the momentum balance equation (3), where ρ is the density and b is the volume force acting in the piezoelectric material.

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} - \nabla \cdot T = b \quad (3)$$

To complete the set of equations to be solved, it is considered a Maxwell equation, given by (4).

$$\nabla \cdot D = 0 \quad (4)$$

2.2. Fluid flow and heat transfer

When the piezoelectric transducer is actuated, the boundary oscillation near the fluid generates acoustic waves that propagate into the fluid, inducing the flow. The flow in the microfluidic domain is governed by the compressible Navier-Stokes equations, which comprise the momentum equation (5) and the continuity equation (6) [25], where ρ is the fluid density, u the velocity field vector, p the pressure, η the dynamic viscosity, κ the dilatational viscosity, F the volume force field, I the identity matrix and $-pI + \eta(\nabla u + (\nabla u)^T) - \left(\frac{2\eta}{3} - \kappa\right)(\nabla \cdot u)I = \Sigma$ the Newtonian stress tensor.

$$\rho \frac{\partial u}{\partial t} + \rho u \cdot \nabla u = \nabla \cdot [-pI + \eta(\nabla u + (\nabla u)^T) - \left(\frac{2\eta}{3} - \kappa\right)(\nabla \cdot u)I] + F \quad (5)$$

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (6)$$

The compressible Navier-Stokes equations are applied since the fluid density varies as a result of pressure oscillations (due to the compression and decompression of the acoustic waves) [25], [26].

The great difference between the timescales of piezoelectric vibration (period of 0.1 μ s) and global heating (minutes) leads to the necessity of developing an accurate approach to overcome that difference and evaluate the heating of the microfluidic domain. The problem was decomposed in two parts, one intended for short time scales and another one for long time scales. Therefore, the numerical approach to solve the acoustic streaming and heat transfer problems considers an expansion of the variables presented in the Navier-Stokes equations – density, pressure and velocity – as a sum of constant, first order and second order values [14], [27]. The first order components (equations (7) and (8)) represent the damped propagation of the acoustic wave and provide an analysis of the instantaneous flow. After determining the time average values of the first order terms, the second order system (equations (9) and (10)) can be solved. The second order system considers the first order solution as known data and describes the mass and body force sources, evaluating the mean global flow through the acoustic streaming effects in a large time scale [14], [18].

$$\rho^{(0)} \frac{\partial u^{(1)}}{\partial t} - \nabla \cdot \Sigma^{(1)} = 0 \quad (7)$$

$$\frac{\partial \rho^{(1)}}{\partial t} + \rho^{(0)} \nabla \cdot u^{(1)} = 0 \quad (8)$$

$$\rho^{(0)} \frac{\partial \bar{u}^{(2)}}{\partial t} - \nabla \cdot \bar{\Sigma}^{(2)} = \langle -\rho^{(1)} \frac{\partial u^{(1)}}{\partial t} - \rho^{(0)} (\nabla u^{(1)}) u^{(1)} \rangle \quad (9)$$

$$\frac{\partial \bar{\rho}^{(2)}}{\partial t} + \rho^{(0)} \nabla \cdot \bar{u}^{(2)} = \langle -\nabla \cdot (\rho^{(1)} u^{(1)}) \rangle \quad (10)$$

The superscripts (0), (1) and (2) represent the equilibrium, first and second order values, respectively, of ρ , u and Σ , and $\langle \rangle$ represents a time average term. Based on the first order velocity values it can be determined the dissipation factor, as described in (11), where φ_V is the instantaneous dissipation term, u_x the first order velocity in x direction and u_y the first order velocity in y direction.

$$\varphi_V = 2 \left[\left(\frac{\partial u_x}{\partial x} \right)^2 + \left(\frac{\partial u_y}{\partial y} \right)^2 \right] + \left[\frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y} \right]^2 - \frac{2}{3} \left[\frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} \right]^2 \quad (11)$$

The instantaneous dissipation term is integrated over time and it is obtained a time average value. Multiplying the average dissipation term by the fluid viscosity, it is obtained the viscous dissipation factor, which is applied to the heat transfer equation (12), which includes conductive and convective terms, in order to determine the temperatures within the domain. The dissipation caused by the second order velocities can be despised, since this term presents lower velocities and gradients and, therefore, is negligible.

$$\rho C_p \left(\frac{\partial T}{\partial t} + u_{x2} \frac{\partial T}{\partial x} + u_{y2} \frac{\partial T}{\partial y} \right) = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + \eta \overline{\varphi_v} \quad (12)$$

In (12), $\overline{\varphi_v}$ is the time average dissipation term, T is the second order temperature, C_p is the specific heat capacity, k is the thermal conductivity of the fluid, u_{x2} the second order velocity in x direction and u_{y2} the second order velocity in y direction [28].

