HEAT REMOVAL ENHANCING IN CAPILLARY ELECTROPHORESIS

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Abstract. The problem of heat removal from capillaries applied in Capillary Electrophoresis is studied using the ANSYS CFX 5.7® simulation software. Simulations show that the addition of an external cylindrical cover of a dielectric material with a good thermal conductivity increases the efficiency of heat dissipation. A system made by multi-capillaries sandwiched between two glass plates also presented a good efficient head dissipation when the space between capillaries and plates are filled with dielectric material with a good thermal conductivity coefficient. For mean operations condictions, a order of the temperature difference of about 5°C was observed between the liquid core of the capillaries and the external circulating air when good conductivity materials are used to externally cover the capillaries. Electroosmosis also does not affect the dynamics of heat dissipation, except by the fact that a fresh liquid with a not regulated temperature continuously enters the inlet of the capillary.

Keywords: capillary electrophoresis, heat dissipation, micro-channel, micro-scale, electroosmosis.

1. Introduction

The number of technologies requiring the manipulation of liquids in micro-channels is growing fast and already has an important role nowadays. These technologies includes micro-generation of energy, micro-reactors, micro-mixers, micro and nano-dispensers, and in analysis equipment based on capillaries or micro-channels used in chemistry, biochemistry, genetics, biotechnology and clinical analysis. It is a huge challenge to handle fluids in channels with diameter measuring less than $100~\mu m$ in deep. Conventional technologies use pressure gradients to move liquids in tubes. In the micro-scale however, extreme large pressure gradients are required, because the cross sections are very small. Moreover, micro-pumps are not reliable regarding delivery precision and control in this scale (Maynes and Webb, 2002).

An interesting alternative is the use of the phenomenon of *electroosmosis*, which is the effect of fluid flow through micro channels due to the application of an electric potential difference between the capillary ends. Usually dielectric material made micro-channels is used to move polar (usually aqueous solutions) liquids in the axial direction of the micro-channel. The resulting fluid flow velocity is proportional do the applied electric field. For instance, microchannels made of fused-silica (or amorphous quartz) and filled with a neutral pH water solution, have an electroosmotic flow from the anode reservoir to the cathode reservoir. Up to 1000 Volts/cm can be applied, resulting in an electroosmotic velocity of the order of a few millimeters per second and the Reynolds number is normally 0.05 (Kist, 1993). This allows a practical, reliable and precise flow control. Another remarkable property of this flow is that the velocity profiles of the liquid is constant across the channel and drops to zero only very close to the walls (also shown by Kist (1993)). This differs drastically from the pressure driven flow, which is parabolic (Poisseuille flow). Electroosmosis is largely used in Capillary Electrophoresis. In this a piece of a cylindrical capillary having typically 50cm, 50 µm internal diameter and 350 µm outer diameter is filled with an aqueous solution and the ends introduced into two reservoirs containing the same or other aqueous solutions. The application of an electrostatic potential difference between capillary ends promotes a flow of the fluid through the capillary called electroosmosis. The molecules from samples to be analyzed are electroosmoticaly driven from the micro channel inlet (where a small sample plug is injected) through the capillary to the opposite end. Simultaneously to the electroosmosis phenomenon also the electrophoresis phenomena occur, separating the samples ions or molecules among them.

One of the major problems encountered in Capillary Electrophoresis is the Joule heating caused by the high voltage used in this technique. Water made buffer solutions have a little conductivity that renders ionic currents of the order of 10 to 100 μ A. This produces a few watts of heat per meter of capillary when 10 to 30 kV are applied. Therefore, good heat extraction strategies must be developed in order to get a good temperature control. Temperature changes of more than 5°C from run-to-run makes the technique useless because migration times (the time for one sample component to

reach the other end) will fluctuate too much. Therefore, it's very important to keep temperature fluctuations from run-to-run under 0.2°C.

In this work a few methods of heat removal are studied with ANSYS CFX $5.7^{\text{®}}$ software simulations. One of the main challenges is the fact that the capillaries have only 10 to 75 µm internal diameters and 180 to 375 µm outer diameters. In other words, there is a significant heat generated inside the liquid phase (liquid core) of the capillary and a relatively small area for dissipation in the liquid-solid interface and solid-external phase interface. Therefore, this work is focused on the following topics: a) to simulated the rate o heat transfer when dielectric materials with good thermal conductivity coefficient are used to externally cover the capillaries in order to increase the area of heat exchange; b) to use simulations to study the heat dissipation efficiency of alternative geometrical parameters. The final results will be the temperature difference between the centre of the capillary and the external circulating air.

