Electro-osmotic flow in rectangular microchannels: geometry optimization

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Abstract. Micro-flow devices have turned over the years from the subject of fundamental research to fully-fledged industrial applications. Although for some cases the transport phenomena in micro-devices can be handled satisfactorily by using the same approach as for their larger-size counterparts, micro-effects such as electro-osmotic flow (EOF) are typical of small scales and can be employed to circulate coolant through heat sinks by means of electro-osmotic pumping. In order to obey the constraints that different engineering applications impose, design criteria must be employed to optimize the performance of the devices according to the criteria chosen. In this work optimization of the cross-sectional area of a microchannel where EOF and heat transfer at the walls occur is employed to demonstrate how approaches based on the first or second law of thermodynamics may yield opposite results, which are strongly dependent on the peculiarities of EOF, i.e. the ratio of Joule heating to heat transfer at the walls.

1. Introduction
Starting from the early years of this century microchannels have gradually evolved from the subjects of fundamental research to constitutive elements of so-called micro-flow devices (MFDs), as can be seen by comparing older reviews on the subject to more recent ones [1; 2]. In spite of some research still being addressed to fundamental subjects [3–9], MFDs have now progressed beyond the level of prototypes and find applications in several fields [10]; in particular, micro heat exchangers (MHXs) are employed in air conditioning systems [11] and heat pumping equipment [12]. Only at small scales, however, can flow devices exploit micro-effects such as electro-osmosis, which allows the motion of a liquid relative to a charged surface (e.g. due to chemical equilibrium between the surface and an electrolyte), induced by an applied external potential gradient across a microchannel, which acts on the layer of mobile ions, known as Electric Double Layer (EDL) [13]. Electro-osmotic flow in microchannels have received considerable theoretical attention, both for traditional geometries, such as circular ducts and parallel plates[14; 15], but also for more complex geometries such as rectangular, elliptical and triangular ducts [16; 17] and the use of electro-osmotic pumps (EOPs) has been investigated both theoretically and experimentally [18; 19] to circulate a polar fluid through the channels of heat sinks. As in several other engineering fields [20; 21] also MHXs are liable to optimization in order to enhance their performance or to reduce manufacturing and pumping costs. This can be achieved e.g. through changes of the basic configuration, treating the problem from the perspective of the first law of thermodynamics, which has led to the introduction of performance evaluation criteria, (PECs) [22; 23]. PECs adopt the view of the first law of thermodynamics, but the works of Bejan
[24; 25] through the entropy generation minimization (EGM) stress the importance of the second law. More recently, researchers have dealt with the optimization of micro heat exchangers [26–28] combining both approaches, with new and interesting results obtained when also conjugate effects are considered.

Among the many shapes of the ducts of heat exchangers which have been investigated, square cross-sections with smoothed corners have recently been studied in two works [29; 30], for laminar flow and H1 and H2 boundary conditions, whilst Lorenzini and Morini [31] and Lorenzini [32] extended the analysis to the case of rectangular and trapezoidal cross-sections, with and without viscous dissipation. So far, to the best of the Author’s knowledge, no attempt has been made to optimize microchannels where an electro-osmotic flow occurs combining first- and second-law approaches through PECs and EGM. Hence the motivation for this work, where the effect of the change in the shape of the cross-section on the flow and heat transfer performance of an electro-osmotic flow is investigated in terms of maximum heat transfer and minimum entropy generation.

2. Mathematical Model

The non-dimensional concentration of the ions is obtained by solving the incompressible Nernst-Planck equation for negligible Peclet numbers, which yields the so-called Boltzmann distribution

$$c_i^* = \exp \left( \mp z_i e_0 \psi \over \kappa_B T \right)$$

where $c_i^*$ is the concentration of the i-th species normalized by the average concentration of the same species $c_0$, $z_i$ its valence, $e_0$ the unit electric charge, $\psi$ the potential of the electric field, $\kappa_B$ is the Boltzmann constant, and $T$ the thermodynamic reference temperature of the fluid. The $\mp$ sign depends on whether co-ions or counter-ions are involved. Knowledge of the concentration of co-ions and counter-ions allows the calculation of the density of charge in the fluid, which can be used in the constitutive equation for the electric field to obtain the potential distribution function in non-dimensional form $\psi^* = \psi \over \kappa_B T$ by solving the Poisson-Boltzmann equation:

