



Low Reynolds number mass transfer past regular square arrays of cylinders in cross flow

N. Cancilla , M. Ciofalo , A. Tamburini *, G. Micale

Dipartimento di Ingegneria, Università degli Studi di Palermo, Viale delle Scienze Ed. 6, Palermo 90128, Italy

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ABSTRACT

Computational results were obtained for low Reynolds number steady and fully developed cross flow with mass transfer past an infinite regular square array of cylinders. For a fixed porosity of 0.5 the Reynolds and Schmidt numbers and the orientation of a forcing term (representing the driving pressure gradient) were made to vary in a broad range, and their influence on local and overall mass transfer was investigated. Both uniform mass flux and uniform concentration conditions at the cylinder-fluid interface were considered. In the Reynolds number range investigated (from $Re = 10^{-4}$ to $Re \approx 10^2$, which is the largest value for which steady-state conditions can conservatively be assumed), an extremely complex dependence of the local and mean Sherwood number on the forcing term orientation was observed, which became increasingly strong and Schmidt number-dependent as the Reynolds number increased. For all Schmidt and Reynolds numbers considered, the mean Sherwood number correlated well with the Péclet number, exhibiting a flat behavior up to $Re \approx 2$ and a ~ 0.25 -power law increase for larger Re . Boundary conditions significantly affected local Sherwood numbers, but much less corresponding mean values. The applicability of existing heat transfer correlations for tube banks to the present conditions was critically discussed.

1. Introduction

Tube or rod arrays are commonly found in a variety of industrial equipment, such as heat exchangers [1], boilers [2], condensers [3], hollow-fiber contactors [4] and shell-and-tube reactors [5].

The study of the tube-side fluid dynamics and heat or mass transfer is fairly simple and is usually approached by the elementary theory (Hagen-Poiseuille law if the flow is laminar) or by adopting semi-empirical correlations for the transport coefficients [6].

The modelling of shell-side flow and simultaneous mass or heat transfer phenomena deserves more attention. While there is a rich literature on tube banks, usually involving transitional and turbulent flow, the knowledge of flow and mass transfer in hollow-fiber bundles, usually involving low Reynolds numbers (almost invariably < 100 , and often < 1) and high Schmidt numbers, is more limited [7–11].

Over the years, the intensive use of hollow-fiber devices has led to the need for more accurate predictions and has prompted much research on this topic. In computational studies, the simplest approach assumes fully developed axial flow with scalar transport in regular square or hexagonal lattices [12]. Some authors, however, have also addressed

randomly packed fibers [13,14]. The case of developing axial flow in a bundle of rods has also been investigated over the years [15,16]; in many applications, notably involving membrane contactors (e.g. hemodialysis), the equipment length is not sufficient for mass transfer to attain fully developed conditions [17].

The condition of cross flow, which will be the one investigated in the present work, commonly occurs in heat exchangers when the shell side fluid flows perpendicular to the tube axes [18], but is encountered also in membrane separation processes [19,20] involving mass transfer.

Fig. 1 is a schematic representation of a typical cross flow hollow-fiber contactor. In the first half of the module, the shell-side fluid enters an inner cylindrical mixing space, flows radially outwards from multiple openings, perpendicular to the fibers, and is collected into an outer annular mixing space. In the second half, it flows radially inwards and is collected in the inner mixing space, from which it exits the module. A partition separates the two halves preventing axial flow in the shell side.

In cross flow, the angle formed by the mean flow direction with the rows of rods, tubes or fibers in the generic cross-sectional plane (flow attack angle) plays a role in determining both hydrodynamics and heat / mass transfer [21]. However, most of the literature has been limited to

* Corresponding author.

E-mail address: alessandro.tamburini@unipa.it (A. Tamburini).

Nomenclature		x, y	Cartesian coordinates (m)
		z	Cartesian coordinate parallel to the cylinders (m)
		Greek symbols	
A	fluid area (m ²)	γ	forcing term angle (deg)
A_{tot}	total area (m ²)	ε	porosity (-)
C	periodic component of the scalar concentration (mol m ⁻³)	λ	Darcy-Weisbach friction coefficient (-)
D	scalar diffusivity (m ² s ⁻¹)	μ	dynamic viscosity (Pa s)
d	diameter of the cylinder (m)	ρ	density (kg m ⁻³)
F	forcing term compensating the large-scale pressure gradient (Pa m ⁻¹)	φ	azimuthal angle (deg)
F_0	reference pressure gradient (Pa m ⁻¹)	χ	dimensionless concentration (-)
f	dimensionless forcing term (-)	Subscripts	
J	local scalar flux (mol m ⁻² s ⁻¹)	b	bulk value (mass flow averaged)
L	side length of the domain corresponding to the pitch of the square lattice (m)	loc	local value
K	normal hydraulic apparent permeability (m ²)	m	mean value
k	dimensionless normal hydraulic apparent permeability (-)	max	maximum value
n_{FV}	number of finite volumes (-)	s	direction of the forcing term F
Nu	Nusselt number (-)	w	wall value
p	periodic component of the pressure (Pa)	x, y, z	Cartesian coordinates
Pe	Péclet number (-)	Superscripts	
Pr	Prandtl number (-)	n, m	exponents in the power-law dependence $Sh_m \sim Re^n Sc^m$
Re	Reynolds number (-)	Averages	
S	wet surface of the computational domain (m ²)	$\bar{\cdot}$	azimuthal average (with respect to φ)
Sc	Schmidt number (-)	$\langle \cdot \rangle$	superficial average
S_C	source term compensating the large-scale scalar gradient (mol m ⁻³ s ⁻¹)	$\{ \cdot \}$	angular average (with respect to γ)
Sh	Sherwood number (-)	$ \cdot $	vector magnitude
$\mathbf{u}$	local velocity vector (m s ⁻¹)		
V	volume (m ³)		

two attack angles only (for square arrays, these correspond to the so called “in-line” and “staggered” configurations) so far. In the authors’ opinion, mass or heat transfer phenomena associated with intermediate orientations deserve a more in depth scrutiny. Therefore, in the present study the effect of the flow attack angle was investigated by letting the orientation of a forcing term vary in small angular steps.

Besides the flow attack angle, two other crucial parameters investigated in the present work are the Reynolds number Re and the Schmidt number Sc (to be replaced by the Prandtl number Pr in the context of heat transfer).

In regard to the Reynolds number, as mentioned above, a vast literature exists on heat or mass transfer phenomena in the range from transitional to fully turbulent regimes (e.g., from $Re \approx 100$ to $Re \approx 40,000$ or larger). In this range, several correlations have been proposed to predict the Nusselt or Sherwood numbers as functions of geometrical parameters and of the Reynolds and Prandtl or Schmidt numbers [22–27]; many of these can be found in textbooks on transport phenomena [28].

For example, Janjua et al. [29] report computational results for flow and heat transfer across single cylinders with different cross-sectional

shapes at a Prandtl number of 0.71 and Reynolds numbers in the range 100–40,000. Also Jiang et al. [30] report computational results but for pulsatile flow and heat transfer from a tube bank to a liquid metal at Reynolds numbers in the range 1000–100,000.

However, the low-Reynolds number region (say, $Re < 100$) has not been fully explored. Yet this condition, although unusual in heat exchangers, is common in hollow-fiber membrane units or mini heat exchangers operating in the laminar steady regime. For example, in hemodialysis modules characterized by radial shell-side inlets and outlets, cross flow velocity components are some orders of magnitude lower with respect to the axial one (cross flow Reynolds number ≈ 0.1 –1).

