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1 **JOURNAL: Microfluidics and Nanofluidics**

2

3 **Brief Communication**

4

5 **Fluid flow-based description of the geometrical features in fluidic channels using the Shannon's**
6 **information theory: an exploratory study**

7

8 **S. Ripandelli^{1*}, D. Pugliese^{2*}, M. Sotgiu¹, U. Morbiducci¹**

9 ¹Politecnico di Torino, Department of Mechanical and Aerospace Engineering, 10129 Torino,
10 Italy

11 ²Politecnico di Torino, Department of Applied Science and Technology and RU INSTM, 10129
12 Torino, Italy

13

14 *corresponding authors: simone.ripandelli@gmail.com; ORCID: 0000-0001-7867-9461

15 diego.pugliese@polito.it; ORCID: 0000-0002-6431-1655

16

17 **Keywords**

18 Shannon Entropy, microfluidics, information theory, thermodynamics, fluids

19

20 **Abstract**

21 Inspired by Nature, where storing information is an intrinsic ability of natural systems, here we
22 investigate the capability of interacting systems to transport/store the information
23 generated/exchanged in the interaction process in the form of energy or matter, preserving it
24 over time. In detail, here we test the possibility to consider a fluid as a carrier of information,
25 speculating about how to use such information. The final goal is to demonstrate that
26 information theory can be used to illuminate physical observations, even in those cases where
27 the equations describing the phenomenon under investigation are intractable, are affected by
28 a budget of uncertainty that makes their solution not affordable or may not even be known. In
29 this exploratory work an information theory-based approach is applied to microfluidic data. In
30 detail, the classical study of the fluid flow in a microchannel with obstacles of different
31 geometry is faced by integrating fluid mechanics theory with Shannon's theory of information,
32 interpreted in terms of thermodynamics. Technically, computational fluid dynamics
33 simulations at Reynolds' numbers (Re) equal to 1 and 50 were carried out in fluidic channels
34 presenting obstacles with rectangular and semicircular shape, and on the simulated flow fields

35 the Shannon's information theory was applied evaluating the fluid dynamics information
36 entropy content. It emerged that the Shannon Entropy (SE) evaluated at the outflow section of
37 the flow channel depends upon the geometric features (i.e. position, shape, aspect ratio) of the
38 obstacles. This suggests an interpretation of the fluid dynamics establishing in a flow channel
39 presenting obstacles in terms of information theory, that can be used to identify *a posteriori*
40 the geometric features of the obstacles the fluid interacts with. The proposed approach can be
41 applied to flow data at the boundaries of fluid domains of interest to extract information on the
42 process occurring inside a system, do not making any appeal to the governing equations of the
43 phenomenon under observation or intrusive measurements.

44

45 **1 Introduction**

46 In principle, the behavior of fluids in motion can be fully described by three equations: an
47 equation describing the conservation of mass, a second equation based on the second Newton's
48 law of motion, and a third equation based on the conservation of energy (Cox 2015; Khasanov
49 2011; Merdasi et al. 2018).

50 A condition for a real fluid to be in motion is that sufficient energy is to be spent. It follows
51 that the fluid in motion is a system that modifies its internal energy, thus generating a variation

52 of entropy (S) of the system in a purely thermodynamic meaning. The concept of entropy (not
53 univocally accepted indeed), which can be explained as the level of disorder of a system
54 describing its evolution under the effect of the external environment, was taken up by Claude
55 Shannon in 1948 (Shannon 1948) and applied to the field of information theory in order to
56 describe the level of complexity of a signal in data communication systems. In general, it is still
57 uncommon to apply information theory for the purpose of the analysis of flow fields
58 characterized by different levels of complexity (Ikeda and Matsumoto 1986). Indeed, the idea
59 of considering a fluid in motion as an information carrier is not new, inspired by the fact that
60 Nature uses fluids to transport a plethora of biochemicals. Looking at a fluid in motion as an
61 information carrier (e.g. nutrients to cells, proteins through blood, etc.), a parallelism between
62 fluid flow and information theory based on the definition of the SE can be easily established.

