Tsallis Entropy applied to microfluidic channels analysis

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Abstract

This work investigated the possibility to describe the fluid flow in a microchannel from a thermodynamic point of view, exploring the possibility to evaluate the presence of obstacles (or, more in general, geometry imperfection) and their influence on the fluid. Tsallis entropy concept was employed. This form of entropy was introduced in 1988 by Costantino Tsallis as a basis for generalizing the standard statistical mechanics and as a generalization of the standard Boltzmann-Gibbs entropy. Inspired by nature, where storing information is an intrinsic ability of natural systems, here we investigate the capability of interacting systems to transport/store the information generated/exchanged in the interaction process in the form of energy or matter, preserving it over time. In detail, here we test the possibility to consider a fluid as a carrier of information, speculating about how to use such information. The final goal is to demonstrate that information theory can be used to illuminate physical observations, even in those cases where the equations describing the phenomenon under investigation are intractable, are affected by a budget of uncertainty that makes their solution not affordable or may not even be known. In this exploratory work, an information theory-based approach is applied to microfluidic data. In detail, the classical study of the fluid flow in a microchannel with an obstacle of a specific geometry is faced by integrating fluid mechanics theory with Tsallis entropy. Technically, computational fluid dynamics simulations at Reynolds' numbers (Re) equal to 1 were carried out in fluidic channels presenting a rectangular obstacle and on the simulated flow fields.

Tsallis Entropy

Introduced by physicist Tsallis, it is a form of non-extensive entropy (not dependent on the "size" of the phenomenon) that, in its limit, returns Shannon entropy, thus being a generalization of the same entropy.

This formalism has already been applied in the field of fluid dynamics, particularly to determine velocity profiles in an open channel hydraulic system.

The idea would be to apply the Tsallis formalism to a microfluidic channel, similar to the one investigated in Marta's work, and study the possible correlations that may arise between entropy, Shannon entropy, velocity profile, and obstacle geometry. The aim of applying this concept to microfluidics is to consolidate and practice using this approach, but there are no limitations to its applicability.

In 1989, Chiu [1] presented an application of this entropy by studying the velocity profile of a current in a hydraulic channel. Starting from the definition of entropy itself, the author derived a function for the free surface current profile by analyzing experimental data. The analytical solution of the flow in the channel involved certain variables that appeared when solving the equations derived from the application of the entropy theory, which were subsequently obtained by comparing the analytical function with the experimental data.

In a more recent study on Arxiv, Manotosh Kumbhakar [2] and colleagues revisited Chiu's treatment, aiming to deepen certain aspects, particularly in seeking a physical meaning for those parameters that Chiu empirically estimated using experimental data. This study is still under investigation.

The utilization of Tsallis entropy to derive fluid velocity

To derive the velocity, we start directly from the definition of Tsallis entropy, a generalized version of Shannon entropy. Tsallis entropy (TE - Tsallis Entropy) can be written in one of its integral formulations as follows:

$$H_q[f(\hat{u})] = \frac{1}{q-1} \cdot \int_{\hat{u} \epsilon \theta} f(\hat{u}) \cdot \left[1 - \left(f(\hat{u})\right)^{q-1}\right] d\hat{u} \qquad (1)$$

Where $f(\hat{u})$ is the probability density function (PDF) of the variable û: in this case, we use the letter u to work with velocity, but this discussion could apply to any other variable. The parameter q or entropic parameter appears in equation (1) For q→1 comes the Shannon Entropy (SE) (i.e. limit case).

In the specific case, the value û represents the normalized velocity with respect to the maximum measured or estimated velocity; $\hat{u} = u/u_{max}$.

The parameter q is generally associated with an interaction between the system under examination and a "thermal bath," as defined in thermodynamic language or in more traditional treatments. The system, in other words, exchanges energy or information with the external environment or, in general, with the space it interacts with.

Once the entropy is defined in this way, the principle of maximum entropy is applied to the system using this relationship. The objective is to maximize the value of this relationship (i.e., searching for maxima). How is this achieved? Through the method of Lagrange multipliers, which relies on the constraints of the function itself. What are these conditions?