2.3. Domain, initial and boundary conditions

The problem was solved in a simple 2D domain, representing a piezoelectric film of β -PVDF (solid subdomain) above a rectangular microcuvette (fluid subdomain), as shown in figure 1. The two subdomains were solved sequentially. First, the equations for the solid subdomain were solved to obtain the amplitude of the mechanical stress in the solid-liquid interface [18]. Afterwards, the amplitude of the mechanical stress was used as an input to solve the equations of the fluid subdomain.

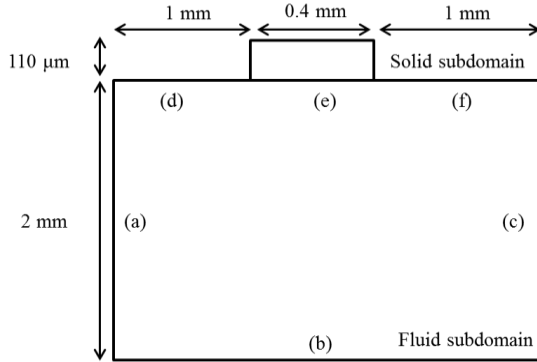


Figure 1. Multiphysics problem domain, representing the solid and fluid subdomains geometries and dimensions. The characters (a) to (f) represent the domain boundaries.

Relatively to the solid subdomain, correspondent to the piezoelectric transducer, COMSOL Multiphysics solves piezoelectric equations in a matrix form (ϵ , s and d coefficients given by [21]). The definition of appropriate boundary conditions is critical. Relatively to the solid subdomain, two groups of boundary conditions are considered: mechanically, the lateral tips of the β -PVDF film are fixed, and the lower and upper boundaries present no mechanical restrictions, which implies that the film vibrates vertically; and electrically: the inferior boundary is connected to the ground, the superior boundary is connected to a sinusoidal voltage of 10 MHz frequency and 20 V amplitude, and the lateral boundaries present electrical continuity. Relatively to the fluidic subdomain, different groups of boundary conditions are applied, for solving the Navier-Stokes and the heat transfer equations. In order to solve the first order Navier-Stokes equations, the fluid subdomain refers to a liquid bounded by walls (a), (b), (c), (d) and (f) where the velocity is zero. In the solid-liquid interface (e) the fluid pressure follows a function sinusoidal in time and uniform in space. Since the microfluidics heating is the main focus of this paper, the piezoelectric effect was simplified. The mechanical stress generated by the transducer was replaced by an oscillatory pressure function (uniform in space) applied to the fluid, with a frequency of 10 MHz and an amplitude peak equal to the peak of the mechanical stress obtained for the solid-liquid interface (around 20 MPa). In the second order Navier-Stokes equations, all the fluid boundaries are defined as walls with zero velocity, expressed by a no slip condition: $u=0$.

Relatively to the heat transfer mode, the piezo-fluid boundary presents heat transfer by conduction, while the other boundary conditions in the domain are defined as walls with natural convective heat transfer between the domain and the exterior. It was considered a $5 \text{ W}/(\text{m}^2\cdot\text{K})$ constant convective heat transfer coefficient. Relatively to the initial conditions, the initial velocities and pressure are zero, and the initial temperature of the liquid in the microcuvette is set to $22 \text{ }^\circ\text{C}$. The domain was meshed with a quadrilateral structured uniform grid with 41664 cells (168 x 248 elements).

3. Results

The following results present the evaluation of microflows generated by acoustic streaming and the consequent heating within a microscale fluidic domain.