63 Motivated by the possibility of interpreting a fluid as information carrier, in this study
64 information theory is applied to microfluidics, where its capability to discriminate the shape of
65 obstacles in a channel based on the knowledge of the motion of fluid particles upstream and
66 downstream of the obstacle is tested. In detail, the capability of the SE to discriminate the shape
67 of the obstacle based on the distortion of fluid streamlines is tested, with the final aim to use
68 the SE of the system as a *fingerprint* of the obstacle shape-specific flow perturbation. The

69 potency of the herein proposed approach has not been largely explored. To cite a valuable
70 example, Pozo et al. (Pozo et al. 2017) analyzed the flow complexity in open systems,
71 approaching the distortion of fluid streamlines in a channel at the level of information
72 transmission.

73 Technically, here computational fluid dynamics (CFD) solutions of laminar flow in channels
74 presenting obstacles were compared to an “ideal communication” channel where the
75 transmitted and received messages are identical and SE was applied to CFD data. The
76 characterization of microflows as information carriers finds several applications, e.g. to assess
77 mixing efficiency in micromixers (Camesasca et al. 2006; Pennella et al. 2010; Pennella et al.
78 2012) or in microreactors and in scaffolds and bioreactors for tissue engineering applications
79 (Eijkel and Van den Berg 2005; Bilen and Yapici 2002; Yojina and Ngamsaad 2010; Tariq et al.
80 2020) and in many other technological fields like solar energy (Ali 2020), nanofluids for
81 manufacturing processes (Wang et al. 2020), heat and mass transfer (Chen et al. 2020; Sajjad
82 et al. 2020; Sözen et al. 2021).

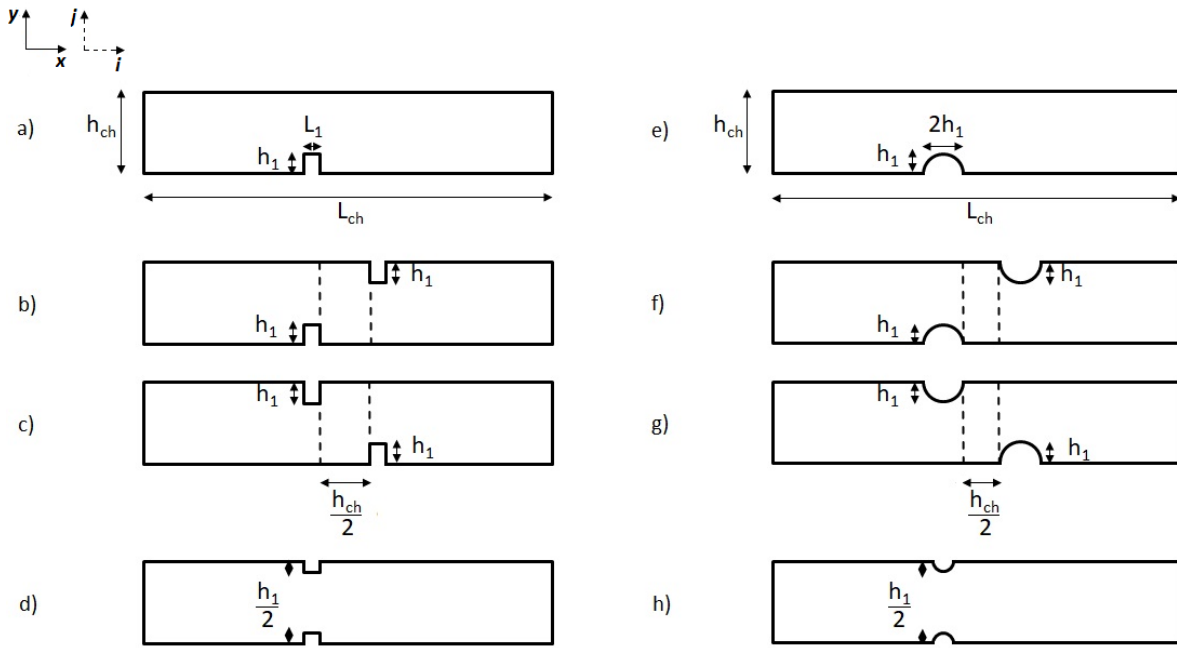
83 The principal aim of this study, and the reason of its novelty, was to investigate the behavior
84 of a fluid that flows in a channel in presence of obstacle/s characterized by different shape,
85 multiplicity and disposition and employing the information theory. This exploratory study

86 highlights that at defined conditions a simplified approach based on the information theory can
87 be applied to extract information on the processes occurring within closed systems, and that
88 this can be done by measuring only the “information” at systems’ boundaries.