2. Cases studied and description of the model.

2.1. Capillary tubing

In Capillary Electrophoresis the molecules are separated inside capillaries. The capillaries are made of fused silica and externally covered with a polymeric material (used to give mechanical protection against the fragile capillary). In the most practical applications the capillaries used have 50 cm in length, 50 µm internal diameter, a fused silica wall of 130 µm tick and covered by a layer of 20 µm polymer (poliimide), as shown in Figure 1.

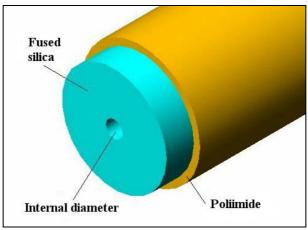


Figure 1. Layers of the capillary.

The capillary is always filled with a buffer solution. These aqueous buffer solutions are used to keep the pH fixed at desired values. The application of high voltages creates currents of the order of micro Amperes. Consequently, heat is generated with power of the order of 1 watt per meter of capillary. In most cases temperature is regulated by direct external circulation of air. Therefore, heat diffuses through the capillary wall, through the polymer coating, and finally to the air.

The main disadvantage of using air to remove temperature is its low heat conductivity coefficient. On the other hand, it presents advantages like, availability and electric isolation. The late being very important because usually very high voltages (up to 30 KV) are used.

The low head removal capacity of air can be partially solved by increasing the area of heat exchange. Therefore, the first problem simulated was a capillary covered with an external cylindrical cover of a good dielectric material. This is the subject of the next section.

2.2. A covered capillary

As discussed in the previous section, it is expected that the addition of a layer of dielectric material should increased the rate of head removal. Therefore, as shown in Figure 2, two situations will be simulated and compared: (a) a capillary in the center of a tube with thermal paste; and (b) a capillary eccentrically positioned inside a tube filled with thermal paste.

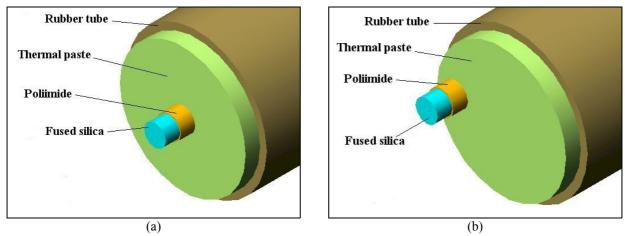


Figure 2. Capillary tube positioned at the center (a) and eccentrically (b) inside a rubber tube filled with thermal paste.

There are many advantages of using thermal paste in these applications: first it is easy to handle, can be easy used to fill tiny pores and spaces, and it sticks well, decreasing the thermal resistance of contacts. However, it is difficult to garanty that the capillary stays at the centre of the tube at the end of the manufacturing process. That is the reason why this situation is also studied in the simulations.

Another problem studied is the use of a multi-capillary system where the capillaries are sandwiched between two dielectric plates (like glass or quartz), spaced by 1 mm from each other, and dielectric materials are used to fill the space between capillaries and plates. In this case two filling dielectrics where simulated: epoxy glue and thermal paste.

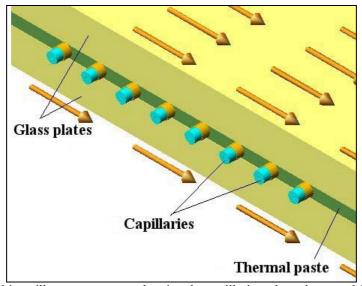


Figure 3. Multi-capillary array system showing the capillaries, glass plates, and filling material.

2.3. Physical model

Temperature in the buffer solution is the main variable to be solve, due to the fact that the excessive heating of this solution may compromise the analysis of capillary electrophoresis. As presented in the introduction of this paper, the buffer solution flow has a flat profile, where the electroosmosis forces are dominant. This laminar flow can be considered to be almost uniform and constant, and convective effects can be neglected in this flow. Heat transfer will be modeled as diffusive along the capillary inner radius.

Heating of the buffer solution comes from Joule effect (Ohm law) and is constant along both the interface with the fused silica wall (*Ri* in Figure. 4) and along the entire length of the capillary. Boundary condition in the external surface of the capillary is always convective (*Re* in Figure. 4), where air is used as a cooling fluid. The first two proposed study cases (with and without covering) have cylindrical geometries, whereas the last one (multi-capillary array) has flat interfaces.

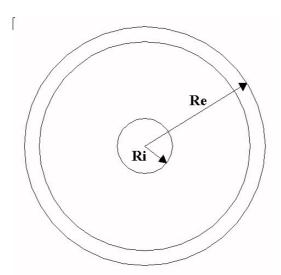


Figure 4 – Schematic picture of the capillary cross section, with *Ri* is the interface between the buffer solution and the internal fused silica wall and *Re* is de external surface.