3.1. Acoustic streaming results

Figure 2 presents the instantaneous pressure, resulting from the acoustic propagation within the microfluidic domain after a $1 \text{ } \mu\text{s}$ total simulation time, with a $0.01 \text{ } \mu\text{s}$ timestep, determined by solving the first order compressible Navier-Stokes flows. Figure 3 presents the velocity field correspondent to the steady mean global flow, after solving the second order equations in a stationary case.

The instantaneous acoustic propagation leads to a pressure profile formed by high and low pressure bands, with peak amplitudes decreasing as the acoustic wave moves away from the transducer. The distribution of the first order velocity within the domain (not presented in the figures) has the same pattern as the pressure. In figure 3, it can be seen that the actuation of the acoustic transducer generates a global flow with fluids recirculation.

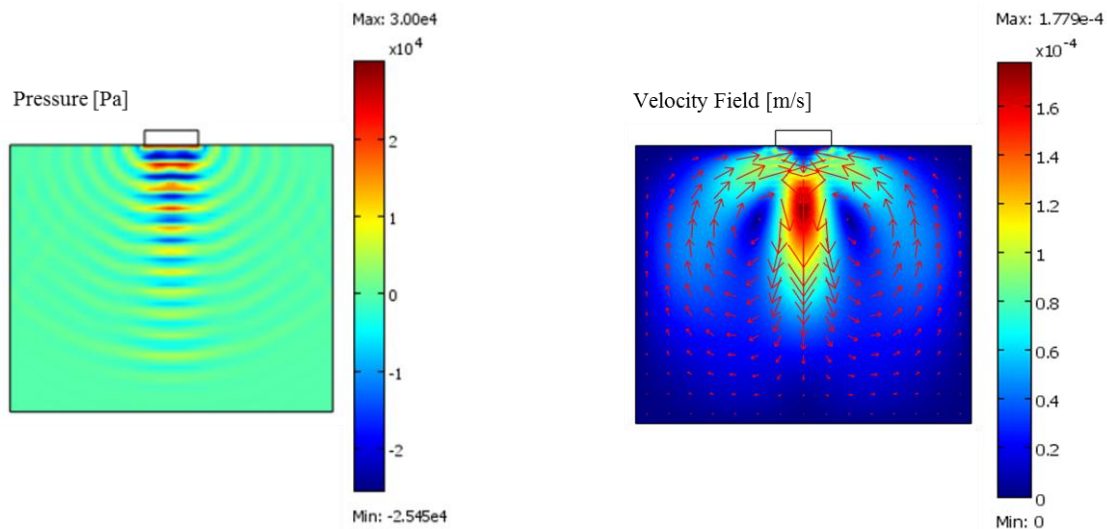


Figure 2. Instantaneous pressure (Pa) in a $2 \text{ mm} \times 2.4 \text{ mm}$ microcuvette filled with a $1 \text{ Pa}\cdot\text{s}$ viscosity fluid and excited with a 20 MPa and 10 MHz sinusoidal pressure, after $1 \text{ } \mu\text{s}$.

Figure 3. Steady velocity field (m/s) in the microcuvette filled with a $1 \text{ Pa}\cdot\text{s}$ viscosity fluid and excited with a 20 MPa and 10 MHz sinusoidal pressure, in a stationary simulation.

3.2. Fluid heating

Based on the first order Navier-Stokes flows, presented in section 2.2, the heat transfer variables were determined. Figure 4 presents the time average viscous dissipation term (a)), calculated during a $1 \text{ } \mu\text{s}$ simulation time, with a $0.01 \text{ } \mu\text{s}$ timestep, and the temperature (b)) after a 10 minutes total simulation time, with a 1 second timestep, within the microscale fluidic domain.