89

90 **2 Methods**

91 In this study a microchannel geometry without and with obstacles of different shape and
 92 position was investigated. Overall, as depicted in Fig. 1, nine configurations were considered,
 93 i.e. one without obstacles and 8 with obstacles. The ratio between the height of the channel h_{ch}
 94 and the characteristic obstacle dimension h_1 was set to $h_1 = h_{ch}/6$. In microchannel
 95 configurations where more than one obstacle was considered, inter-distance was set equal to
 96 $h_{ch}/2$ (Fig. 1).



97

98 **Fig. 1** Schematic illustration of the investigated channel geometries with obstacles ($h_1 = h_{ch}/6$). The
 99 analysis on models a, d, e and h is presented in the Results Section. Coordinates (i, j) correspond to the
 100 logical coordinates useful for the computational analysis

101 The analytical solution of the fluid motion in the microchannel without obstacles can be easily
102 obtained from Navier-Stokes equations. In detail, for an incompressible, homogeneous,
103 Newtonian fluid in steady-state laminar condition, the law of motion in the microchannel can
104 be expressed as:

$$105 \quad u_x = -\frac{1}{2\mu} \cdot \frac{dp}{dx} \cdot (y_0^2 - y^2) \quad (1)$$

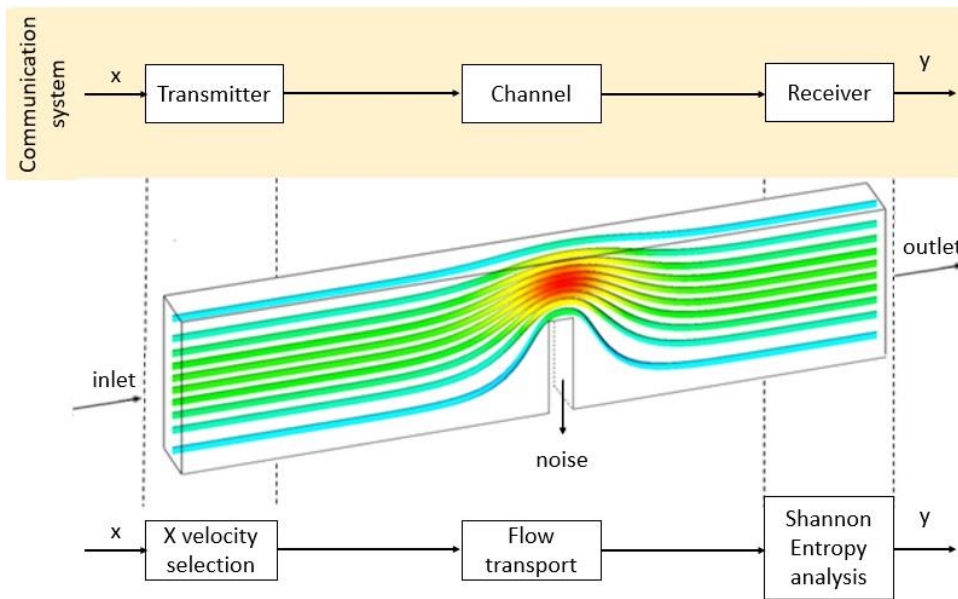
106 where u_x is the velocity in axial (x , see Fig. 1) direction, μ the dynamic viscosity, p the pressure,
107 y the general position in vertical direction (Fig. 1) and y_0 the coordinate of the microchannel
108 wall, where velocity is equal to 0 (i.e. no-slip conditions).

109 The finite volume-based CFD commercial code Fluent (ANSYS Inc., USA) was adopted to solve
110 the discretized governing equations of fluid motion in microchannels with obstacles. In detail,
111 the Navier-Stokes equations in their discretized form and under steady-state laminar
112 conditions were solved using a second order pressure discretization and a second order
113 upwind momentum discretization scheme. The fluid was assumed to be isotropic,
114 incompressible and Newtonian with a density value ρ equal to 998.2 [kg·m⁻³] and a dynamic
115 viscosity μ equal to 10⁻² [kg·s·m⁻²]. To ensure grid-independence of the solution, based on a
116 mesh sensitivity analysis, quad-mesh with elements size of 1·10⁻⁴ m was adopted. On average,
117 the resulting computational grids consisted of 24000 elements and 24381 nodes. Two different

118 flow regimes, characterized by Re equal to 1 and 50, were simulated by applying Dirichlet
119 conditions at the inflow section of the microchannel geometry (in terms of flat velocity profile),
120 while the reference pressure Neumann boundary condition was imposed at the outflow section.
121 Walls were assumed to be rigid, and the no-slip condition was imposed.