Few authors have addressed such cases. Among them, Ishimi et al. [31] studied mass transfer past periodic arrays of cylinders and solved the flow and heat transport governing equations for the case of uniform wall concentration boundary conditions. Sangani and Acrivos [32] proposed semi-analytical solutions but restricted their analysis to low Péclet numbers and uniform heat flux. Antonopoulos [21] provided numerical solutions for different values of the Prandtl number. In regard to experimental work, Wilk [33] investigated mass and heat transfer in mini-channels. He reported also many literature results for different

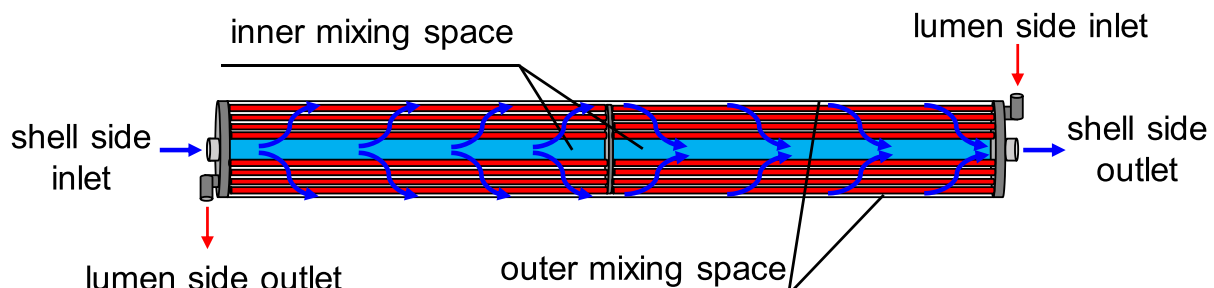


Fig. 1. Schematic of a hollow-fiber membrane unit operating in cross flow.

values of the Schmidt (or Prandtl) number. Some of the most relevant correlations applicable to cross flow with mass or heat transfer in square lattices of cylindrical elements at Reynolds numbers < 100 will be summarized and compared with the present results in the Appendix.

In regard to the Schmidt or Prandtl numbers, Table 1 reports the values investigated in this work and indicates a possible physical application for each range of values.

In earlier research, the present authors have extensively studied shell-side hydrodynamics and scalar transport in a variety of configurations. Reference [12] deals with regular square and hexagonal lattices. The effect of the bundle porosity was investigated in [34]. The influence of channelling (due to the presence of localized regions with different porosities) on friction and mass / heat transport coefficients was studied in [35] for axial flow and in [36] for cross flow. The case of undulated fibers was investigated in [37,38]. The hydrodynamic characteristics of square lattices of circular rods, square lattices of elliptic rods, and randomly distributed circular rods were compared in [39].

The present work focuses on low-Reynolds number scalar transport in cross flow past square lattices of circular cylinders. The analysis spans a broad range of Reynolds numbers Re (based on superficial velocity and cylinder diameter, see Eq. (7)), from creeping flow conditions (down to $Re = 10^{-4}$) to a conservative upper limit for steady flow ($Re \leq \sim 50$ –70), thereby restricting the investigation to the steady laminar flow regime. According to Williamson [40], for an isolated cylinder, vortex shedding arises in the wake and the steady-state assumption fails when $Re > \sim 50$. A similar transitional value for the switch from steady flow to vortex shedding past a single tube ($Re = 40$) is mentioned by Zukauskas [26].

For arrays of cylinders, there are indications that their mutual interaction causes an increase of the critical Re value. Although quantitative results cannot be found in the literature for the bundle porosity considered in the present paper (0.5), the critical Re appears to increase as the bundle porosity decreases. For example, Zukauskas [26] generically described as “predominantly laminar” the flow regime occurring in tube banks at Reynolds numbers Re_{max} (based on the bulk velocity in the restricted section, see Appendix) below 1000; for square arrays, this corresponds to a Reynolds number Re (present definition) of ~ 200 for a bundle porosity of 0.5 and ~ 500 for a bundle porosity of 0.8. Beale and Spalding [41], based on numerical simulations, reported that in both in-line and staggered tube banks with a porosity of ~ 0.8 instabilities occur for $Re > 50$ (present definition). Nishimura et al. [42], based on experimental results, stated that, for square arrays with a bundle porosity of 0.8, the critical Reynolds number for the onset of vortex shedding is ~ 100 , with the in-line configuration exhibiting a larger amplitude of the velocity oscillations. The considerable scatter between critical Re values suggested by different authors should be observed.

Finally, the influence of adopting different boundary conditions (i.e., Dirichlet or Neumann) on mass (or heat) transfer was also assessed.

Table 1

Schmidt / Prandtl numbers investigated in the present work with the relevant possible physical meaning or practical application.

Schmidt / Prandtl number	Possible application
500	Mass transfer, several solutes in water (urea in hemodialysis, ions in electrodialysis); heat transfer, heavy organic liquids (e. g., engine oil)
10–100	Heat transfer, light organic liquids (e.g., fuels)
5	Heat transfer (cold water in heat exchangers, seawater in membrane distillation, refrigerants)
0.5–1	Mass transfer (gas separation); heat transfer (all gases)
0.01–0.1	Heat transfer (liquid metals)

2. Models and methods

2.1. General assumptions

The simulations were performed using the commercial finite volume code Ansys-CFX® 2023 R2 [43].

In the modelling, the following simplifying assumptions were made:

1. all cylinders are aligned with the longitudinal z axis and have identical diameter d ;
2. the cylinders are organized in a regular square lattice configuration;
3. the fluid flows perpendicular to the cylinders under laminar, fully developed and steady-state conditions;
4. the fluid physical properties (density, dynamic viscosity and scalar diffusivity) are constant.

Assumptions (1) through (4) allow the use of the unit cell approach. This methodology, wherein the computational domain is a repetitive periodic unit of the array encompassing a single cylinder, has been often employed by the present authors in previous works [12,34,36,38,39].

2.2. Governing equations

The steady-state continuity and momentum equations for the flow of a Newtonian incompressible fluid, given assumptions (1)–(4) above, can be written:

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

$$\rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{F} \quad (2)$$

in which $\mathbf{u}$ is the velocity vector, p is the periodic component of the pressure, ρ and μ are the density and the dynamic viscosity of the fluid. The forcing term $\mathbf{F}$ is a driving pressure gradient compensating the large-scale pressure loss.

Simulations were carried out by applying a uniform forcing term $\mathbf{F}$ across the computational domain. For ease of comparison, the forcing term can be expressed in a dimensionless form as

$$\mathbf{f} = \mathbf{F} \frac{\rho d^3}{\mu^2} \quad (3)$$

where $F_0 = \mu^2 / (\rho d^3)$ is a reference pressure gradient scale. For example, F_0 is $\sim 1 \text{ Pa m}^{-1}$ in water for a cylinder diameter of 1 mm.

The convection-diffusion transport equation governing the scalar distribution is:

$$\mathbf{u} \cdot \nabla C = D \nabla^2 C + S_C \quad (4)$$

where C is the periodic component of the scalar concentration and D the scalar diffusivity in the fluid. The source term S_C compensates the large-scale scalar gradient; it can be shown that it can be expressed as follows:

$$S_C = - \left(\frac{\bar{J}S}{V} \right) \cdot \frac{u_s}{\langle u_s \rangle} \quad (5)$$

in which $\bar{J}$ is the surface-averaged wall scalar flux from the cylinder walls to the fluid, S is the wet surface and V is the volume of fluid. The wall scalar flux can either be imposed in the simulations (when Neumann boundary conditions are applied) or calculated as part of the solution (in the case of Dirichlet or Robin boundary conditions). The quantity $\bar{J}S/V$ is the average value of the source term while the last fraction in Eq. (5) is a dimensionless local correction, u_s being the local velocity component along the direction of the forcing term $\mathbf{F}$ and $\langle u_s \rangle$ its superficial average, i.e. its average computed over the whole computational domain (fluid + cylinder). For an in-depth discussion of the unit-cell approach, refer to [12].

