Tutorial 6

Inverse problems in a microchannel

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Abstract. The aim of this work is to present new techniques for the estimation of thermophysical properties in microfluidic devices. The estimations are performed from the experimental measurements of the front face temperature fields of microfluidic chips, using InfraRed (IR) thermography. The inverse methods developed are based on a correlation coefficient. It allows estimating parameters like the thermal diffusivity, the velocity, and also the source term. Different applications will be shown. In the first experiment, we demonstrate how to use our methods for the estimation of Fourier and Peclet numbers in the case of transient flows in microchannels. Then, we will apply those methods for the kinetics characterization of an acid/base chemical reaction. This experiment is realized in co-flow configuration in microchannels and is used to quantify the enthalpy of reaction. Finally, phase change is studied, from freezing of single droplets on free surfaces to crystallization in microchannels. This part of the work focuses on the estimation of source term and its location. All experiments are realized with an IR Camera and rapid image processing using MATLAB software.

1. Introduction

The objective of this tutorial is to present a simple inverse technique and its application to experimental microfluidic problems. During the experiments, the front face temperature field of a microfluidic chip will be recorded by InfraRed (IR) thermography. Then, this temperature field will be processed in order to estimate thermal and flow parameters. The method, based on the calculation of a correlation coefficient, is described for transient state problems. We will see different applications of the method:

- Flow characterization in transient state.
- Application to chemical reaction
- Phase change (ice formation)

2. Key notions

2.1 Experimental setup

Figure 1 shows a scheme of the experimental setup. Measurements are performed thanks to an infrared camera with a lens of focal 25 mm. The flow rate is controlled from the bottom of the chip, thanks to syringe pumps. We impose a 1-D temperature gradient, which is controlled via two Peltier elements:

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we heat on one side and cool on the other one. The gradient has to be orthogonal to the channels we want to look at.

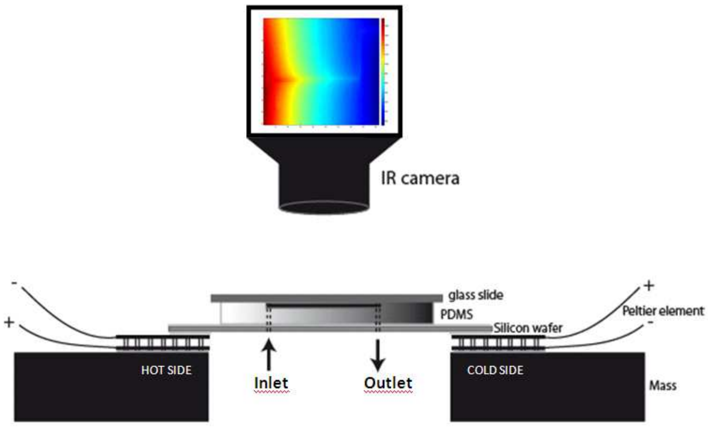


Figure 1. Scheme of the experiment

2.2 Modeling of the system

As presented in the figure. 1. the microfluidic chip to characterize is deposited on a silicon plate where heat fluxes are imposed in order to obtain a thermal gradient. The silicon plate is a high thermal conductive material (λ = 100 $W.m^{-1}.K^{-1}$) with the following dimensions: diameter 50 mm, and thickness 250 µm. As shown on figure 2, the microfluidic chip is composed of insulated PDMS material (λ = 0.1 $W.m^{-1}.K^{-1}$) with a thickness close to 1 cm. The microchannel of 250 µm thickness is surrounded over three faces by this insulator. A thin glass plate covers one face of the channel which is a relative good thermal conductor (λ = 1 $W.m^{-1}.K^{-1}$). The thickness of the glass (e_g) is around 170 µm. Due to the very low thickness of the glass and the very low thermal conductivity of the PDMS in comparison with the one of the glass; we assumed that the thermal diffusion in z direction (i.e., in the thickness of the glass) is negligible and that the glass plate acts as a fin body.