122 The concept that a confined fluid in motion is an information carrier, and the parallel with a
123 communication system, was translated into a scheme where: (1) the fluid in the microchannel
124 is the carrier; (2) the inflow section (or more in general a section upstream of the channel
125 segment presenting obstacles) is the transmitter; (3) the outflow section (or more in general a
126 section downstream of the channel segment presenting obstacles) is the receiver; (4) the
127 difference in flow features between the two sections is the information transmitted. In this
128 regard, flow perturbations induced by the presence of obstacles can be regarded as the “noise”
129 affecting the system (Fig. 2). The channel without obstacles was considered as the reference
130 case, i.e. the case where the carrier (fluid) is not disturbed and the transmitted information is
131 not modified.

132



135 **Fig. 2** Schematic illustration of the parallelism between a communication system and a fluidic system

136 Distilling in fluid mechanics terms, at the very low Re laminar flow regimes adopted in
 137 microfluid applications the streamlines deflection induced in the channel by the presence of an
 138 obstacle does represent a modification of the information content carried by the fluid at any
 139 channel location upstream of the obstacle. In the absence of obstacles, fluid streamlines will not
 140 be deflected, following a linear path; any obstacle capable to perturb the flow will deflect fluid
 141 streamlines and ultimately the carried information, in accordance with the conceptual model
 142 of Fig. 1. It is well known from the analytical solution of the laminar fluid motion in the channel
 143 without obstacles, that the flow field is characterized by streamlines parallel to the axis of the
 144 conduit (as well as to the channel's walls). The presence of an obstacle, even maintaining

145 laminar conditions, will perturb the flow with the consequence that streamlines will be
 146 deflected losing their parallelism. This behavior was translated building up a binary matrix,
 147 representative of the phenomena. To build up the representative binary matrix, here fluid
 148 velocity data from CFD simulations were considered (i.e. for each cell of the quad-mesh a value
 149 of velocity was extrapolated). Technically, a $N \times M$ matrix $B_{i,j}^x$ was built:

$$150 \quad B_{i,j}^x = \begin{bmatrix} b_{1,1} & \dots & b_{1,M-1} \\ \vdots & \ddots & \vdots \\ b_{N,1} & \dots & b_{N,M-1} \end{bmatrix} \quad (2)$$

151 with $i = \{1, \dots, N\}$, where N is the number of grid cells in y direction, and $j = \{1, \dots, M - 1\}$, where
 152 M is the number of grid cells in x direction (Fig. 1). The binary elements $b_{i,j}$ of the matrix were
 153 calculated as follows:

$$154 \quad b_{i,j} = \begin{cases} 1, & \frac{\bar{u}_{i,j}^x}{\bar{u}_{i,j-1}^x} \leq \zeta_{i,j} \\ 0, & otherwise \end{cases} \quad (3)$$

155 where $\bar{u}_{i,j}^x$ and $\bar{u}_{i,j-1}^x$ are the values of the x -component of the velocity at grid cell location (i, j)
 156 and $(i, j-1)$, respectively. The threshold values $\zeta_{i,j}$ for matrix $B_{i,j}^x$ binarization were set according
 157 to:

$$158 \quad \zeta_{i,j} = \frac{\bar{u}_{i,j}^{num.}}{\bar{u}_{i,j-1}^{num.}} - \frac{\bar{u}_{i,j}^{ana.}}{\bar{u}_{i,j-1}^{ana.}} = 0 \quad (4),$$

159

160 and depend on the results of CFD analysis and Eq. (1). From this equation, $\bar{u}_{i,j}^{num.}$ and $\bar{u}_{i,j}^{ana.}$ are
 161 the CFD and the analytical velocity values in x direction at grid cell location (i, j) , and $\bar{u}_{i,j-1}^{num.}$ and
 162 $\bar{u}_{i,j-1}^{ana.}$ are the CFD and the analytical velocity values in x direction at grid cell location $(i, j-1)$,
 163 respectively.