$$\nabla^2 \psi^* = (kD_h)^2 \sinh (\psi^*)$$

where $k = \sqrt{2e^2c_0z_i^2/\varepsilon \kappa_B T}$ is the Debye-Hückel parameter, reciprocal to the Debye length, $c_0$ is the average concentration of the species, $\varepsilon$ the electrical permittivity of the medium. To solve the equation, boundary conditions on the potential at the channel wall $\psi_0$ must be given: neglecting the compact layer, this equals the value of the potential at the Stern plane $\zeta$, so that

$$\psi_0^* = \zeta^* = z_i e \over \kappa_B T \zeta$$

The dependence of $\psi^*$ on geometry, $\zeta^*$ and $kD_h$ is thus apparent.

The non-dimensional velocity profile in the channel is obtained by solving the suitable form of the Navier-Stokes equation. The assumptions made in this work are steady, fully-developed laminar flow of a Newtonian fluid with thermophysical properties independent of temperature inside a microchannel of constant cross-section with rigid, non-porous walls. Further, no pressure gradients act along the flow direction and the only body force present is an external electric field along the channel’s axis, $z$, $E_{ext} = E z_i z$. As a consequence, only the velocity component along $z$ is non-zero, and its magnitude at each point of the cross-section depends on the other two coordinates: $\vec{u} = u_z (x, y) \hat{i}_z$. The momentum transport equation in non-dimensional form becomes

$$\nabla^2 u^* = ME_z^* \sinh (\psi^*)$$
where the non-dimensional quantities are $E^* = \frac{E_z L}{\zeta}$ (electric field), $u^* = u/U$ (velocity), and $M = \frac{2\mu_0 \sigma \zeta D_h^2}{\rho u^*}$. The normalizing velocity $U$ is chosen such that $M = 1$, so

$$\nabla^2 u^* = E_z^* \sinh (\psi^*)$$

(5)

The boundary conditions for the problem are given by the no-slip velocity condition at the walls:

$$u_{wall} = u_0 = 0 \Rightarrow u^*_0 = 0$$

(6)

Given the dependence of the velocity problem on the shear layer potential and on the applied electric field, one can write

$$u^* = u^* (\text{geometry}; \zeta^*, \kappa D_h, E_z^*)$$

(7)

The energy equation is then solved to obtain the temperature distribution. Under the additional assumptions of thermally fully developed flow with negligible viscous dissipation effects, heat generation in the fluid due to Joule heating, uniform cross-section area $A_c$ and $H1$ thermal boundary conditions (uniform heat flux along the channel’s axis, $q'$, and uniform temperature over the perimeter of the cross-section), the non-dimensional form becomes

$$\frac{u^* U}{u_m} \left( \frac{1}{A_c^*} + M_z \right) = \nabla^2 T^* + M_z$$

(8)

where $A_c^* = A_c/D_h^2$ and $u_m$ the average cross-sectional velocity defined as

$$u_m = \frac{U}{A_c^*} \int_{A_c^*} u^* dA_c^*$$

(9)

The quantity $M_z$ relates the thermal input due to Joule heating to the linear heat flux $q'$:

$$M_z = \frac{E_z^2 \lambda_0 D_h^2}{q'}$$

(10)

where $\lambda_0$ is the electrical conductivity of the fluid. Imposing $H1$ boundary conditions results in

$$T^* \big|_{P^*} = 0$$

(11)

The line heat flux $q'$, is identified given by specifying the value of $M_z$.

In view of the above discussion, the temperature field is dependent on the flow field and on the heat flux over the cross-section, so that

$$T^* = T^* (\text{geometry}; \zeta^*, \kappa D_h, M_z)$$

(12)

It is to be remarked that the dependence on the non-dimensional external electric field $E_z^*$ has disappeared; this is due to the presence of the $u^*/u_m$ ratio: in the momentum transport equation the term $E_z^*$ introduces but a scaling factor in the solution, which appears both in $u^*$ and in $u_m$.