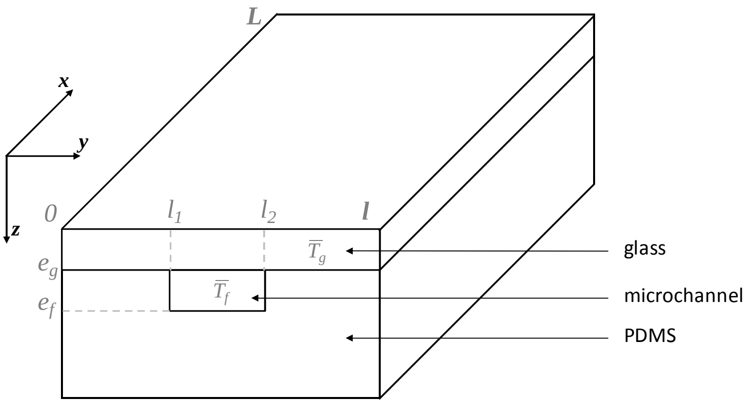


Figure 2. Schematics of the microfluidic chip

The temperature in the glass plate is averaged as expressed in equation (1).

$$\overline{T_g}(x,y,t) = \int_0^{e_g} T_g(x,y,z,t)dz \tag{1}$$

The temperature and the heat source are also averaged in the same way ($\overline{T_f}$ and $\overline{\varphi_f}$). With such conditions, equations in both microchannel and glass plate can be averaged over the z direction as written in equations 2 and 3, repectively.

$$\left|\lambda_f \frac{\partial T_f(x,y,z,t)}{\partial z}\right|_{eg}^{ef} + e_f\overline{\varphi_f}(x,y,t) + \lambda_f e_f\left(\frac{\partial^2\overline{T_f}(x,y,t)}{\partial x^2} + \frac{\partial^2\overline{T_f}(x,y,t)}{\partial y^2}\right) = \rho_f Cp_f e_f\left(v(x,y,t)\frac{\partial\,\overline{T_f}(x,y,t)}{\partial x} + \frac{\partial\,\overline{T_f}(x,y,t)}{\partial t}\right)$$

And the boundary conditions are:

$$-\lambda_f\frac{\partial\,\overline{T_f}(x,y,t)}{\partial x} = \phi_C \quad for\ x = 0 \quad and\ -\lambda_f\frac{\partial\,\overline{T_f}(x,y,t)}{\partial x} = \phi_F \quad for\ x = L \tag{2}$$

$$\frac{\partial\,\overline{T_f}(x,y,t)}{\partial y} = 0 \quad for\ y = l_1 \quad and\ y = l_2$$

$$\overline{T_f}(x,y,t) = 0 \quad for\ t = 0$$

$$-\lambda_f\frac{\partial T_f(x,y,z,t)}{\partial z} = -\lambda_g\frac{\partial T_g(x,y,z,t)}{\partial z} \quad for\ z = e_g$$

$$\frac{\partial T_f(x,y,z,t)}{\partial z} = 0 \quad for\ z = e_f$$

The heat equation in glass plate is written as follow.

$$\left|\lambda_g\frac{\partial T_g(x,y,z,t)}{\partial z}\right|_0^{eg} + \lambda_g e_g\left(\frac{\partial^2\overline{T_g}(x,y,t)}{\partial x^2} + \frac{\partial^2\overline{T_g}(x,y,t)}{\partial y^2}\right) = \rho_g Cp_g e_g\frac{\partial\,\overline{T_g}(x,y,t)}{\partial t}$$

And the boundary conditions are:

$$-\lambda_g\frac{\partial\,\overline{T_g}(x,y,t)}{\partial x} = \phi_C \quad for\ x = 0 \quad and\ -\lambda_g\frac{\partial\,\overline{T_g}(x,y,t)}{\partial x} = \phi_F \quad for\ x = L \tag{3}$$

$$\frac{\partial\,\overline{T_g}(x,y,t)}{\partial y} = 0 \quad for\ y = 0 \quad and\ y = l$$

$$\overline{T_g}(x,y,t) = 0 \quad for\ t = 0$$

$$-\lambda_f\frac{\partial T_f(x,y,z,t)}{\partial z} = -\lambda_g\frac{\partial T_g(x,y,z,t)}{\partial z} \quad for\ z = e_g$$

$$-\lambda_g\frac{\partial T_g(x,y,z,t)}{\partial z} = h\,T_g(x,y,z,t) \quad for\ z = 0$$