164 Here the SE was employed to quantify the level of interaction between fluid flow and the
 165 obstacles in the microchannel, intended as the level of streamlines deflection with respect to
 166 the microchannel without obstacles, binarized according to matrix $B_{i,j}^x$. By definition, the
 167 formulation of the SE is given by:

$$168 \quad SE(X_i) = -P(X_i) \log_2 P(X_i) \quad (5),$$

169 where X_i is a discrete random variable with possible values $\{X_1, \dots, X_n\}$ and $P(X_i)$ is the
 170 probability distribution of X_i . Theoretically, an increase of entropy corresponds to a loss in
 171 information content. In this study, the SE was evaluated according to:

$$172 \quad SE = -P_i \log_2 P_i \quad (6)$$

173 where P_i is given by:

$$174 \quad P_i = \frac{\sum_1^j b_{i,j}}{N} \quad (7)$$

175 Based on Eqs. (6) and (7), the SE ranges between zero (i.e. no information lost or, for the
 176 specific application, no distortion of fluid streamlines) and one (i.e. all the information carried

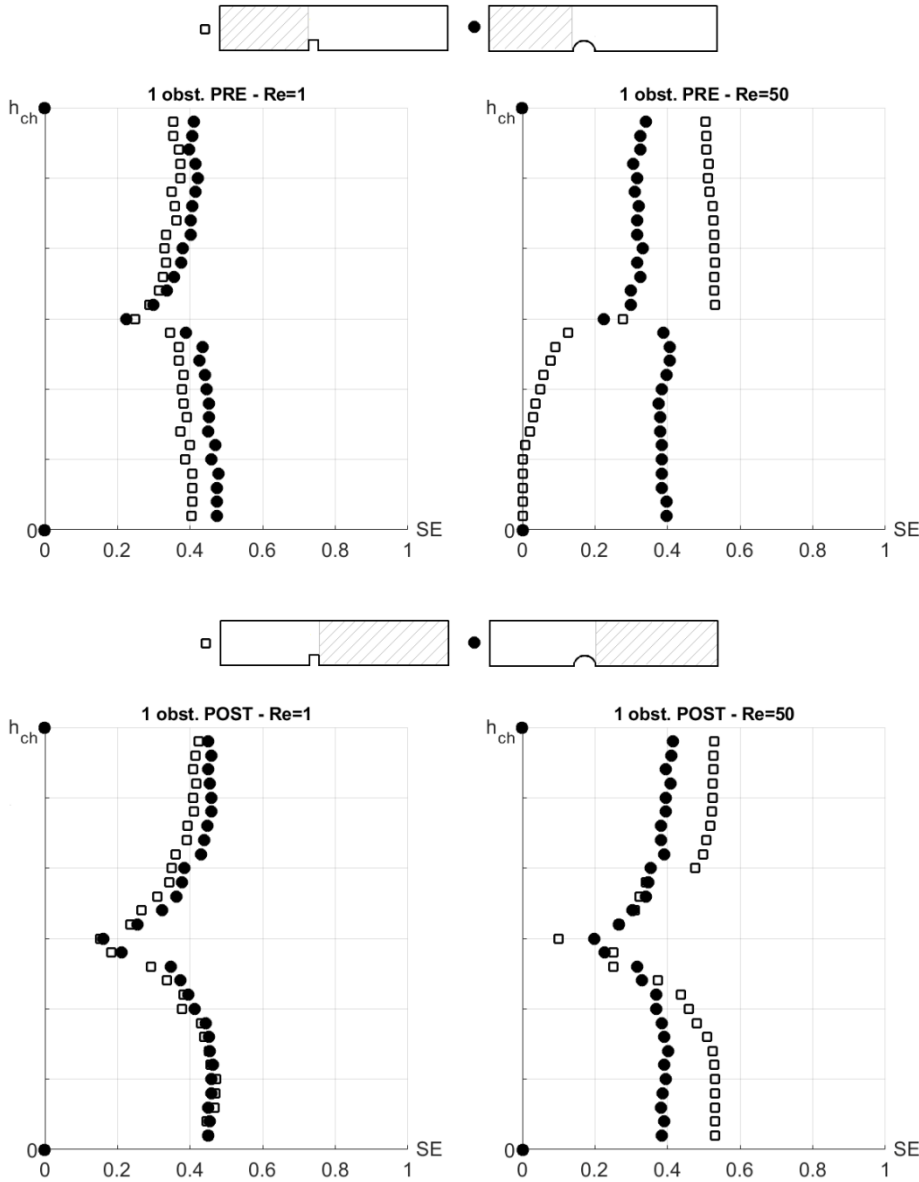
177 by the fluid lost due to the disruption of the flow field as a consequence of its interaction with
178 obstacles in the microchannel).