2.3. Boundary conditions and fluid properties

Following the unit cell approach, periodic boundary conditions were applied to all variables between opposite boundaries of the computational domain. The velocity field on the cylindrical walls was subject to a no slip condition, while in the majority of cases a Neumann boundary condition was applied to the scalar field, with an arbitrary uniform value J assigned to the wall scalar flux. In some simulations, Dirichlet boundary conditions were applied instead by assigning the scalar C a uniform, arbitrary value C_w at the walls (the values chosen for J or C_w have no effect on the predicted Sherwood or Nusselt numbers).

For computational purposes, the fluid physical properties were those of water at 25 °C: density $\rho = 997 \text{ kg}\cdot\text{m}^{-3}$, dynamic viscosity $\mu = 8.89\cdot 10^{-4} \text{ Pa}\cdot\text{s}$ [44]. The scalar diffusivity D was made to vary as to obtain Schmidt numbers $Sc = \mu/(\rho D)$ in the range $0.01 \leq Sc \leq 500$.

2.4. Computational domain and main definitions

Since only pure cross flow is considered, the computational domain is essentially two-dimensional and is shown in Fig. 2. In this work, the porosity $\varepsilon = A/A_{tot}$ was set to 0.5, A being the fluid area and A_{tot} the total area (fluid + cylinder). The cylinder diameter is denoted by d and the side length of the square domain (pitch of the square lattice) by L . Note that in square lattices the d/L ratio and the porosity ε are related by:

$$\varepsilon = 1 - \frac{\pi}{4} \left(\frac{d}{L} \right)^2 \quad (6)$$

For computational purposes, the value of $0.280\cdot 10^{-3} \text{ m}$, typical of hollow fibers for hemodialysis, was chosen for d , yielding $L \approx 0.351\cdot 10^{-3} \text{ m}$ for $\varepsilon = 0.5$. Of course, once the results are cast into a dimensionless form, neither the geometrical scales nor the physical properties are relevant.

The generic azimuthal angle φ was assumed to increase counter-clockwise starting from the x axis direction. The forcing term angle γ was defined as the angle between the forcing term F and the x axis. Note that, due to the possible hydraulic anisotropy of the lattice, the mean

flow direction may not be aligned with the forcing term [39], so that the present definition of the angle γ (which can be arbitrarily set) is more appropriate than that of “flow attack angle” (which is obtained as part of the solution).

The cross flow Reynolds number Re was defined here as:

$$Re = \frac{\rho \langle u_s \rangle d}{\mu} \quad (7)$$

where $\langle u_s \rangle$ is the superficial velocity (defined in Section 2.2) projected on the direction of the forcing term F :

$$\langle u_s \rangle = \langle u_x \rangle \cos \gamma + \langle u_y \rangle \sin \gamma \quad (8)$$

$\langle u_x \rangle$ and $\langle u_y \rangle$ being the superficial velocity components along the x and y directions.

The normal hydraulic apparent permeability K of the bundle when subjected to the forcing term F (driving pressure gradient) was:

$$K = \mu \frac{\langle u_s \rangle}{|F|} \quad (9)$$

Its dimensionless counterpart, k , can be obtained by dividing K by the square of the diameter ($k = K/d^2$). On the basis of Eqs. (7) and (9), the relationship between the dimensionless permeability k and the Darcy-Weisbach friction coefficient λ is:

$$\lambda = \frac{2}{Re} \frac{1}{k} \quad (10)$$

The Péclet number Pe was defined here, as usual in the literature, as the product between the Reynolds number Re and the Schmidt number Sc ($Pe = Re \cdot Sc$).

The local shell-side Sherwood number (dimensionless mass transport coefficient) Sh_{loc} can be defined as:

$$Sh_{loc} = \frac{J}{C_w - C_b} \frac{d}{D} \quad (11)$$

where J is the local scalar flux, C_w is the local scalar concentration at the wall, and C_b is the bulk scalar concentration, i.e. the mass flow-weighted average of the scalar concentration computed on an arbitrary cross section.

However, when mass flux boundary conditions are imposed at the wall, the quantity Sh_{loc} as defined by Eq. (11) may diverge at points where the concentration at the wall, C_w , becomes equal to the bulk concentration, C_b . Sh_{loc} may even attain negative values where $C_w < C_b$ despite a net mass flux into the fluid, or $C_w > C_b$ despite a net mass flux out of the fluid. These conditions, physically unrealizable in simple channel flows with mass transfer, are indeed possible in more complex flows with strong surface non-uniformities [45].

The above phenomenon is illustrated in Fig. 3. This reports maps of the local concentration C for $|f| = 3$ ($Re \approx 0.01$), $Sc = 1$, uniform mass flux boundary conditions and two values of the forcing term angle γ , 0° (a) or 45° (b). C is made dimensionless as $\chi = (C - C_b)/(\bar{C}_w - C_b)$. The thick black line is the isoline $\chi = 0$, i.e. $C = C_b$; it can be observed that it intersects the cylinder wall for $\gamma = 0^\circ$, making Sh_{loc} diverge, but not for $\gamma = 45^\circ$.

The above discussed singularity is more likely to occur at very low Reynolds numbers (creeping flow conditions) and, of course, cannot occur when imposed concentration boundary conditions are adopted at the fluid-solid interface.

For the same reason, the simple wall average of the local Sherwood number, $\overline{Sh_{loc}}$, is not a reliable measure of the mean Sherwood number, and it is preferable to use the alternative quantity:

$$Sh_m = \frac{\bar{J}}{\bar{C}_w - C_b} \frac{d}{D} \quad (12)$$

in which $\bar{J}$ and $\bar{C}_w$ are the wall-averaged scalar flux and concentration at

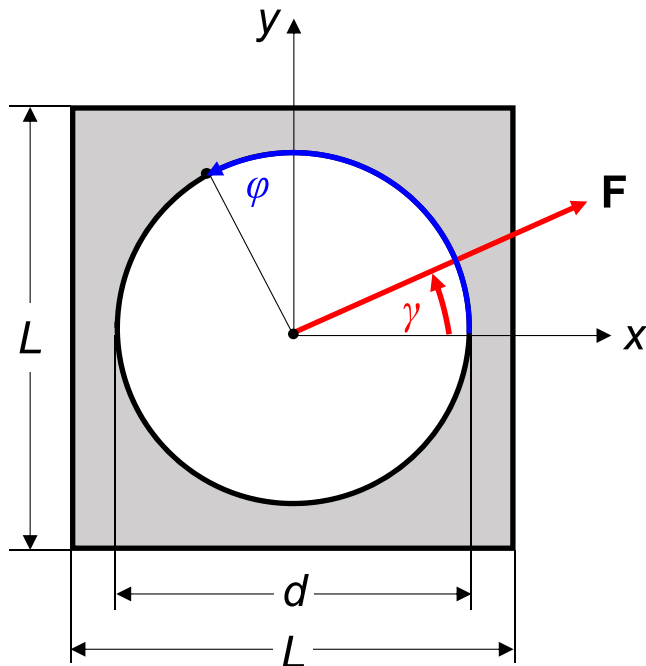


Fig. 2. 2-D computational domain of a regular square lattice with porosity $\varepsilon = 0.5$.