Then, as depicted by Fudym et al. [1]we supposed that a local thermal equilibrium is established between the average temperature in z direction of the channel and the glass plate

$$\overline{T_g} = \overline{T_f} = T \tag{4}$$

Therefore, with this assumption and the application of the thermal continuity at the interface, the general in plane analytical thermal model is a local transient advection diffusion equation such as:

$$-h\,T(x,y,0,t)+\ e_f\overline{\varphi_f}(x,y,t)+\left(\lambda_f e_f+\lambda_g e_g\right)\left(\frac{\partial^2 T(x,y,t)}{\partial x^2}+\frac{\partial^2 T(x,y,t)}{\partial y^2}\right)= \rho_f Cp_f e_f v(x,y,t)\frac{\partial\,T(x,y,t)}{\partial x}+\left(\rho_f Cp_f e_f+\rho_g Cp_g e_g\right)\frac{\partial\,T(x,y,t)}{\partial t} \tag{5}$$

As the observable resulting from the measurement is the temperature field obtained with the IR camera. The inverse processing method is built on a numerical finite difference schema applied on each node (or pixel). The previous equation is then rewritten as follow:

$$H_{i,j}^k T_{i,j}^k+\Phi_{i,j}^k+\Delta T_{i,j}^k={Pe^*}_{i,j}^k Tx_{i,j}^k+\left(\frac{1}{{Fo^*}_{i,j}^k}\right)Tt_{i,j}^k \tag{6}$$

With,

$$\left|\begin{array}{l} H_{i,j}^k=\dfrac{h_{i;j}^k\Delta l^2}{\left(\lambda_f e_f+\lambda_g e_g\right)}\ ,\quad \Phi_{i,j}^k=\dfrac{e_f\overline{\varphi_{i,j}^k}\Delta l^2}{\left(\lambda_f e_f+\lambda_g e_g\right)} \\[2ex] \Delta T_{i,j}^k=(T_{i+1,j}^k+T_{i-1,j}^k+T_{i,j+1}^k+T_{i,j-1}^k-4T_{i,j}^k) \\[2ex] Tx_{i,j}^k=\left(T_{i+1,j}^k-T_{i,j}^k\right)\ ,\qquad Tt_{i,j}^k=(T_{i,j}^{k+1}-T_{i,j}^k) \\[2ex] {Pe^*}_{i,j}^k=K1.\dfrac{v_{i,j}^k\Delta l}{{a_f}_{i,j}^k}\qquad and\quad K1=\dfrac{1}{\left(1+\dfrac{\lambda_g e_g}{\lambda_f e_f}\right)} \\[4ex] {Fo^*}_{i,j}^k=K2.\dfrac{{a_f}_{i,j}^k\Delta t}{\Delta l^2}\qquad and\quad K2=\dfrac{\left(1+\dfrac{\lambda_g e_g}{\lambda_f e_f}\right)}{\left(1+\dfrac{\rho_g Cp_g e_g}{\rho_f Cp_f e_f}\right)} \end{array}\right. \tag{7}$$

Where Pe* and Fo* are the relative Peclet and Fourier numbers characterizing the flow and thermal conditions of the system. Here, *Δl* corresponds to the size of the pixels of the IR camera and *Δt* depends on the acquisition frequency. With the IR lens we used, the size of one pixel is equal to 250 µm and the acquisition rate is around 25 to 100 Hz. With the flow rate we used and the section of the channel, the average value of the velocity is closed to 1 mm/s. For the measurements, the chip is horizontal, so the heat losses coefficient h is taken equal to 10 $W.m^{-2}.K^{-1}$. According to the thermal properties of the fluid (usually water or fluids with properties close to water) and the glass wafer, the non-dimensional numbers could be numerically estimated, such as: $H \approx 10^{-3}$, $Pe^* \approx 1$ and $Fo^* \approx 10$. As the heat losses are very small comparing to the Fo and Pe numbers, we assumed to neglect them. Finally, the complete equation is rewritten as follow:

$$\Delta T_{i,j}^k+\Phi_{i,j}^k={Pe^*}_{i,j}^k Tx_{i,j}^k+\left(\frac{1}{{Fo^*}_{i,j}^k}\right)Tt_{i,j}^k \tag{8}$$

In this work, we adopt a step by step approach on the equation 6, in order to estimate parameters one by one. The first experiment is devoted to the simple flow detection in transient state. No internal heat source is generated when a simple flow of water occurs in the microchannel. In those conditions, we will be able to estimate consecutively the Fourier and Peclet numbers, as a calibration of the microsystem. Then, the method will be used for the study of a chemical reaction, allowing estimating the source term. Finally, the same overall method will be illustrated with a different application, formation of ice in microchannels.