Solving the momentum and energy transport equations yields the velocity and temperature profiles over a cross-section, from which the Poiseuille and Nusselt numbers can be obtained:

$$Po = \frac{f Re}{2} \left( \frac{1}{P^*} \int_{P^*} \frac{\partial u^*}{\partial h} \right)$$

(13)

which is also independent of $E_z^*$, and

$$Nu = -\frac{1}{P_h^*} \int_{P^*} \frac{\partial u^*}{\partial h} dA_c^*$$

(14)
3. Performance Evaluation Criteria and Objective Functions

Microchannels are also employed in the manufacture of heat sinks: indeed, when conjugate effects are not relevant, the performance of the heat sink is determined by the performance of the microchannel. In order to obtain acceptable values of the heat transfer surface, pumping power, thermal power exchanged, every engineering application imposes specific constraints. These are often fewer than the degrees of freedom of the problem, which is thus amenable to optimization.

PECs, [23], define the kind of optimization carried out by specifying which quantities are left unchanged with respect to a reference configuration and the objective functions: in this work only the geometry of the microchannel shall be modified. Starting from a rectangular cross-section with sharp corners, they are rounded progressively up to a radius of curvature corresponding to half the length of the shorter side. The rectangular geometry is uniquely defined by two non-dimensional parameters, the aspect ratio, \( \beta \), and the radius of curvature, \( R_c \), which are defined with reference to Fig. 1 as

\[
\begin{align*}
\beta &= \frac{2a}{2b} \\
R_c &= \frac{r_c}{a}
\end{align*}
\]

The cross-sectional area, \( A_c \) and perimeter \( P \), have the following expressions

\[
\begin{align*}
A_c &= a^2 \left[ 1 - \frac{R_c^2}{\beta} \right] (4 - \pi) \\
P &= 4a \left[ 1 + \frac{1}{\beta} - 2R_c \left( 1 - \frac{\pi}{4} \right) \right]
\end{align*}
\]

which are made non dimensional using the hydraulic diameter, \( D_h \):

\[
D_h = \frac{4A_c}{P} = \frac{a}{\frac{a_{ref}}{4}} \left[ 1 - \frac{R_c^2}{\beta} \left( 4 - \pi \right) \right] \left( 1 + \frac{1}{\beta} - 2R_c \left( 1 - \frac{\pi}{4} \right) \right)
\]

so that \( A_c^* = \frac{A_c}{D_h^2} \), \( P^* = \frac{P}{D_h} \); likewise \( a^* = \frac{a}{D_h} \), \( b^* = \frac{b}{D_h} \).

![Figure 1. Geometry investigated.](image)

For the applications of PECs the modified geometry (i.e. with rounded corners) is compared to the reference one, and three new quantities are defined:

\[
S' = \left( \frac{a}{a_{ref}} \right)^2 \left[ 1 - \frac{\beta}{4} R_c^2 (4 - \pi) \right]
\]

\[
P'_{h} = \frac{a}{a_{ref}} \frac{1 + \frac{1}{\beta} - 2R_c (1 - \frac{\pi}{4})}{1 + \frac{1}{\beta}}
\]

\[
D'_{h} = \frac{a}{a_{ref}} \frac{4/\beta - R_c^2 (4 - \pi)}{1 + 1/\beta} \frac{1 + 1/\beta}{4/\beta}
\]
where the superscript ′ indicates the pertaining ratio between the actual and the reference values. The ratio \( a/a_{\text{ref}} \) appears in all the above equations, further geometrical constraints need to be introduced to obtain expressions that only depend on \( \beta \) and \( R_c \). In this work, \( D_h' = 1 \), and Eq.(21) is used to obtain a suitable expression for \( a/a_{\text{ref}} \).

The objective functions are the heat duty _\( Q_\), the pumping power _\( W_\), the length of the microchannel, _L_, the mass flow rate \( \dot{m} \) and the temperature difference between wall and bulk fluid \( \Delta T = T_w - T_b \). They can be related by applying a mechanical and thermal energy balance to the single channel, and are expressed as the ratio of their values in the modified configuration to those for the reference (\( R_c = 0 \)) geometry:

\[
\frac{Q'}{Q_{\text{ref}}} = \frac{Nu'P_h'L'\Delta T'}{D_h'} \tag{22}
\]

\[
W' = \frac{W}{W_{\text{ref}}} = \frac{\dot{m}^2(fRe)'L'}{S'D_h'^2} \tag{23}
\]

Equations(22) and (23) contain all five objective functions, and these are valid for a fixed geometry; the problems has thus four degrees of freedom, which means that each PEC is defined by holding the three other quantities constant.