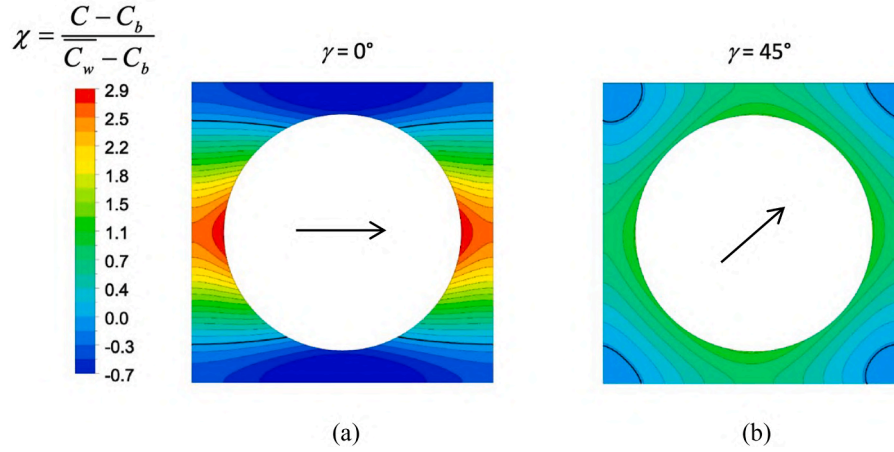


Fig. 3. Color maps of the dimensionless concentration $\chi = (C - C_b)/(\overline{C_w} - C_b)$ for a forcing term magnitude $|f| = 3$, a Schmidt number $Sc = 1$ and uniform mass flux boundary conditions. Forcing term angle: $\gamma = 0^\circ$ (a); $\gamma = 45^\circ$ (b). The thick line represents bulk concentration.

the wall, respectively. This definition is consistent with that commonly used in the literature on heat transfer in tube banks [41,46]. $\overline{Sh}_{loc}$ and Sh_m coincide if uniform concentration boundary conditions are used.

Note that the quantity Sh_m , although it applies to the whole cylinder, is still a function of the forcing term angle γ .

2.5. Finite volume grids and numerical details

The present simulations were limited to pure cross flow and thus were essentially two-dimensional. Therefore, the extent of the computational domain along the longitudinal direction was irrelevant. For compatibility with the code used, it was set to an arbitrary value and discretized by two finite volumes. The computational grids were exclusively composed of hexahedra, which are recognized for providing more accurate results compared to grids made by tetrahedra or hybrid [47].

All simulations were performed in double precision to ensure high numerical accuracy. Advection terms were discretized using a second-order upwind scheme (“high resolution” option of Ansys-CFX®). A stringent convergence criterion was applied, requiring the dimensionless residuals of all variables to drop below 10^{-12} before the solver was stopped.

Fig. 4 reports the computed dimensionless permeability k (a) and mean Sherwood number Sh_m (b) as functions of the number n_{FV} of finite volumes in the 2-D x-y cross section. The test case considered here was characterized by a forcing term magnitude $|f| = 3 \cdot 10^4$ ($Re \approx 50-70$), which is the highest value simulated in the present paper, a forcing term angle $\gamma = 30^\circ$, uniform mass flux boundary conditions and (as far as mass transfer is concerned) all the values of the Schmidt number Sc .

In regard to permeability, this decreases only by $\sim 0.5\%$ as n_{FV} increases from 2000 to 100,000, indicating a very weak grid dependence (note the expanded scale of graph a). In regard to the mean Sherwood number, this exhibits a weak dependence upon n_{FV} up to $Sc = 10$, while the influence of n_{FV} increases rapidly for larger Sc ; for $Sc = 500$, Sh_m decreases from ~ 300 to ~ 90 as n_{FV} increases from 2000 to 100,000. However, the last two grids (with $n_{FV} \approx 64,000$ and 100,000) yield almost identical values of Sh_m (89.26 and 89.40, respectively).

Therefore, it can be concluded that the grid with 100,000 volumes in the cross section provides largely grid-independent results for both hydrodynamics and mass transfer even under the most demanding conditions. This grid was used in all subsequent simulations. It comprises 2000 cells in the azimuthal direction ($0-360^\circ$) and 50 cells in the radial direction, with a radial size near the cylinder wall ranging from $\sim 2.7 \cdot 10^{-3} d$ to $\sim 8.2 \cdot 10^{-3} d$.

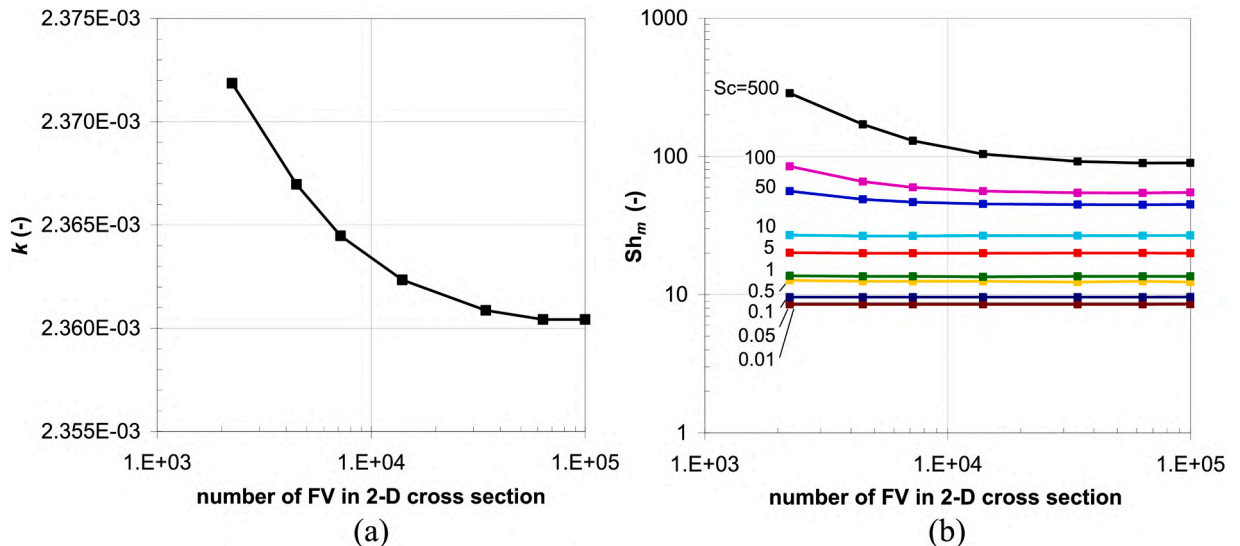


Fig. 4. Dimensionless permeability k (a) and mean Sherwood number Sh_m (b) as functions of the number of finite volumes in the 2-D x-y cross section for a forcing term magnitude $|f| = 3 \cdot 10^4$ ($Re \approx 50-70$), a forcing term angle $\gamma = 30^\circ$, uniform mass flux boundary conditions and different values of the Schmidt number Sc .

3. Results

Even with the present limitation to a single L/d ratio (~ 1.25 , yielding a bundle porosity $\varepsilon = 0.5$), the number of total cases simulated in the present work amounted to 2052:

- for uniform mass flux boundary conditions: 9 values of the forcing term magnitude $|f| \times 10$ values of the Schmidt number $Sc \times 19$ values of the forcing term angle $\gamma = 1710$ cases;
- for uniform wall concentration boundary conditions: 9 values of the forcing term magnitude $|f| \times 2$ values of the Schmidt number $Sc \times 19$ values of the forcing term angle $\gamma = 342$ cases.

Each case required about 5 core-hours of CPU time, for a total of about 10,000 core-hours.

3.1. Hydrodynamics

As anticipated in the Introduction, the present study is partly complementary to a previous investigation [39] in which, among other geometries, regular square arrays of circular cylinders in laminar cross flow were characterized in regard to their hydrodynamic behavior only.

Fig. 5 reports the predicted normal apparent hydraulic permeability, Eq. (9), made dimensionless with respect to d^2 , as a function of the forcing term angle γ for different values of the dimensionless forcing term magnitude $|f|$, Eq. (3), representing the driving pressure gradient. Only the interval $\gamma = 0^\circ$ – 45° is represented since, due to the existing symmetries and periodicities, it is sufficient to account for the overall variation of a quantity in the whole range 0° – 360° .