2.3 The correlation method

The correlation method applied to IR thermography is derived from the Gauss Markov theorem [2].The entire procedure for a transient state estimation of the Fourier number by such correlation method was described by Pradere et al [3]. Such methodology will be applied to the case of microfluidic devices. Here, the correlation method will be explained using the example of the first experiment: microflows characterization in transient state. The main idea is to use the thermal gradient imposed to the microchannel (see experimental set up) as a thermal solicitation and to perform the estimation with the equation 8. In transient state, with a simple flow of water (no source term) the Equation 6 can be rewritten as follow:

$$\Delta T_{i,j}^{k} = Pe{*}_{i,j}^{k} Tx_{i,j}^{k} + \left(\frac{1}{Fo{*}_{i,j}^{k}}\right) Tt_{i,j}^{k} \tag{9}$$

But when the flow rate is stopped inside the microchannel, we are in a purely diffusive model. The system is in relaxation mode and the governing equation is now:

$$\Delta T_{i,j}^{k} = \left(\frac{1}{Fo{*}_{i,j}^{k}}\right) Tt_{i,j}^{k} \tag{10}$$

We work with a IR temperature film which is a three dimension matrix T(I,J,K) as illustrated on figure 3.We calculate a correlation coefficient between the two observables Tt and ΔT according to the following expression, in order to verify if they are correlated.

$$St_{i,j}^{k} = \frac{\sum_{k=n}^{n+Nt} \Delta T_{i,j}^{k} . Tt_{i,j}^{k}}{\sqrt{\left(\sum_{k=n}^{n+Nt} \Delta T_{i,j}^{k}\right)^{2}} . \sqrt{\left(\sum_{k=n}^{n+Nt} Tt_{i,j}^{k}\right)^{2}}} \quad for \quad n \in [1; (K - Nt)] \tag{11}$$

Nt is the length of the temporal window used for the calculation (number of images taken for calculations).

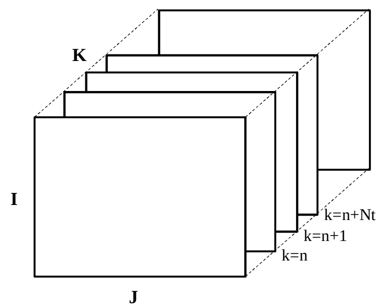


Figure 3. Cubic matrix of frames from the IR recording

If the coefficient is close to 1, *Tt* and ΔT are correlated. It means we are in such conditions that the model defined by equation 10 is valid. In that case we can estimate the Fourier number as follow:

$$\left(\frac{1}{Fo^{*}{}_{i,j}^{k}}\right) = St_{i,j}^{k}\frac{\sqrt{\left(\sum_{k=n}^{n+Nt}\Delta T_{i,j}^{k}\right)^2}}{\sqrt{\left(\sum_{k=n}^{n+Nt}Tt_{i,j}^{k}\right)^2}} \tag{12}$$

These values of the Fourier number are averaged and used as a calibration for the consecutive estimation of the Peclet Number. From the knowledge of Fourier number, Equation 9 can be rewritten as follow:

$$\begin{gathered} Y_{i,j}^{k} = Pe^{*}{}_{i,j}^{k}Tx_{i,j}^{k} \\ with,\quad Y_{i,j}^{k} = \Delta T_{i,j}^{k} - \left(\frac{1}{Fo^{*}{}_{i,j}^{k}}\right)Tt_{i,j}^{k} \end{gathered} \tag{13}$$

Again, the correlation coefficient will be calculated between the two observables, which are now *Y* and *Tx*, according to the expression:

$$Sx_{i,j}^{k} = \frac{\sum_{k=n}^{n+Nt}Y_{i,j}^{k}.Tx_{i,j}^{k}}{\sqrt{\left(\sum_{k=n}^{n+Nt}Y_{i,j}^{k}\right)^2}.\sqrt{\left(\sum_{k=n}^{n+Nt}Tx_{i,j}^{k}\right)^2}} \tag{14}$$

As before, the correlation coefficient is used to find zones where the linear relation of equation 11 is verified.

$$Pe_{i,j}^{k} = Sx_{i,j}^{k}\frac{\sqrt{\left(\sum_{k=n}^{n+Nt}Y_{i,j}^{k}\right)^2}}{\sqrt{\left(\sum_{k=n}^{n+Nt}Tx_{i,j}^{k}\right)^2}} \tag{15}$$