4. Entropy balance and entropy generation number

Optimization through PECs is based ultimately on first-law considerations: in order to obtain information as to how efficiently available energy is transformed, entropy generation rate, \( \dot{S}_{\text{gen}} \), must be calculated, and it can be split into two contributions, one due to heat transfer, the other to pressure drop, and can be derived through the combined use of the energy and entropy balance equations:

\[
\dot{S}_{\text{gen}} = \dot{S}_{\text{gen},\Delta T} + \dot{S}_{\text{gen},\Delta p} \tag{24}
\]

Details for the case of pressure-driven flows with viscous dissipation details can be found in [28]. Under the assumptions of negligible fluid temperature difference between wall and bulk fluid at the inlet as compared to the bulk temperature and of fluid temperature increase as compared to the inlet temperature_\((T_i - T_m)/T_m << 1, (T_c - T_i)/T_i << 1)_), in the case of electro-osmotic flow, the first term of Eq.(24) becomes

\[
\dot{S}_{\text{gen},\Delta T} = \frac{\dot{Q} \Delta T}{T_i^2 \left( \frac{T_e}{T_i} \right)} \left[ 1 + M_cA_c \left( 1 + \frac{T_c}{\Delta T} \right) \right] \tag{25}
\]

And the second term has the same form as for the case of pressure-driven flow

\[
\dot{S}_{\text{gen},\Delta p} = \frac{2\mu \dot{m}^2 fReL}{\rho^2 A_c D_h^2 T_i} \tag{26}
\]

Equations (25), (26) represent the entropy generation rate due to heat transfer and to frictional losses respectively; they can be related by introducing the augmentation irreversibility ratio,

\[
\phi = \frac{\dot{S}_{\text{gen},\Delta p}}{\dot{S}_{\text{gen},\Delta T}} \tag{27}
\]

With a view to comparing the influence of the radius of curvature of the corners on the constrained performance of microchannels of rectangular cross-section, it is expedient to employ
the augmentation entropy generation number $N_S$ as introduced in [24]

$$N_S = \frac{(\frac{d}{\dot{S}_{gen}})_{opt}}{(\frac{d}{\dot{S}_{gen}})_{ref}} = \frac{(\frac{\dot{S}_{gen,\Delta T}}{\dot{S}_{gen,\Delta T}})_{ref} + (\frac{\dot{S}_{gen,\Delta P}}{\dot{S}_{gen,\Delta P}})_{ref}}{1 + (\frac{\dot{S}_{gen,\Delta P}}{\dot{S}_{gen,\Delta T}})_{ref}} = \frac{N_T + \phi_{ref}N_P}{1 + \phi_{ref}} \quad (28)$$

In the case of $N_T$, $T_i/T_{ref}T_e' = 1$ and

$$N_T = \frac{\dot{Q}'\Delta T'}{T_e'} + \frac{1 + M_z A_c^*}{1 + M_{z,ref} A_c^*} \left(1 + \frac{\Delta T}{\Delta T_{ref}}\right) \quad (29)$$

the normalized exit temperature $T_e'$ is obtained from an energy balance

$$T_e' = \frac{T_i}{T_{e,ref}} + \left(1 - \frac{T_i}{T_{e,ref}}\right) \frac{\dot{Q}'}{\dot{m}'A_c\Delta T_{ref}} + 1 + M_{z,ref} A_c^* \quad (30)$$

For $N_P$

$$N_P = \frac{\dot{m}^2(fRe)^{1/2}L'}{A_c^2D_h^2} = W' \quad (31)$$

The entropy generation number is thus expressed in terms of the objective functions, Eqs. (22) and (23), shown above. Some quantities must be known to compute $\dot{S}_{gen}$, and for this work their value has been chosen as follows: $T_i/T_{ref} = 0.95$, $\Phi_{ref} = 0.1$, $\Delta T/T_{ref} = 20$ and $M_{z,ref} = 0.001 - 0.01 - 0.1$.