179

180 **3 Results**

181 The analysis was extended to all the microchannels with different obstacles geometry and
182 number summarized in Fig. 1. As first explanatory example, the SE values computed along two
183 cross-sections (proximal and distal to the obstacle, respectively) of the two microchannels with
184 single obstacles of rectangular and semicircular shape, at two different Re numbers (1 and 50),
185 are presented in Fig. 3. At $Re = 1$, as expected, moderate differences are highlighted by the SE
186 both between the upstream and downstream sections (flow field distortion consequence of the
187 presence of the obstacle) and between the two microchannels (consequence of the different
188 shape of the obstacles). Marked differences in SE distribution (and in absolute values as well)
189 along the cross-sections emerge at $Re = 50$ (Fig. 3): as expected, the presence of the rounded
190 (semicircular) obstacle, which is expected to distort fluid streamlines less than the obstacle
191 with rectangular shape, modifies trans-obstacle SE values markedly less than the rectangular
192 single obstacle (the semicircular shape maintains almost unaltered the SE of the system even
193 increasing the inertial effects by one order of magnitude, as stated by the Re). The results of Fig.

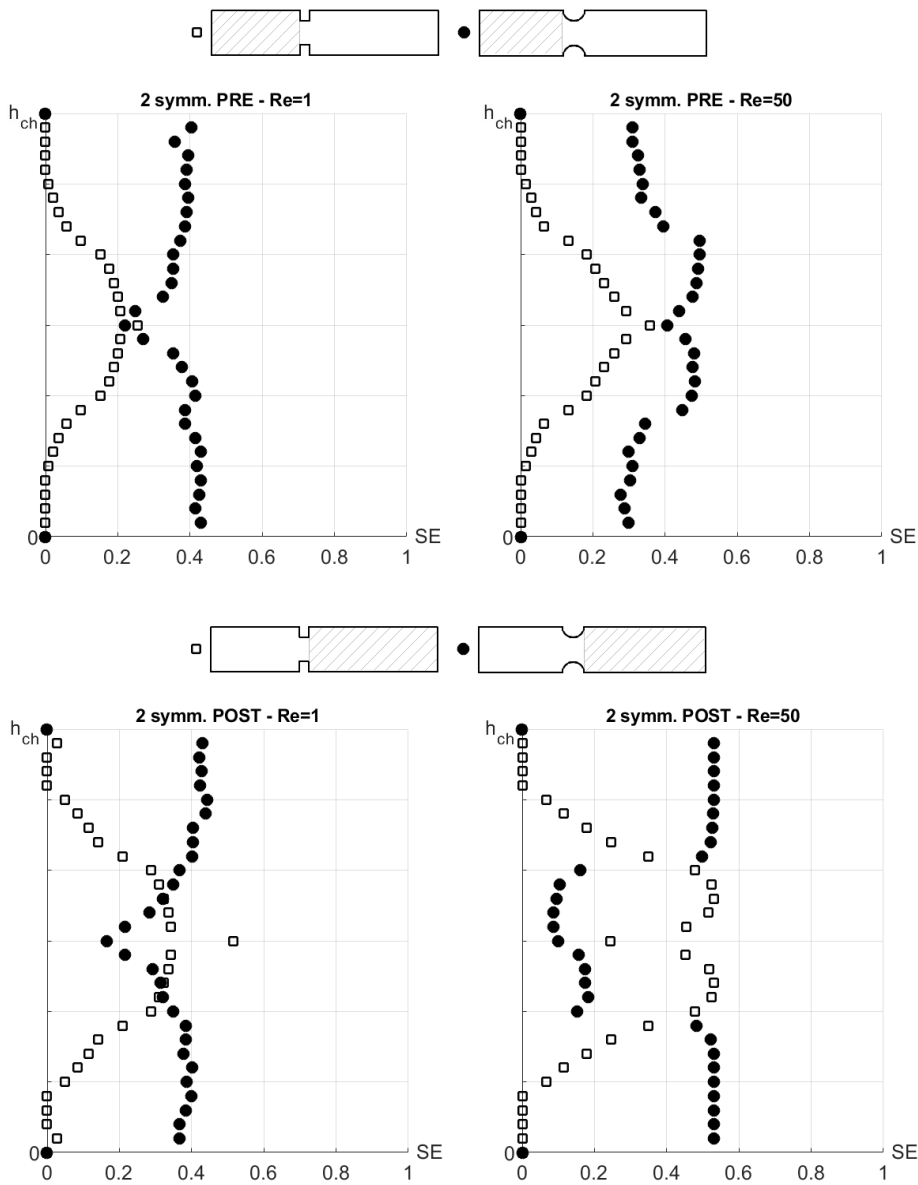
194 3 confirm the capability of the SE of discriminating between obstacle shapes, properly
 195 capturing thermodynamically-induced variations in the microchannel system.