Note that, as demonstrated by Cancilla et al. [39], in the present configuration the hydraulic permeability becomes anisotropic when the Reynolds number exceeds a value of unity order. In these circumstances the Reynolds number, as defined by Eq. (7), associated with any given value of $|f|$ depends on the angle γ , so that only approximate values or ranges of Re can be indicated in the legend.

The figure shows that all the simulated cases at $Re \leq 1$ (i.e. $Re = 10^{-4}$, 10^{-3} , 10^{-2} , 10^{-1} , 1) yield a Darcyan and isotropic permeability, independent both of Re and of the angle γ . Only above a threshold corresponding to $|f| \approx 300$ or $Re \approx 1$, the permeability decreases with increasing $|f|$ (Re), due to the increasing importance of nonlinear

(Forchheimer) terms in the pressure drop – flow rate relation, and becomes a function of the forcing term angle γ . For values of $|f|$ larger than 3000 ($Re > \sim 9.5$), the permeability exhibits in the range 0° – 45° two local maxima for $\gamma = 0^\circ$ and 45° , which are directions of geometrical symmetry, and a relative minimum at some intermediate angle ($\gamma \approx 15^\circ$ for $|f| = 9000$, or $Re \approx 25$, and $\gamma \approx 5$ – 6° for $|f| = 30,000$, or $Re \approx 50$ – 70).

In the following Sections, the analysis will be extended to mass transfer.

3.2. Influence of the boundary conditions at the cylinder-fluid interface

As discussed in Section 2.4, uniform concentration boundary conditions offer the advantage that a local Sherwood number Sh_{loc} can be defined without incurring in singularities or unphysical negative values, and that the mean Sherwood number Sh_m can be obtained as the circumferential average of Sh_{loc} . However, in most practical applications, notably involving hollow fibers, and, in general, whenever the mass transfer resistance of the wall thickness is a large fraction of the overall resistance (lumen side film + wall thickness + shell side film), actual boundary conditions will be very close to those of uniform mass flux [48]. This explains why these latter conditions were used throughout most of the present study, as well as in most previous work by our group.

The question arises whether results are significantly affected by the choice of the boundary conditions. To answer this question, Fig. 6 reports polar charts of the mean Sherwood number Sh_m as a function of the forcing term angle γ for four increasing amplitudes $|f|$ of the forcing term, from $|f| \leq 0.3$ ($Re \leq 1 \cdot 10^{-3}$) (chart a) to $|f| = 30,000$ ($Re \approx 50$ – 70) (chart d). Each chart is drawn for two values of the Schmidt number Sc (1 and 500) and the two boundary conditions investigated here (uniform flux or uniform concentration).

The dependence of Sh_m on the forcing term angle γ might be represented in the form of Cartesian, rather than polar, charts and, for symmetry reasons, the γ range might be limited to the interval 0° – 45° (see “Supplementary Material”, Figure S1). Clearly, this alternative representation allows a more accurate reading of specific values but loses something in terms of clarity.

The general features of the charts in Fig. 6 will be discussed in the following Section 3.4. Here, we only stress that the influence of boundary conditions on the angular profiles of the mean Sherwood number is small. Boundary conditions may have a larger influence on

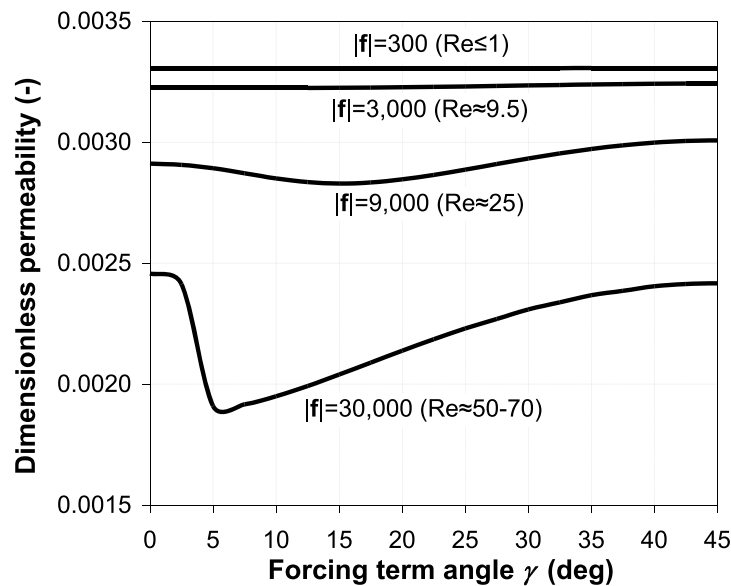


Fig. 5. Dimensionless normal apparent hydraulic permeability as a function of the forcing term angle γ at different values of the dimensionless forcing term magnitude $|f|$.