Two constraints were defined:

- Imposing the integral of the PDF function,

$$\int_{\hat{u}\epsilon\theta} f(\hat{u}) d\hat{u} = 1 \qquad (2)$$

- Physical constraint. When discussing velocity, one can consider and apply the principle of conservation of flow rate, which states that

$$Q = \int u \, dA = u_{max} \int \hat{u} \, dA = u_{max} A \bar{\hat{u}} \qquad (3)$$

Once the constraints are defined, you can write the Lagrangian as follows:

$$L(f, \lambda) = \frac{1}{q-1} \cdot \int f(\hat{u}) \cdot \left[1 - \left(f(\hat{u})\right)^{q-1}\right] d\hat{u} \; + \; \lambda_0 \int f(\hat{u}) \, d\hat{u} + \; \lambda_1 \int \hat{u} \cdot f(\hat{u}) \, d\hat{u} \qquad (4)$$

The Euler–Lagrange relation[1] leads to the equation of the PDF function for velocity.

$$f(\hat{u}) = \left[\frac{q-1}{q} \cdot \left(\frac{1}{q-1} + \lambda_0 + \lambda_1 \cdot \hat{u}\right)\right]^{1/q-1} \qquad (5)$$

Application of the Euler-Lagrange principle

$$\frac{\partial L}{\partial f} - \frac{\partial}{\partial \hat{u}}\left(\frac{\partial L}{\partial f'}\right) = 0$$

Decomposing (4) seeing it as the sum of $L_1()+L_2(f,\lambda)+L_3 f,\lambda()$, applying the Euler–Lagrange derivation we get:f,λ

$$\frac{\partial L_1}{\partial f} - \frac{\partial}{\partial \hat{u}}\left(\frac{\partial L_1}{\partial f'}\right) = \frac{1}{q-1} - \frac{q}{q-1} \cdot f(\hat{u})^{q-1}$$

$$\frac{\partial L_2}{\partial f} - \frac{\partial}{\partial \hat{u}}\left(\frac{\partial L_2}{\partial f'}\right) = \lambda_0$$

$$\frac{\partial L_3}{\partial f} - \frac{\partial}{\partial \hat{u}}\left(\frac{\partial L_3}{\partial f'}\right) = \lambda_1 \hat{u}$$

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[1] Of which I have all the steps done: see section "Application of the Euler-Lagrange principle" at the bottom of the page

$$\frac{1}{q-1} - \frac{q}{q-1} \cdot f(\hat{u})^{q-1} + \lambda_0 + \lambda_1 \hat{u} = 0$$

From which one obtains precisely the relation (5) through one or two algebraic steps.

This function can be integrated on the domain $[0,\hat{u}]$ to obtain the cumulative distribution function (CDF).

$$F(\hat{u}) = \int_0^{\hat{u}} f(\hat{u}) d\hat{u} = \frac{1}{\lambda_1} \cdot \left(\frac{q-1}{q}\right)^{\frac{q}{q-1}} \left\{ \left(\lambda_0 + \lambda_1 \hat{u} + \frac{1}{q-1}\right)^{\frac{q}{q-1}} - \left(\lambda_0 + \frac{1}{q-1}\right)^{\frac{q}{q-1}} \right\} \ (6)$$

The next step is to relate this function to the geometric domain of the "channel".

There is a simple case, 2D, and a complex case, 3D, not treated here.

Let's start with the simple case.

Speed is a function of position, namely:

$$\hat{u} = g\ (y) = \breve{g}\ (\Psi)\ (7)$$

Having considered that x is the direction of the flow and y is the vertical of the channel.

Always starting from Chiu's studies, the same researcher used generalized coordinates that allowed him to deal more easily with the 3D case. Starting from the same generalized coordinates, re-reducing them to the 2D case leads to a range of values $Y_{min}= 0$ and $Y_{max} =1$ con $Y= y/D$ where D represents the maximum height of the channel or the light of the channel.

In this simple case, then the following report can be written.

$$F(\hat{u}) = \int_0^{\hat{u}} f(\hat{u}) d\hat{u} = \int_{g^{-1}}^{g^{1}} f(g(\Psi)) \frac{d\hat{u}}{d\Psi} \cdot d\Psi = \int_{g^{-1}}^{g^{-1}} f(g(\Psi)) \frac{d\hat{u}}{d\Psi} \cdot d\Psi = \int_{\Psi_{min}}^{\Psi} \breve{f}(\Psi) d\Psi = \frac{y}{D}\ (8)$$

which is obvious for the 2D case, less for the 3D case (not reported here).

At this point (8) must be equal to (6).