196
 197 **Fig. 3** SE computed on two cross-sections (proximal to the obstacle, upper panel; distal to the obstacle,
 198 lower panel) of two microchannels presenting single obstacles with different shape (rectangular and
 199 semicircular), at two different Re (1 and 50). h_{ch} is the general height of the channel

200 Figure 3 also highlights an expected lack of symmetry (more pronounced at $Re = 50$) in the SE
201 cross-sectional distribution, reflecting the absence of geometrical and fluid dynamical
202 symmetry in the two microchannels with single obstacles. In this regard, the second
203 explanatory example of Fig. 4 reports the SE values computed along two cross-sections
204 (proximal and distal to the obstacle, respectively) of the two microchannels presenting
205 obstacles with rectangular and semicircular shape, symmetrically located with respect to the
206 microchannel axis. In this case, the cross-sectional SE distributions: (1) confirm the capability
207 of capturing the different influence of the shape of the obstacle in the flow field, with marked
208 differences related to the obstacle shape clearly evident also at $Re = 1$; (2) adequately reflect
209 the presence of a geometrical (and fluid dynamical) symmetry of the microchannel system.

210 Summarizing, the cross-sectional distributions of Figs. 3 and 4 clearly demonstrate that SE
211 is an indirect measure of the impact that obstacles with different shape and configuration have
212 on the microchannel fluid dynamics, suggesting that SE can be adopted to *a posteriori*
213 discriminate the shape of obstacles (e.g. cultured cells in biomicrofluidic applications) in
214 systems without optical access. This is like to say that SE can be used as a sort of *fingerprint*
215 that specific obstacles leave on fluid streamlines, depending upon their shape, configuration
216 and fluid dynamics conditions (as defined by the Reynolds' number).



217

218 **Fig. 4** SE computed on two cross-sections (proximal to the obstacle, upper panel; distal to the obstacle,