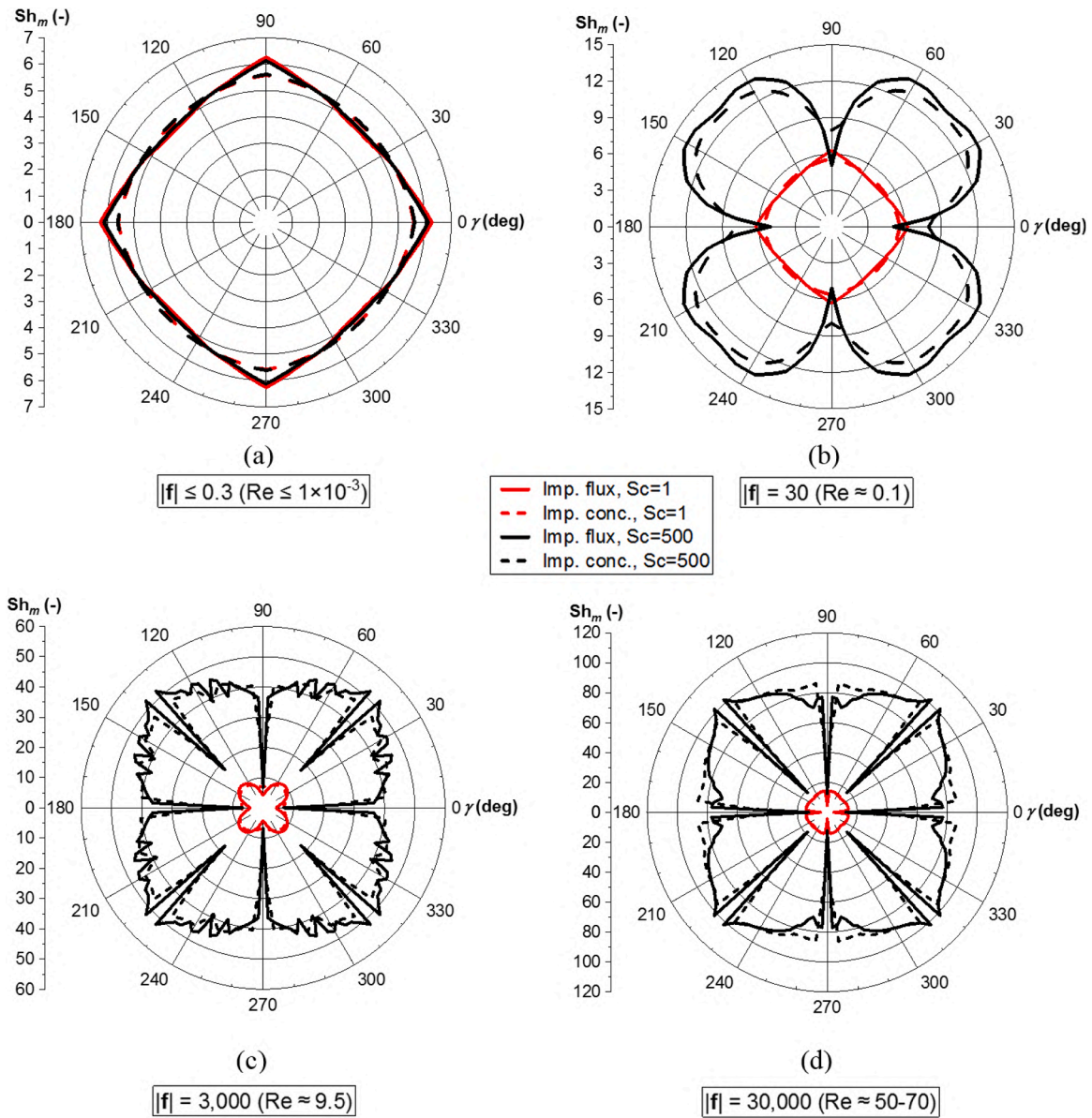


Fig. 6. Polar chart of the mean Sherwood number Sh_m as a function of the forcing term angle γ for two values of the Schmidt number Sc and different boundary conditions. Solid lines: uniform flux; broken lines: uniform wall concentration. Black lines: $Sc = 500$; red lines: $Sc = 1$. Forcing term magnitude (and average Reynolds number): (a) $|f| \leq 0.3$ ($Re \leq 1 \times 10^{-3}$); (b) $|f| = 30$ ($Re \approx 0.1$); (c) $|f| = 3000$ ($Re \approx 9.5 - 9.6$); (d) $|f| = 30,000$ ($Re \approx 50 - 70$).

the *local* distribution of the Sherwood or Nusselt numbers, as discussed in the following Section 3.3.

3.3. Local Sherwood number

A few authors have investigated the profiles of the local Nusselt number along the periphery of a tube, either isolated or belonging to a tube bank. Experimental data were provided by Zukauskas [23,26] but they were obtained at high Reynolds numbers. Computational results were presented by Antonopoulos [21] and Mandhani et al. [49]. For example, Fig. 7 compares the present results for the local Sherwood number Sh_{loc} , as defined by Eq. (11), with the simulations by Antonopoulos [21] for heat transfer in-line arrays with $\varepsilon = 0.5$, Sc (Pr) = 10, $Re = 30$ and uniform flux boundary conditions. The local Sherwood number is normalized by its circumferential average and is reported as a function of the azimuthal angle φ (its direction is defined in the inset). Note that, at this relatively high Reynolds number, no singularity of the type discussed in Section 2.4 occurs.

For this configuration, the local Sherwood or Nusselt number exhibits minima both in the upstream stagnation point ($\varphi = 180^\circ$) and in the downstream point opposite to it ($\varphi = 0^\circ$), while it attains its maximum values at $\varphi \approx 90^\circ$. This, however, is not always true as the following discussion shows.

Fig. 8 reports polar charts of the local Sherwood number Sh_{loc} , Eq. (11), as a function of the azimuthal angle φ for $|f| = 3000$ (yielding $Re \approx 9.5$), two values of the Schmidt number (1, left column, charts a-c-e, and 500, right column, charts b-d-f) and three values of the forcing term angle γ (0° , top row, charts a-b; 15° , middle row, charts c-d; and 45° , bottom row, charts e-f). Solid lines are for uniform mass flux boundary conditions, broken lines for uniform concentration ones.

An extremely complex scenario emerges. For $\gamma = 0^\circ$ and 45° , which are directions of geometrical symmetry (top and bottom row, respectively), but not for $\gamma = 15^\circ$ (middle row), the polar charts exhibit bilateral symmetry about the direction of the forcing term. A peculiar feature of the charts is that the front stagnation point $\varphi = \gamma + 180^\circ$ corresponds for both boundary conditions to a deep minimum of Sh_{loc} .

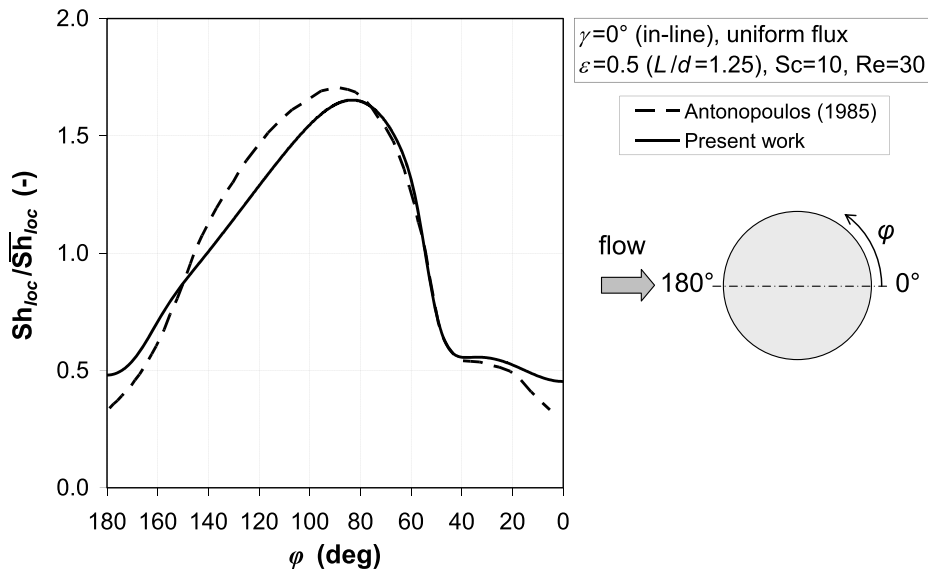


Fig. 7. Comparison of the present results (solid line) for the local Sherwood number with the simulations by Antonopoulos [21] (broken line) for in-line ($\gamma = 0^\circ$) arrays with $\varepsilon = 0.5$, Sc (Pr) = 10, $Re = 30$ and uniform flux boundary conditions. The Sherwood number is normalized by its circumferential average. The inset illustrates the direction of the azimuthal angle ϕ .

for $\gamma = 0^\circ$ ($\phi = 180^\circ$, charts a-b), but to a flat maximum of Sh_{loc} for $\gamma = 45^\circ$ ($\phi = 225^\circ$, charts e-f) as a consequence of the different structure of the flow field.

In the low-Schmidt number cases $Sc = 1$, left column, Sh_{loc} levels are higher for uniform flux than for uniform concentration at all forcing term angles γ . When $Sc = 500$, right column, Sh_{loc} levels are higher for uniform flux than for uniform concentration only for $\gamma = 15^\circ$, chart (d), whereas the opposite is true for $\gamma = 0^\circ$, chart (b). For $\gamma = 45^\circ$, chart (f), maxima of Sh_{loc} at $\phi = 225^\circ$ (front stagnation point) are higher for uniform concentration, but this is compensated by deeper minima at the opposite point $\phi = 45^\circ$ and lower levels in some intermediate angular intervals.

The increase of the Schmidt number from 1 to 500 has completely different effects depending on the forcing term angle γ and the boundary conditions.

For $\gamma = 0^\circ$, charts (a)-(b), and uniform flux, maxima of Sh_{loc} decrease about twofold when Sc increases from 1 to 500. However, for the same γ but uniform concentration, maxima of Sh_{loc} increase by $\sim 30\%$.

For $\gamma = 15^\circ$, charts (c)-(d), which is a generic direction not associated with any geometrical symmetry, the polar charts exhibit no symmetry. As Sc increases from 1 to 500, Sh_{loc} levels increase ~ 4 times ($= 500^{0.22}$) for uniform flux and ~ 5 – 6 times ($= 500^{0.26-0.29}$) for uniform concentration (note the use of different scales), while the overall shape of the polar diagrams changes markedly.