In Eqs. (29) and (30) no direct or indirect (i.e. through objective functions) of the quantity $M_z$ on the geometrical parameters $\beta$ and $R_e$ has been shown yet. This is a point deserving attention: when $Nu$ is computed, a certain value of $M_z$ is chosen, which binds $E_z$ to $q'$. A similar problem is encountered when imposing $E_z^*$, which relates $L$ and $E_z$, but $fRe$ is independent of $E_z^*$, so using the Poiseuille number is sufficient to overcome the difficulty. In the case of $M_z$, $E_z$ is decoupled from $q'$ if $M_z$ is written in terms of the objective functions. It can be demonstrated that this leads to the following expression

$$M_z = \frac{(fRe)^2}{D_h^2A_c^2Q'}M_{z,ref} \quad (32)$$

Equation (32) is not explicit, as $\dot{Q}'$ depends on $M_z$ through $Nu$, yet a dependence $M_z = M_z(R_e, \beta)$ can be established once the PEC has been defined.

5. Results

5.1. Velocity and temperature distribution

The Poiseuille and Nusselt numbers must be calculated in order to carry out the optimization procedure. To this extent, the velocity and temperature distributions for different radii of curvature were computed by solving Eqs. (2), (5), (7) considering $D_h = 24 \mu m$ and a fully heated perimeter. For all simulations, an externally imposed electric field $E_z = 100 kV \cdot m^{-1}$ was chosen, while the microchannel length was $L = 0.01 m$. The fluid considered was de-ionized ultra-filtered water (DIUF), with $n_0 = 10^{-6} mol \cdot m^{-3}$ at a reference temperature was $T = 293 K$ and with $\zeta = 0.2 V$. The corresponding non-dimensional quantities appearing in the equations become $\zeta^* = 8$, $E_z^* = 5000$, $\kappa D_h = 9.85$, 78.84. For each geometry four different aspect ratios
were considered ($\beta = 0.1, 0.25, 0.5, 1.0$), radii of curvature from $R_c = 0.0$ to $R_c = 1.0$ in steps of 0.1 and $M_z = 10^{-3}, 10^{-2}$ and $M_z$ from 0.1 to 1.0 in steps of 0.1.

The Poiseuille numbers for a given hydraulic diameter are independent of $M_z$ and can be expressed as a function of the non-dimensional radius of curvature and of the aspect ratio of the channel in the form

$$fRe (\beta, R_c) = \sum_{i=0}^{3} d_i R_i^c$$

(33)

where $d_0 = fRe_0 (\beta)$ is the value of the Poiseuille number for the reference cross-section.

The Nusselt number is likewise expressed as

$$Nu (\beta, R_c, M_z) = Nu (\beta, R_c, M_{z,ref}) - [a (\beta, R_c)] M_z$$

(34)

$$Nu (\beta, R_c, M_{z,ref}) = \sum_{i=0}^{3} c_i R_i^c$$

(35)

where $c_0 = Nu_0 (\beta, M_{z,ref})$ is the value of the Nusselt number for the reference cross-section.

Once the functional forms of the Poiseuille and Nusselt numbers are known, they can be used in the expressions of $\dot{Q}'$ and $P'$ to apply the PECs and to compute $N_S$.

5.2. PEC and entropy analysis:FG1a ($L', m, \Delta T' = 1; \dot{Q}'$)

In the following the results of the application of the FG1a PEC (fixed-geometry, with $\dot{Q}'$ as objective function) are analysed and compared to the conclusion of a second-law analysis. The results are presented as two- and three-dimensional plots with quantities normalized by dividing them for a reference configuration with $R_c = 0$ and $\beta = 1$. The two-dimensional plots are useful for engineering problems where $\beta$ is assigned, whereas the three-dimensional counterparts can be employed when the aspect ratio may be chosen freely. The length, mass flow rate and temperature difference remain unchanged. Equation (22) becomes

$$\dot{Q}' = Nu' P_h'$$

(36)

and $M_z$ takes a form which only depends on the geometrical parameters and which must be solved numerically

$$M_z = \frac{(fRe')^2}{A^2 Nu' P_h'} M_{z,ref}$$

(37)