Thus, during the experiment we will switch OFF and ON the flowrate successively, and record a thermal film of the whole scene for further estimation, as illustrated below:

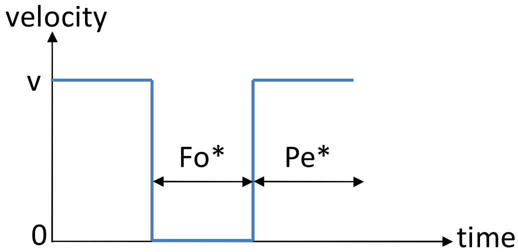


Figure 4. Control of velocity during the experiments for consecutive estimation of Fo* and Pe*

3. Experimental procedure

3.1 Microflow characterization(Pe and Fo* estimation)*

- Connect the water syringes with the microchannel
- Open Altair software (IR images acquisition)
- Control the focusing of the lens
- Turn on the Peltier elements to create the thermal gradient and wait for equilibrium
- Switch ON the flow rate, and wait for equilibrium
- Start recording
- Immediately switch OFF the flow rate=> 1st Thermal transient state for Fo* estimation
- Switch the flow rate back ON =>2nd Thermal transient state for Pe* estimation
- Stop recording
- Repeat for different flow rates

3.2 Acid/base chemical reaction

- Replace the water syringes by Acid and Base
- Turn OFF the Peltier elements to eliminate the thermal gradient and wait for equilibrium
- Control the focusing of the lens
- Carry out a reference image
- Switch ON the flow rate, and wait for equilibrium
- Start recording in steady state (750 frames)
- Repeat for different flow rates

3.3 Phase change

The microchannel is now filled with water and the flow rate is stopped so that the water remains stagnant. In this experiment, only one Peltier element is used to decrease the temperature below 0°C.

- Deposit the microchannel on the Peltier surface.
- Decrease the temperature of the Peltier element progressively.
- Increase Camera frequency to its maximum (freezing is a very fast phenomenon)
- Start recording when the temperature is just below 0°C.
- Stop recording after freezing.

3.4 From the bench to MATLAB

The IR images are stored in a film only readable by Altait software. The file extension is *.ptw*. We will see how to import the files in Matlab. The films should be cut in Altair to eliminate the zones where data are not relevant, this will save time and memory for importation.