The following assumptions are made in our simulations:

- a) Fundamentals of Mechanics of the Continuum are assumed valid (Kist, 1993);
- b) Physical properties of the materials involved are constant and isotropic;
- c) Only the steady state regime of the electrophoresis phenomena is considered;
- d) Thermal contact resistance between materials is considered negligible. This assumption is based on the fact that the buffer solution is a liquid and the thermal paste also sticks to the materials making a good thermal contact.

2.4. Assumptions regarding the aqueous solution

- a) Transport properties of the aqueous solutions are considered to be the same as water.
- b) Aqueous solution filling the capillaries is the only source of heat and considered a homogeneous distributed heat source. This is based on the assumption that the current density is constant in all points inside the liquid phase.
- c) It is assumed that heat propagation from the solution to the capillary wall occurs only by diffusion and not by other means, for instance by convection. It means that there are no mass convection events inside the capillary. This assumption is in the literature (Vinther and Soeberg, 1991).

2.5. Mathematical model.

Conservation equations are written in order to solve the problem. Expressed for a generic variable ϕ , in steady state regime, they assume the following generic form:

$$\vec{\nabla} \cdot \left(\rho \overline{\phi} \, \vec{V} \right) = \vec{\nabla} \cdot \left(\Gamma \vec{\nabla} \, \overline{\phi} \right) + \overline{S^{\phi}} \tag{1}$$

where \vec{V} is the velocity vector of the flow, r is its density and $\overline{S}^{\,\phi}$ is the source term. Quantity ϕ can assume convenient values that enable the expression of conservation of mass, momentum and energy, respectively, as well as the diffusive coefficient Γ . Mass conservation is obtained with $\Gamma=0$, $\phi=1$. The source term $S^{\,\phi}=0$ because there is no mass generation in this specific problem. Momentum conservation has $\Gamma=\mu$ (absolute viscosity), $\phi=V$ (velocity) and $S^{\,\phi}=0$, once its a forced convection problem. Energy conservation is obtained with $\Gamma=k$ (thermal conductivity), $\phi=h$ (specific enthalpy) and $S^{\,\phi}=0$, because there is no hest generation in this physical model.

3. Results

By using the software ANSYS CFX 5.7[®], the effect of air velocity on the liquid temperature is simulated. The air crosses orthogonally the capillary (see Fig. 1) and is the only heat removal mechanism present in all cases studied: a naked capillary, a capillary with a cylindrical cover of thermal paste and capillaries sandwiched between glass plates. In

all simulations the capillaries have $350 \, \mu m$ outer diameter, $50 \, \mu m$ internal diameter and $50 \, cm$ long. The values used for thermal conductivity in the simulations are given below (Table 1).

Table 1	Values used for the	thermal con	ductivity of	the materials	in the simulations
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Material	k [W/(mK)]	Material	k [W/(mK)]
Air	0.0261	Polyimide	0.1549
Epoxi glue	0.44	Rubber	0.13
Fused silica	1.5	Thermal paste	2.0
Glass	1.4	Water (T=300 K)	0.613

The other parameters of the simulation are: temperature of the cooling air is 15°C; the sides of the tetrahedrons used in the finites volumes vary from 2 to 100µm; the convergence criterion of 10⁻⁶ was used. Three rates of heat generation are considered in the simulations: 0.25W, 0.5W, and 1.0W. These values where chosen based on typical values observed in capillary electrophoresis. For each level, curves are plotted showing the center capillary temperature as a function of cooling airflow velocity. Also, different thermal paste layer thicknesses are studied.

Figure 5 shows the results for the situation of generation 0.25 W of heat per meter.

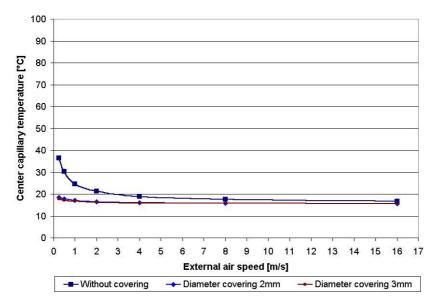


Figure 5 – Temperature in the center of the capillary as a function of cooling air flow velocity and the diameter of thermal paste tube inside which the capillary is located. All simulations were made for a power of 0.25W.

The curves above represent three different conditions of capillary tube covering: without covering and with 2 and 3mm of covering material.

Note that for low velocities (0.25m/s), the temperature of the uncovered capillary increases significantly. But using the covering reduces the temperature inside the capillary because the surface of the interface air-solid is increased. For very high airflow velocities the temperature inside the capillary goes to similar values for all situations.

The next figure (Fig. 6) shows the results for a heat dissipation of 0.5W.