Finally, for $\gamma = 45^\circ$, charts (e)-(f), as Sc increases from 1 to 500, Sh_{loc} levels increase by $\sim 40\%$ for uniform flux and $\sim$ twice for uniform concentration (note the use of different scales), while the overall shape of the polar diagrams changes markedly in the former case and less in the latter case.

Thus, any change in the forcing term angle γ affects the whole circumferential profiles of the local Sherwood number Sh_{loc} and, as a consequence, also its mean values. This will be shown in detail in the following section.

3.4. Mean Sherwood number

A quantity that is of even greater significance than the local mass transfer coefficient, and does not suffer from the singularity problems of this latter under any imposed boundary condition, is the mean Sherwood number Sh_m , Eq. (12). For uniform wall concentration conditions,

but not for uniform mass flux ones, Sh_m coincides with the circumferential average of the local Sherwood number Sh_{loc} . Note that, although it is a mean value holding for the whole cylinder, Sh_m is still a continuous function of the forcing term angle γ , and one may wish to know what the profiles $Sh_m(\gamma)$ look like under different values of the Reynolds and Schmidt numbers.

A comprehensive summary of this behavior is reported in Fig. 9. This shows, in the form of polar charts, the circumferential profiles of Sh_m at different Schmidt numbers for uniform flux boundary conditions. These charts, in which the independent variable is γ , should not be confused with those in the previous Fig. 8, which report *local* values of Sh and have ϕ as the independent variable. Each chart corresponds to a value of the dimensionless forcing term (and thus, approximately, to a Reynolds number), from $|f| \leq 0.3$ ($Re \leq 1 \cdot 10^{-3}$), chart (a), to $|f| = 30,000$ ($Re \approx 50 - 70$), chart (f). The notation “ $|f| \leq 0.3$ ” and similar means that all profiles for $|f| < 0.3$ practically coincide with that for $|f| = 0.3$.

The lowest Reynolds number case $|f| \leq 0.3$ ($Re \leq 1 \cdot 10^{-3}$) is illustrated in Fig. 9(a). A noteworthy feature of this case is that the circumferential Sh_m profiles are independent also of the Schmidt number (in the broad range $0.01 \leq Sc \leq 500$), and thus collapse on a single diamond-shaped circumferential profile exhibiting four maxima of ~ 6.2 for $\gamma = i \cdot 90^\circ$ (“in line” configuration) and four minima of ~ 5 for $\gamma = 45^\circ + i \cdot 90^\circ$ (“staggered” configuration). Here, of course, $i = 0, 1, 2$ or 3 .

For values of $|f|$ larger than 0.3 (i.e., for Reynolds numbers larger than 1×10^{-3}), as shown in charts (b) through (f), the circumferential Sh_m profiles become increasingly complex as either $|f|$ or Sc increases, and those corresponding to different Schmidt numbers start to depart from one another. This is already quite evident in the case $|f| = 3$ ($Re \approx 0.01$), chart (b), where the limiting Schmidt number beyond which the profiles separate is ~ 10 . This trend continues with increasing $|f|$ (or Re); the limiting Schmidt number (in the above sense) is ~ 5 for $|f| = 30$ ($Re \approx 0.1$), ~ 0.5 for $|f| = 300$ ($Re \approx 1$), and ~ 0.1 for $|f| = 3000$ ($Re \approx 9.5$). At the highest $|f|$ investigated (30,000, corresponding to $Re \approx 50$ – 70 depending on the forcing term angle γ) all Sh_m profiles pertaining to different values of Sc , from 0.01 to 500, are different.

For example, at the highest Sc (500), the Sh_m profile for $|f| = 3$ ($Re \approx 0.01$) in chart (b) exhibits an inversion of maxima and minima with respect to the asymptotic case $|f| \rightarrow 0$ ($Re \rightarrow 0$) in chart (a): the directions $\gamma = i \cdot 90^\circ$ become associated with minima and those $\gamma = 45^\circ + i \cdot 90^\circ$ ($i = 0, 1, 2, 3$) with maxima. The same inversion is observed for any

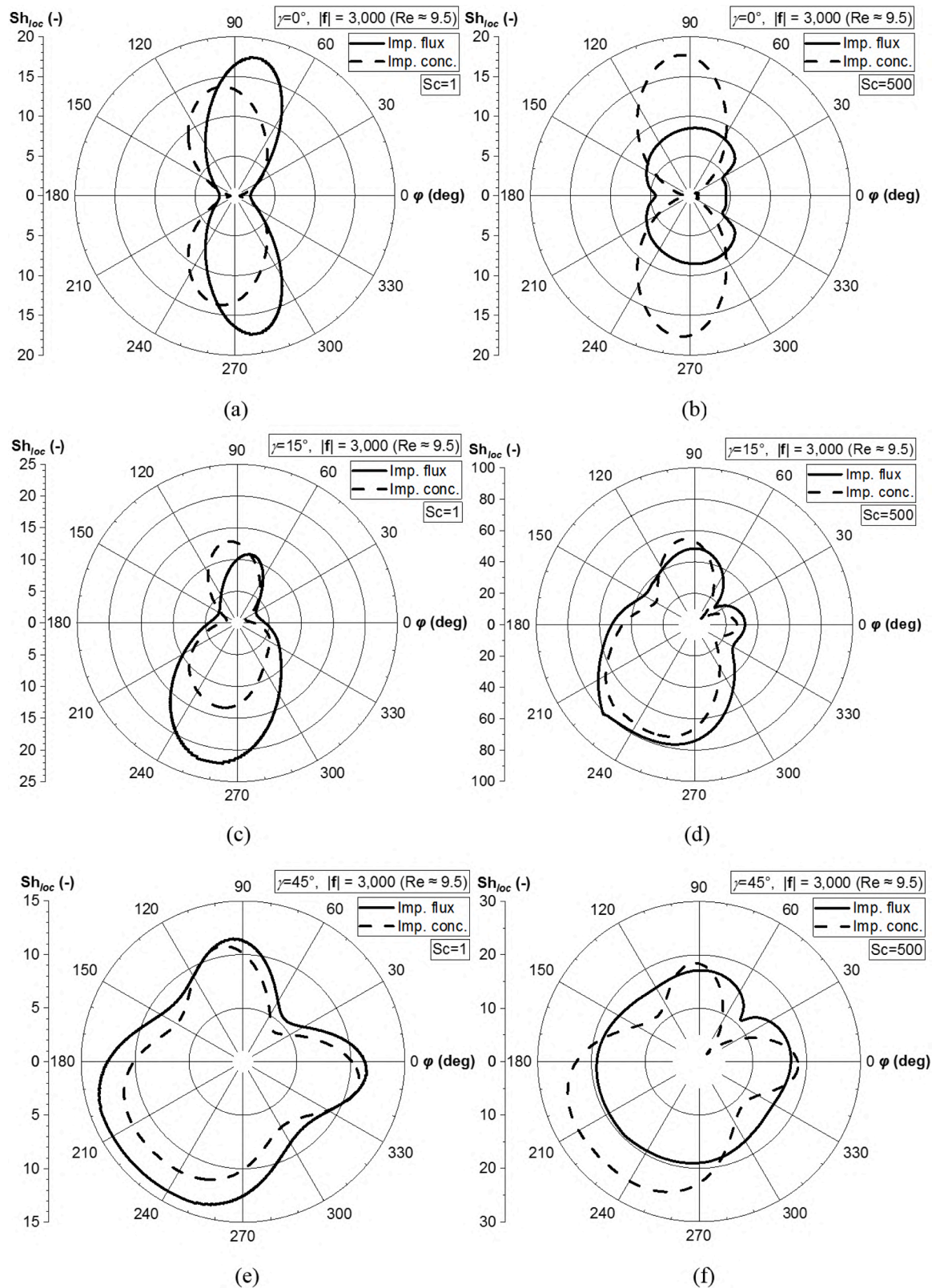


Fig. 8. Polar charts of the local Sherwood number Sh_{loc} as a function of the azimuthal angle φ for a forcing term $|f| = 3000$, yielding an average Reynolds number of ~ 9.5 . Solid lines: uniform flux; broken lines: uniform concentration. Left charts: $Sc = 1$; right charts: $Sc = 500$. Top row: $\gamma = 0^\circ$; middle row: $\gamma = 15^\circ$; bottom row: $\gamma = 45^\circ$.