You get the relation of $\hat{u}$ from equality:

$$\frac{1}{\lambda_1}\cdot\left(\frac{q-1}{q}\right)^{\frac{q}{q-1}}\left\{\left(\lambda_0+\lambda_1\hat{u}+\frac{1}{q-1}\right)^{\frac{q}{q-1}}-\left(\lambda_0+\frac{1}{q-1}\right)^{\frac{q}{q-1}}\right\}=\frac{y}{D} \tag{9}$$

This report would lead to the $\hat{u}$ that would be a function of the two Lagrange multipliers and the entropic factor q of Tsallis. Explaining as a function of $\hat{u}$ yields the relation (9b).

$$\hat{u}=-\frac{\lambda_1+\frac{1}{q-1}}{\lambda_2}+\frac{1}{\lambda_2}\cdot\left\{\left(\lambda_1+\frac{1}{q-1}\right)^{\frac{q}{q-1}}+\lambda_2\cdot\left(\frac{q}{q-1}\right)^{\frac{q}{q-1}}\cdot\frac{y}{D}\right\}^{\frac{q-1}{q}} \tag{9b}$$

By merging some terms (see also equations (13) and (14)), we obtain in contracted form:

$$\hat{u}=-\alpha_2+\left\{(\alpha_2)^{\alpha_1}+\{(1+\alpha_2)^{\alpha_1}-{\alpha_2}^{\alpha_1}\}\cdot\frac{y}{D}\right\}^{\frac{1}{\alpha_1}} \tag{10}$$

To evaluate the goodness of the relation (10) to represent the current profile of a laminar flow in a fluidic channel, we moved on to perform a numerical simulation with SW OpenFOAM for a micro-channel with a water-type fluid under conditions of Re = 10 (laminar conditions). The results of the simulation were then compared, taking some sections, with the current profiles generated (or generable) through the relation (10) to the variation of the unknown parameters.

It was immediately noted that the report (10) is not able to describe the phenomenon correctly. $\hat{u}$ it is in fact correlated with the height in relation to the diameter D (or the depth of the channel) in a 1 to 1 “coupling“. This behavior does not represent reality correctly. The velocity in a closed channel can in fact assume the same value along the vertical coordinate more than once (parabolic profile): there is no univocal relationship between the two quantities. In order to describe the phenomenon using the approach presented, it was therefore necessary to find a new relationship that uniquely correlated the velocity with the y-coordinate (velocity value associated only with a spatial coordinate).

The first step was to consider the report proposed by Chiu *et alii* (1989).[2] The report was in fact proposed to address the problem of open channels with free surface, where the maximum speed is below the free surface of the liquid current: there was no linear and unambiguous correlation between velocity and geometric coordinate. The proposed report took the form of:

$$\xi=\frac{y}{D+h}\cdot\exp(1-\frac{y}{D+h}) \tag{11}$$

Where **h** is the height at which the maximum speed is had. For values of h <0 the maximum speed is below the free surface of the current.

[2] C.L.Chiu; Velocity distribution in open channel flow, 1989, Journal of Hydraulic Engineering.

This first correlation if replaced in (10) instead of the y/D value, is able to describe well the current profile between the wall and the axis of symmetry, but far from any obstacle or in fully developed conditions and considering the symmetric profile with respect to the axis. The presence of an obstacle, in fact, represents a further complication, because, in the vicinity of the latter, the current profile presents a flex to the passage of the fluid due to the presence of a restriction.

The report (11) proved unable to provide a sufficiently accurate description of the current profile in the areas close to the obstacle.

The work, therefore, shifted to looking for a new correlation that would be able to take into account this new current profile (Figure 1 blue and orange lines) in the presence of an obstacle[3].