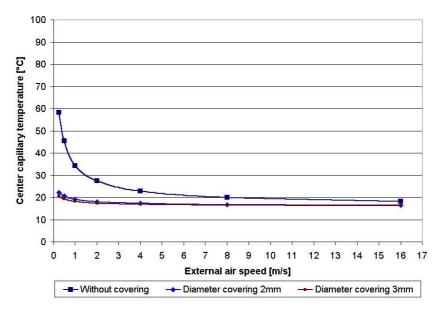


Figure 6 – Temperature in the center of the capillary as a function of air velocity for a capillary dissipating 0.5W.

Note that now the temperature inside the center of the capillary is even higher for low air velocities. The next figure (Fig. 7) shows even higher rates of heat generation (1W).

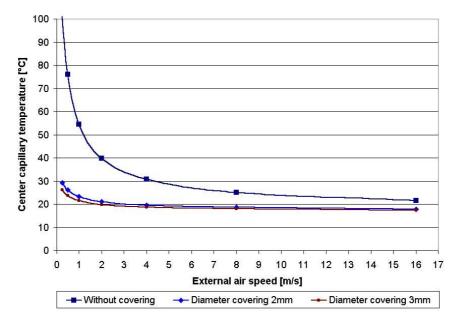


Figure 7 – Temperature in the center of the capillary as a function of air velocity and thermal paste thickness and a rate of generation 1 W.

Even at this high rate of heat generation the temperature in the center of the capillaries stayed at acceptable values while in the case of naked capillaries the temperature of the aqueous phase passed the boiling point of pure water at 1 atm. Moreover, it is evident also that increasing the air velocity beyond 4 m/s has minimum effect on the temperature. Another simulation was made for a capillary located eccentrically inside the tube filled with thermal paste (Fig. 8).

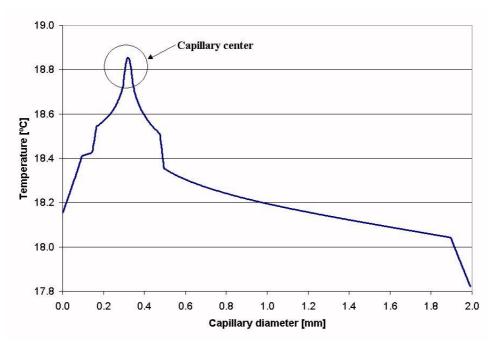


Figure 8 – Temperature on covered capillary symmetry line, 2 m/s cooling air flow speed, 0.5W heat generation rate.

The Figure 8 shows no significant asymmetry in the temperature profile inside the aqueous phase (capillary center). Finally, the problem of using many capillaries, regularly spaced on from another, and placed between two plates was also simulated (see Fig. 3). In our simulations the plates are made of glass and two materials were used to fill the spaces between capillaries and glass plates: epoxy glue and thermal paste.

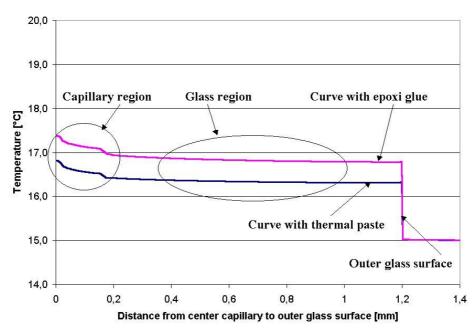


Figure 9 – Temperature profile when epoxy glue (red) and thermal paste (blue) were used to fill the space between capillaries and glass plates.

As shown in Figure 9 a small temperature difference was observed. Basically, a difference of 0.5°C was observed between epoxy glue and thermal paste when the dissipation per capillary was 0.5W and air velocity was 2 mm/s and at 15°C.

4. Conclusions

Heat transfer modeling in capillary channels was applied in this work in order to study the separation of molecules by capillary electrophoresis. Willing to enhance the thermal exchanges, different types of external covering to the capillary were proposed. A fist type was built with thermal paste and a plastic external protection. Air in cross-forced flow was chosen to work as a cooling fluid because of its dielectrical proprieties. As the simulation results showed a good enhancing of heat removal of the capillary, a second alternative was investigated, considering the situation where the capillary lays out of the centerline. In this case, the asymmetry of the temperature profile in the buffer solution could be neglected.

A multi-capillary array was also proposed and simulated, where several capillary tubes were placed in parallel and covered by glass made slabs. Inner spaces can be both filled with thermal paste or by epoxy glue, and the simulated temperature of the buffer solution was 0.5°C, only. This multi-capillary array showed to be a efficient heat removal device, enabling to keep the buffer solution temperature in acceptable levels. Multi-capillary arrays can allow the multiplexing of the capillary electrophoresis analysis.

5. References

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