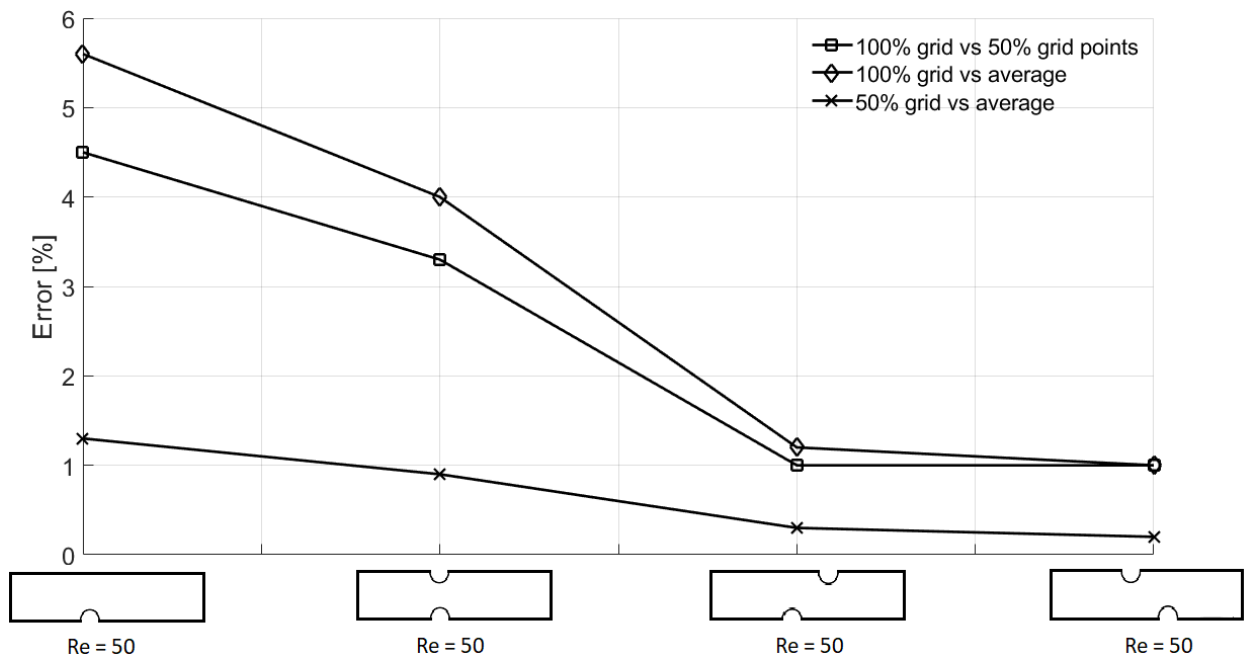
219 lower panel) of two microchannels presenting obstacles with rectangular and semicircular shape, at Re

220 $= 1$ and 50 . Obstacles are symmetrically located with respect to the axis of the microchannels. h_{ch} is the

221 general height of the channel.

222

223 In order to check for the robustness of SE with respect to the CFD grid cardinality (i.e. the
 224 number of nodes considered for the SE calculation), a sensitivity analysis was carried out where
 225 nodes were decimated. Technically, the average value of the SE was calculated considering the
 226 entire microchannel fluid domain as follows: (1) considering the 100% of the mesh grid
 227 elements; (2) considering only 50% of the mesh grid elements; (3) averaging the velocity
 228 values of two adjacent mesh grid elements. The percentage differences among the average SE
 229 values, summarized in Fig. 5 for microchannels with four different semicircular shape obstacle
 230 configurations, clearly show that a substantial reduction (50%) in the number of mesh grid
 231 elements weakly influences SE evaluation (with differences lower than 6%).



232 **Fig. 5** Impact of the number of mesh grid elements on microchannel average SE values. The analysis was
 233 carried out considering the 100% and the 50% of the mesh grid elements, as well as averaging the
 234

235 velocity values of two adjacent mesh grid elements. The results refer to four microchannels with
236 different configurations of semicircular obstacles

237

238 **4 Conclusions**

239 In this study the fluid dynamics in microchannels with obstacles was investigated using the
240 concept of entropy, here approached in a different way compared to the present state-of-the-
241 art (Camesasca et al. 2006, Pozo et al. 2017, Rocha et al. 2008). The analysis suggests that a
242 quantity linked to entropy, SE, is capable to discriminate among different shapes and
243 configurations of obstacles within a microchannel. In the microfluidic field the capability to
244 infer presence and configuration of obstacles in microsystems from SE differences between
245 inflow and outflow sections could allow to monitor e.g. cells shape and growth in
246 microbioreactors, as well as mixing of species in the microsystem itself. Applications other than
247 biomicrofluidics, where fluid streamlines entropy can be employed to describe the physics
248 within the microsystem just looking at SE input and output variations are manifold, ranging
249 from microelectronics to chemistry (Ghaneifar et al. 2021, Shahsavar et al. 2020, Khalid et
250 al. 2021). In this sense, the here presented results represent a starting point for future

251 dedicated applications where the extraction of information on the processes occurring inside a
252 not accessible system is critical.

253 Integrating statistical mechanics with information theory, in the long run will allow to
254 establish a clearly distinguishable link between thermodynamics perturbation of a system and
255 the level of interaction of the individual elements of which a system is made.

256

257 **Conflicts of interest**

258 The authors declare that they have no competing interests.

259

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