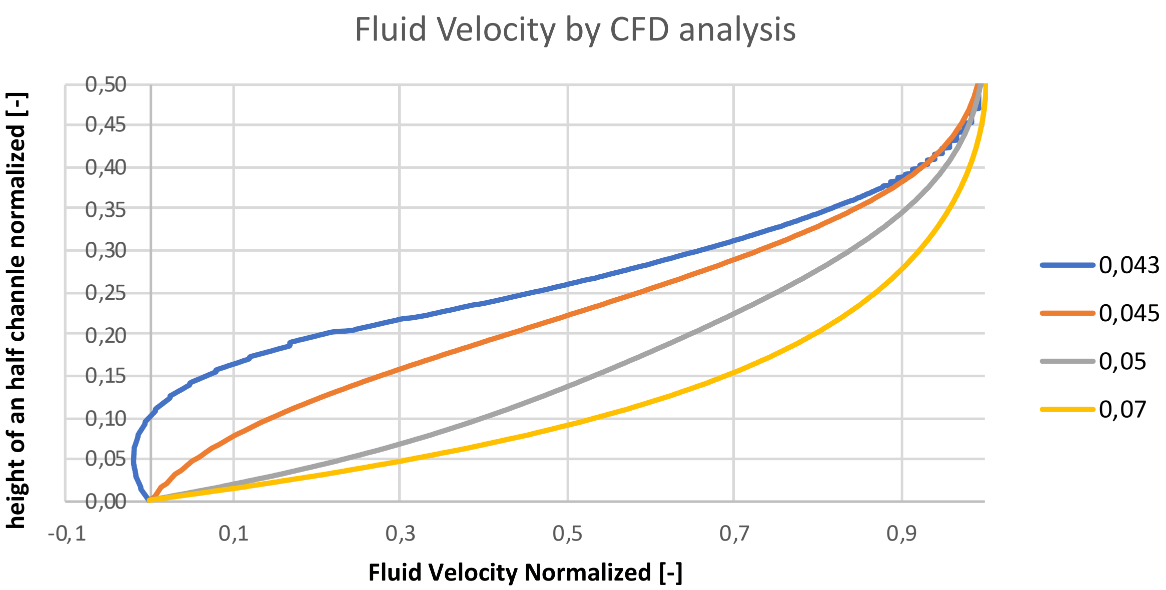

Figure 1. Current profiles downstream of the obstacle. The curves are associated with the distance (e.g., 43 = 4.3 mm after the obstacle).

The new correlation relation proposed to link velocity and relative position within the channel has been designed starting from (11) and proposing a new equation:

$$\xi_1 = \left(\frac{y}{D+h}\right)^{n+1} \cdot \exp\left(1 - \frac{y}{D+h}\right) \qquad (12)$$

In (12) the variable n has been introduced, which away from the obstacle takes the value 0 for a fully developed profile: we then return to the relation (11).

[3] Please note that for a first approach, a rectangular obstacle was chosen, in a 0.5 mm channel, with a height of 0.1 mm and a width of 0.5 mm.

Starting from the proposed relationship, therefore, the shape of the curve is governed at this point by 4 parameters.

$$\alpha_1 = \frac{q}{q-1} \tag{13}$$

$$\alpha_2 = \frac{1-G}{G} \ con \ G = \frac{\lambda_1}{\lambda_1 + \lambda_2 + \frac{1}{q-1}} \tag{14}$$

$$n = const. = \zeta_1 \tag{15}$$

$$h = const. = \zeta_2 \tag{16}$$

In which the factors α_1 e α_2 depend directly on the entropic value of *Tsallis*, while the n and h values are factors of obstacle position and shape of the current profile, respectively.

This relationship made it possible to obtain, by successive approximations of the variables (13)(14)(15)(16), current profiles with a trend able to reflect what was simulated (Figures 2 and 3).