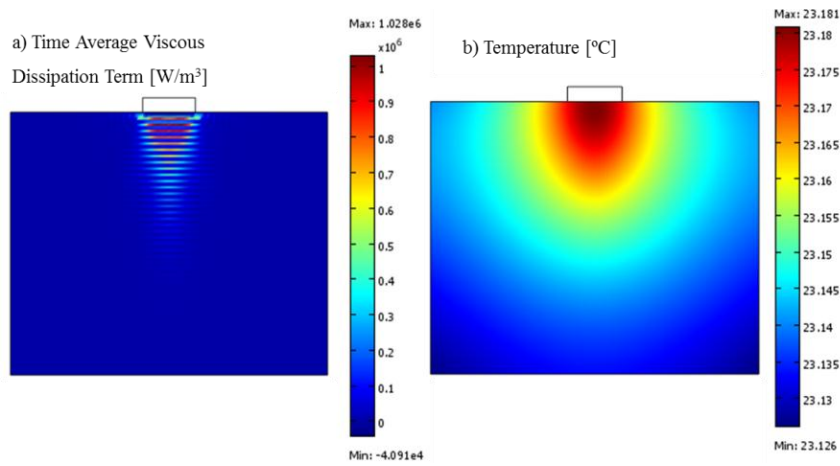


Figure 4. a) Time average viscous dissipation term (W/m^3) and b) Temperature ($^{\circ}\text{C}$) after 10 minutes in the microcuvette filled with a 1 Pa.s fluid and excited with a 20 MPa and 10 MHz sinusoidal pressure.

The viscous dissipation term is highly dependent on the first order Navier-Stokes variables. The peak amplitudes decrease with the distance to the transducer, similarly to the mean acoustic force [29]. The determination of this term was necessary for evaluating the heating of the fluid, over a 10 minutes simulation time. Taking into account the room temperature (22°C), the achieved rise of temperature is less than 1.5°C . There is also a tiny difference in the temperatures in the domain, with a decrease of 0.06°C in the temperature from the top to the bottom of the microcuvette. The temperature differences are minimum since the present model considers only the compressible flow in order to evaluate the heat transfers without external sources. It ignores the heating effect from the piezoelectric transducer, which is expected to help to increase the temperature in the fluid (as preliminary tests by the research team have demonstrated [30]).

3.3. Viscosity effect

It was studied the effect of fluid viscosity in the internal fluid heating. Figure 5 shows the distribution of temperature ($^{\circ}\text{C}$) through the microcuvette, considering fluids with two different viscosities: 1 Pa.s and 0.1 Pa.s.

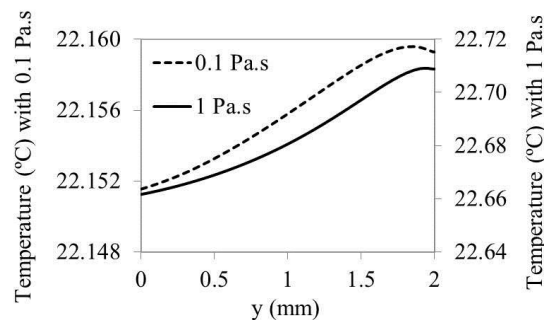


Figure 5. Distribution of temperature ($^{\circ}\text{C}$) after 10 min through a 2 mm depth microcuvette excited by a 10 MHz oscillatory pressure, considering fluids with two different viscosities, simulated in COMSOL Multiphysics. In x-axis, 0 m represents the bottom of the microcuvette and 0.002 m represents the upper limit, near the acoustic source.

From the results it is visible the variation of the temperature with the distance from the transducer, and it is notorious the influence of the viscosity in the achieved results. The 0.1 Pa.s viscosity fluid, has a maximum increase of temperature of 0.236 °C (when compared with the room temperature), while the 1 Pa.s viscosity fluid increases 1.18 °C.

These results suggest that the fluid viscosity has a significant impact in the heat transfer within the domain and, the higher the viscosity, the higher the temperature increase, which is in agreement with the theoretical predictions (section 2.2), which state that the dissipation is higher for higher viscosities. Therefore, it is expected that low viscosity fluids, as water, present insignificant results.

4. Conclusions

This paper presented a model to describe the heat transfer in a microfluidic domain. It was concluded that the heat transfer due to the acoustic wave propagation, without external heat sources, is not able to increase significantly the fluid temperature. It was also concluded that the increase of the fluid viscosity helps improving the viscous dissipation term and, as consequence, leads to superior temperatures. However, the present study doesn't include the heating effect from the piezoelectric transducer, which is expected to favour the increase of the fluid temperature.

Work is ongoing to continue studying the parameters that influence the heating and to implement the dissipation of heat in the polymeric piezoelectric film. After determine the heating in the transducer, results will be compared with the experimental ones achieved by our group, which showed that the acoustic energy generated by a piezoelectric transducer, when transmitted to a fluid, causes its heating [30].

5. References

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