Figure 2 shows the dependence of $M_z$ on the radius of curvature at a reference value of $M_{z,ref} = 10^{-3}$; it is to be remarked that increasing $M_{z,ref}$ only scales the results accordingly, without any changes in the shape or relative position of the curves, and therefore no other such plots are shown. This behaviour is readily explained by recognizing that in Eq.(37) $M_{z,ref}$ only appears as a proportionality factor. The same holds true for all PECs. It is clear that $M_z$ is always increasing with the radius of curvature, and is higher for larger values of the aspect ratio. Considering the constraints imposed by the FG1a criterion, this implies that the line heat flux at the walls $q'$ decreases with increasing radius of curvature, and this trend is more pronounced the higher the aspect ratio: all the others quantities being the same, $M_z$ is inversely proportional to its denominator, $q'$. This is confirmed by the trend of $\dot{Q}'$, see Fig. 3, which is in fact unaffected by the value of $M_{z,ref}$: this can be understood if one considers how $Nu'$ can be expressed through Eq.(37), that is as a function of geometrical parameters only.
Without considering a second-law approach, it can be concluded that under FG1a constraints the maximum heat transfer is achieved by a cross-section with sharp corners. Also, a geometry with high aspect ratio is less sensitive to the variation of $R_c$ and could be therefore preferable, as it can compensate possible manufacturing imprecisions more efficaciously. If the entropy generation number is also considered, the value of $M_{z,ref}$ does play a significant role, as shown in the Figs. 4-6, whose trends are easily explained if one considers the forms of Eqs. (29)-(31). When $M_{z,ref}$ is low, so is $M_z$, and $N_T$ depends almost exclusively on $\dot{Q}'$, and for this reason
the trends of the quantities is almost the same: entropy generation is caused for the most part by actual heat transfer, also thanks to the modest relative contribution of $N_P$ ($\phi_{ref} = 0.1$). When $M_{z,ref}$ increases, the trends are inverted up to about $R_c = 0.2$, then are partially restored; for large enough values of $M_{z,ref}$, the trends are fully inverted, increasing with $R_c$ and decreasing with $\beta$. This means that Joule heating gives an ever increasing contribution to entropy generation, which is opposite in trend to that of $\dot{Q}$. Hence $N_s$ exhibits a maximum at $R_c \approx 0.2$: below this value, heat transfer from the walls dominates, above it Joule heating prevails. As $M_{z,ref}$ increases further, Joule heating becomes the only significant contributor to $N_S$. The factor that guarantees the maximum heat transfer is that with the lowest aspect ratio ($\beta = 0.1$), $R_c$ giving a much smaller contribution. The entropy generation number has a dependence on the aspect ratio which is very similar to that of $\dot{Q}$, Figs. 8 and 9, which was to be expected, since such a high increase with $\beta$ of the thermal power transferred could not leave entropy generation unaffected. Concerning the influence of $R_c$, as $M_{z,ref}$ varies, the same considerations made for the bi-dimensional plots can be made, and the inversion in the trend of $N_S$ can be seen from comparison of Fig. 8 and Fig. 9. Also, the increase in the contribution of Joule heating to $N_S$ makes the variation of this latter quantity with $\beta$ and $R_c$ smaller as $M_{z,ref}$ increases. Finally, it should be noticed that the minimum value of $N_S$ for $M_{z,ref} = 10^{-3}$ is obtained at low $\beta$ and $R_c = 1$, whereas for $M_{z,ref} = 10^{-1}$ the geometry that minimizes entropy generation is a square cross section with sharp corners. In such cases optimization becomes multi-objective.

6. Conclusions
In this work the influence of the smoothing of the corners of rectangular microchannels on the transport phenomena associated to electro-osmotic flow has been studied using an
approach that combines techniques based on the first law (PECs) and the second law (EGM) of thermodynamics. Although sometimes the outcomes are concordant, it has been demonstrated that for cases such the FG1a criterion (maximize $\dot{Q}$ when $\dot{m}$, $L$ and $\Delta T$ remain constant) for fixed $D_h$ the configuration that maximizes $\dot{Q}$ is also that which corresponds to maximum entropy generation, in particular when the value of $M_{z,ref}$ are high enough, i.e. when Joule heating within the fluid gains of importance with respect to heat transfer. When the aspect ratio has not been dictated by some constraints, wall heat transfer is maximized at low aspect ratios, whereas the combination of $\beta$ and $R_c$ for minimum entropy depends on $M_{z,ref}$. In such cases the problems becomes one of multi-objective optimization.

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