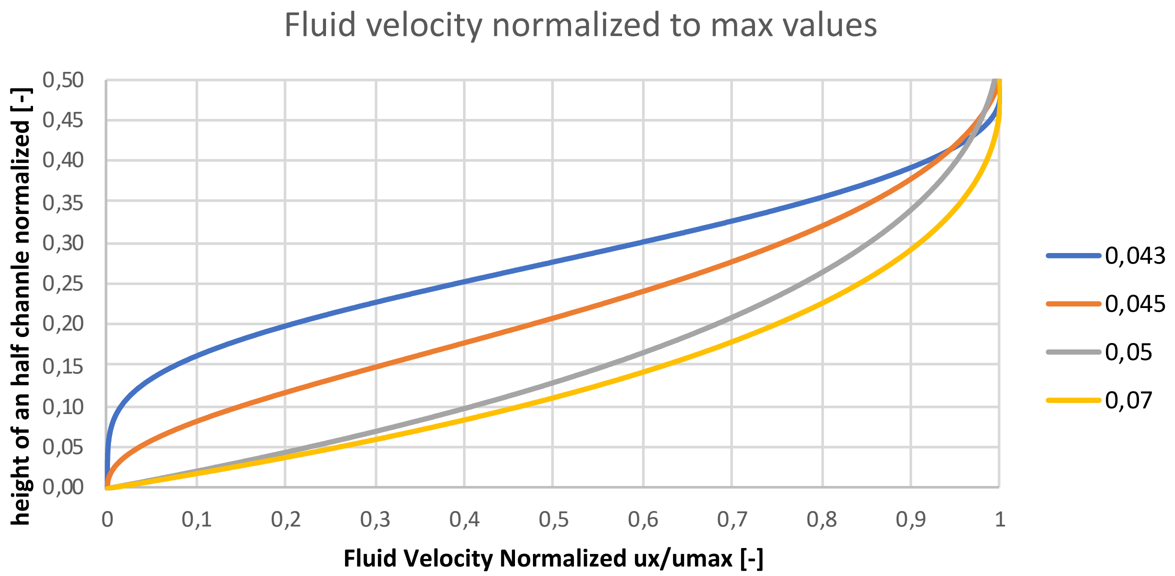

Figure 1. Current profiles downstream of the obstacle derived from the report (10) introducing the speed/position relationship proposed in the report (12). The curves are associated with the distance after the obstacle (e.g. 0,043 are equal to 0,043 mm after the obstacle)

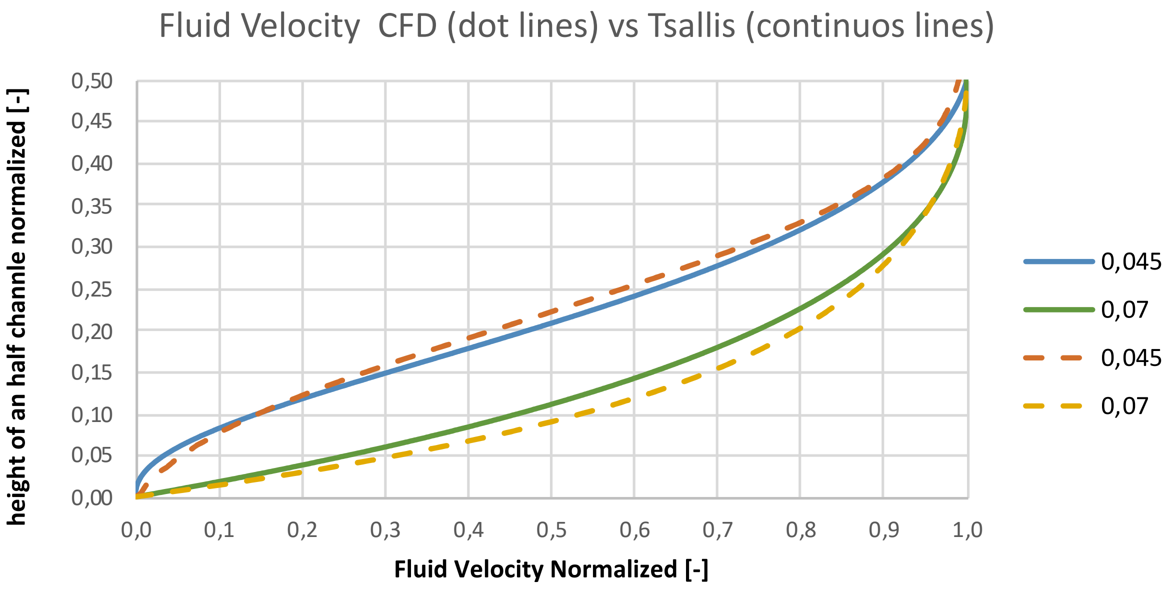

Figure 2. Comparison between simulated (hatch) and theoretical (continuous) current profiles at two different distances from the obstacle.

In this exploratory study, the determination of the parameters takes place iteratively, minimizing waste.

In Figure 3 what was obtained by analyzing the behavior with the first obstacle.