4. Preview of Results

4.1 Microflow characterization

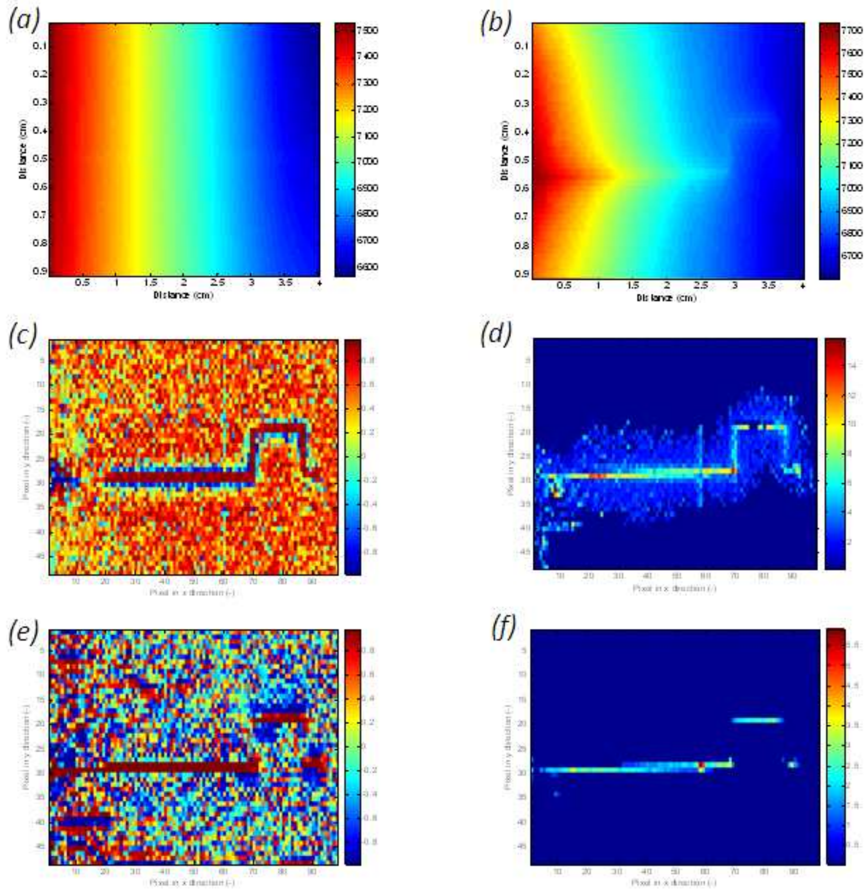


Figure 5. Results examples of microflow characterization. IR temperature field of the thermal gradient without (a) and with (b) flow rate of 500µL/h. Correlation coefficient St (c) and Fo* estimation (d). Correlation coefficient Sx (e) and Pe* estimation(f).

4.2 Acid/base chemical reaction

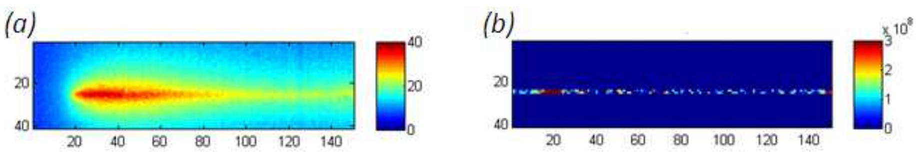
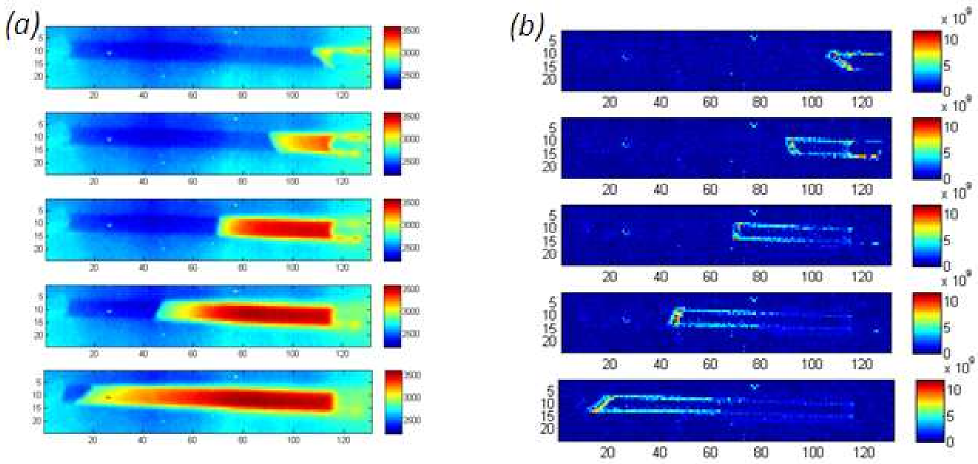


Figure 6. Results examples of an acid/base chemical reaction at 500µL/h. IR temperature field (a) and estimated source term (b)

4.3 Phase change



ıre 7. Results examples of phase change. IR temperature field of the phase change propagation (a). Estimated source term propagation (b)

5. Conclusion

In this work, we have presented the correlation method applied to some microfluidic problems. The method is currently used for qualitative estimations of parameters, such as source terms, and relative Fourier and Peclet numbers. The advantage of the method is the processing of temperature fields, which gives a detailed cartography of the estimated parameters. Thus, it is a very convenient way of localizing moving heat sources, as seen with the phase change example. The method is also very fast and can be applied to several applications (physics, chemistry, biology…).

The drawback of the method lies mainly in the calculations of numerical derivative using finite differences, which introduces little errors in the system. So, one of the objectives is to work on the improvement of the derivative method.

[1]. **O, Fudym, C, Pradere, JC, Batsale.** An analytical two temperature model for convection-diffusion in multilayered systems: Applications to the thermal characterization of microchannel reactors. *Chemical Engineering Science.* 2007, Vol. 62, pp. 4054-4064.

[2]. **Bamford, M.** Méthodes flash et thermographie infrarouge pour la cartographie de propriétés thermophysiques : Application à la caractérisation en thermomécanique. 2007.

[3]. **Pradere, C., Morikawa, J. , Toutain, J., Batsale, J.C, Hayakawa, E., Hashimoto, T.** Microscale thermography of freezing biological cells in view of cryopreservation. *QIRT Journal.* 2006, Vol. 6, 1, pp. 37 - 61.