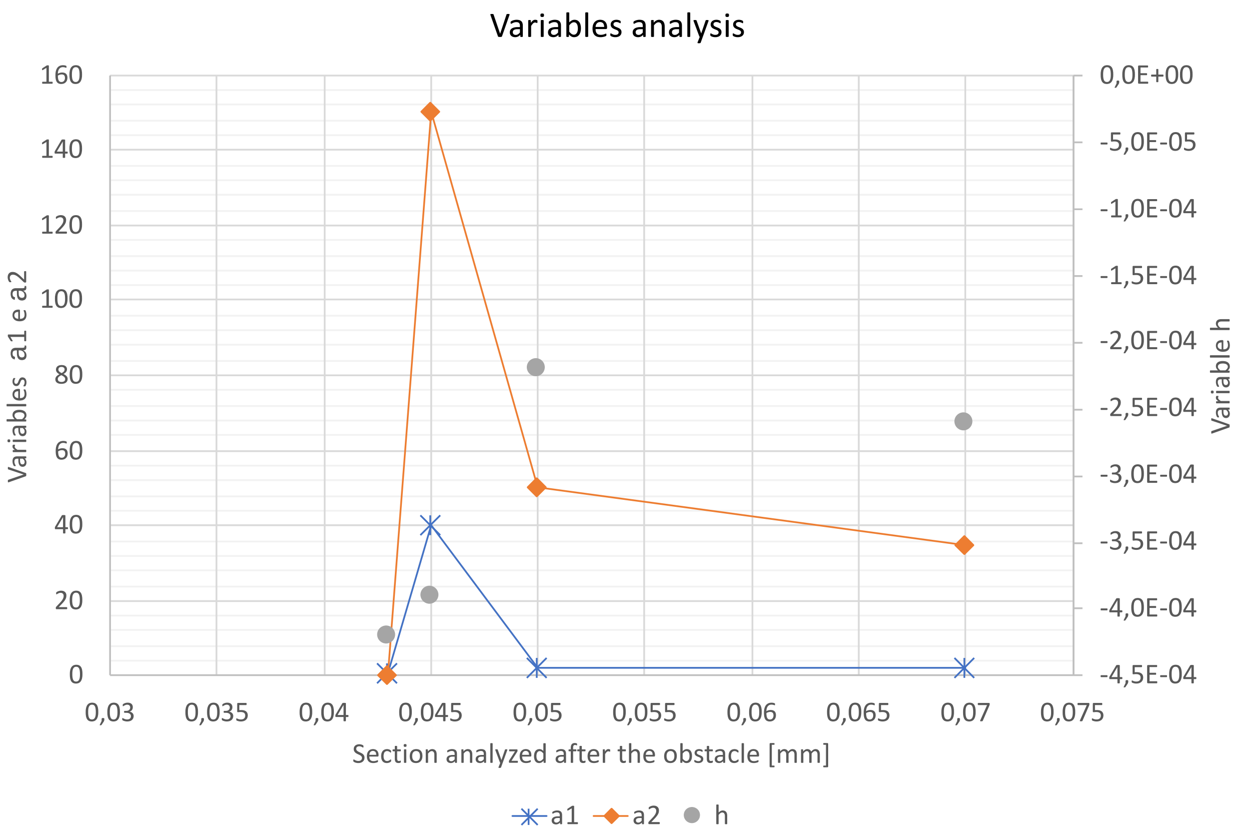

Figure 3. Trend of the values of alfa1, alfa2 and h for the rectangular single obstacle case studied

Conclusions and possible developments

The Tsallis entropy showed its potential to describe a fluid flow in a microchannel. Thanks to this approach a deeper analysis about the influence of the channel geometries on the fluid behavior can be done.

The next steps will be related to the estimation of factors α_1, α_2, n, and h, looking for a correlation between the entropic factor and the internal geometry of the channel, in particular of the obstacle.

In this sense, the first considerations have been made starting from the equation (9 - 9b - 10).

A new evaluation of the position of the correlation between velocity and geometric coordinate (eq 11) to cover the entire channel should be studied.

The relationship (10) explained for the determination of the velocity was used, downstream of numerical simulations in a laminar regime on a simple microchannel (2D), rectangular in shape, without and with a single rectangular obstacle in turn, to determine the parameters q, a_1 and a_2 for the reconstruction of the current profile. In the first instance, the determination of the parameters took place by trial and error starting from the simple channel conditions: undisturbed case.

It is useful to recall that the report (9) had to be amended in order to be used in the presence of an obstacle. Moreover, the same relation proved to be able as developed to reconstruct the current profile **only** on the “hemi-channel“ (half of the channel from the wall to the axis) taking into account the presence of a restriction of the channel itself. This limitation is yet to be investigated and is believed to be related to the function used for the position of the function (10).

The reconstruction and determination of the parameters have made it possible to:

1. verify the goodness of the relationship in the description of current profiles
2. observe the influence of the obstacle in terms of entropic factors along the development of the channel as a function of the nature of the obstacle

Also Manotosh, Kumbhakar [2] and colleagues addressed the problem of giving physical sense to the Lagrangian parameters and the entropic factor by going to work on the calculation of the first and second moments of the PDF distribution function and related to the velocity. It would be an interesting topic to be explored always in relation to microfluidic applications.

Bibliography

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