$|f|$ (i.e., any Re) when the Schmidt number exceeds a certain value, e.g. ~ 10 for $|f| = 30$ ($Re \approx 0.1$, chart c).

This behavior is at odds with that of the hydraulic permeability,

Fig. 5, which starts to exhibit anisotropy (i.e., dependence upon the angle γ) only for $|f| > \sim 300$ ($Re > \sim 1$). Once again, this shows that, for sufficiently high values of the Schmidt number, tiny changes in the flow

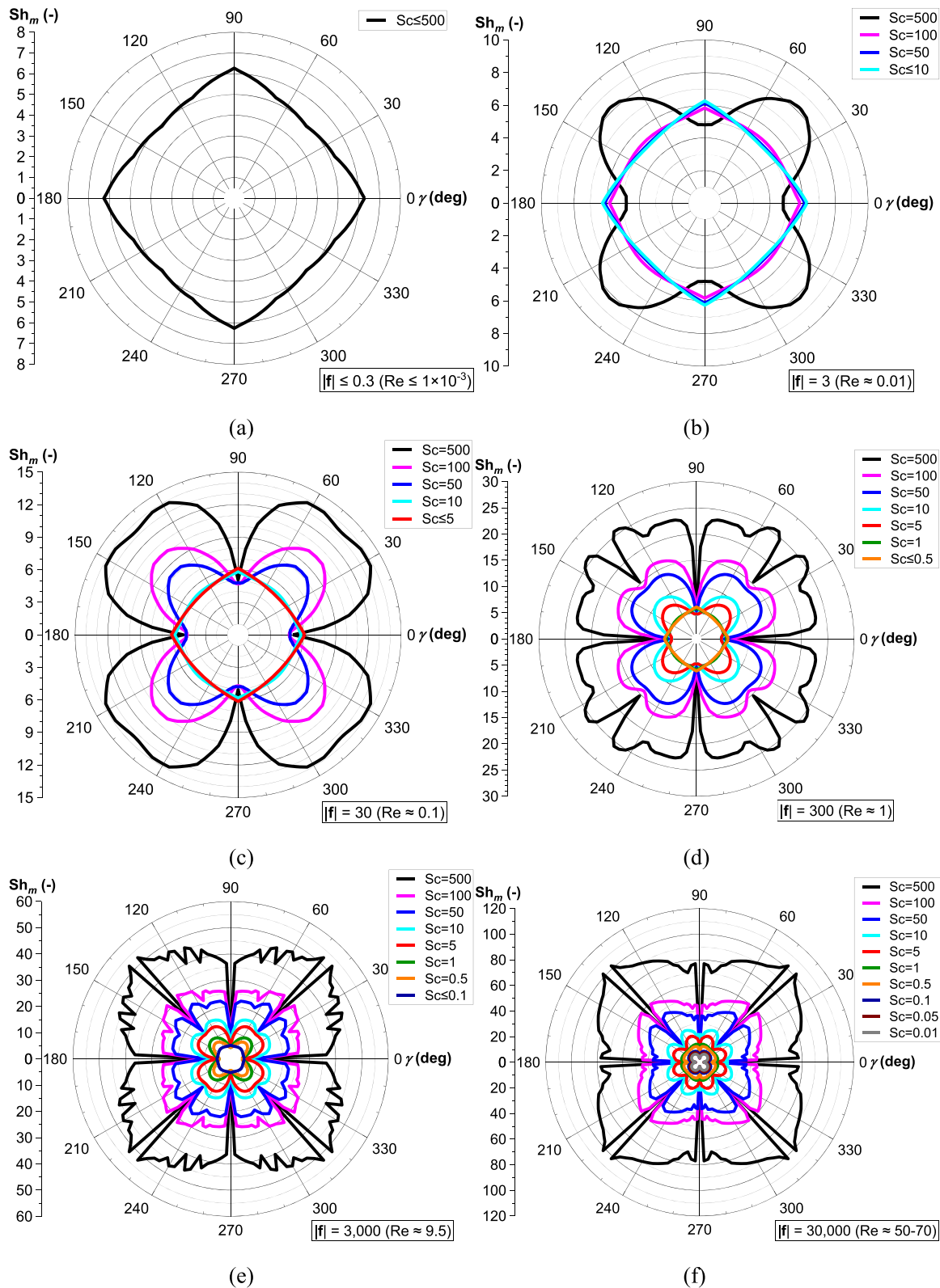


Fig. 9. Polar charts of the mean Sherwood number as a function of the forcing term angle γ at different Schmidt numbers and uniform flux boundary condition. Dimensionless forcing term (and average Reynolds number): (a) $|f| \leq 0.3$ ($Re \leq 1 \cdot 10^{-3}$); (b) $|f| = 3$ ($Re \approx 0.01$); (c) $|f| = 30$ ($Re \approx 0.1$); (d) $|f| = 300$ ($Re \approx 1$); (e) $|f| = 3000$ ($Re \approx 9.5 - 9.6$); (f) $|f| = 30,000$ ($Re \approx 50 - 70$).

field as γ varies are amplified yielding large changes in mass transfer.

A further noteworthy, and somewhat unexpected, feature of the polar charts in Fig. 9 is that, at sufficiently high $|f|$ (i.e., Re) and Sc , the directions of geometrical symmetry (both $\gamma = i \cdot 90^\circ$ and $\gamma = 45^\circ + i \cdot 90^\circ$

for $i = 0, 1, 2, 3$) become associated with deep and narrow minima of Sh_m , whereas all intermediate directions exhibit larger values of Sh_m . Oddly, these minimum transfer directions are (i) just those (occurring in-line or staggered tube banks in cross flow) that have received most

attention in the literature, (ii) are the subject of most existing heat or mass transfer correlations, and (iii) are probably most frequently chosen in actual equipment.

As for Fig. 6, the same dependence of Sh_m on the forcing term angle γ might be represented in the form of Cartesian, rather than polar, charts and, for symmetry reasons, the γ range might be limited to the interval 0° – 45° (see “Supplementary Material”, Figure S2).

Yet another way to represent the combined effects of the Reynolds and Schmidt numbers on the γ -dependent mean Sherwood number is to

plot polar charts of Sh_m for a fixed value of Sc and increasing values of $|f|$ (i.e., Re). For example, Fig. 10 reports Sh_m as a function of γ for $|f|$ increasing from 0.3 to 30,000 and (a) $Sc = 1$; (b) $Sc = 500$.

The figure makes it clear that, for moderate Schmidt numbers ($Sc = 1$, chart a), the curves coincide up to $|f| = 30$ ($Re \approx 0.1$) and separate only for larger values of $|f|$ (i.e., Re). The inversion from maxima to minima at $\gamma = i \cdot 90^\circ$ (and vice versa at $\gamma = 45^\circ + i \cdot 90^\circ$) occurs between $|f| = 300$ and $|f| = 3000$, i.e. between $Re \approx 1$ and $Re \approx 10$. Contrariwise, at high Schmidt number ($Sc = 500$, chart b), the single curves separate for

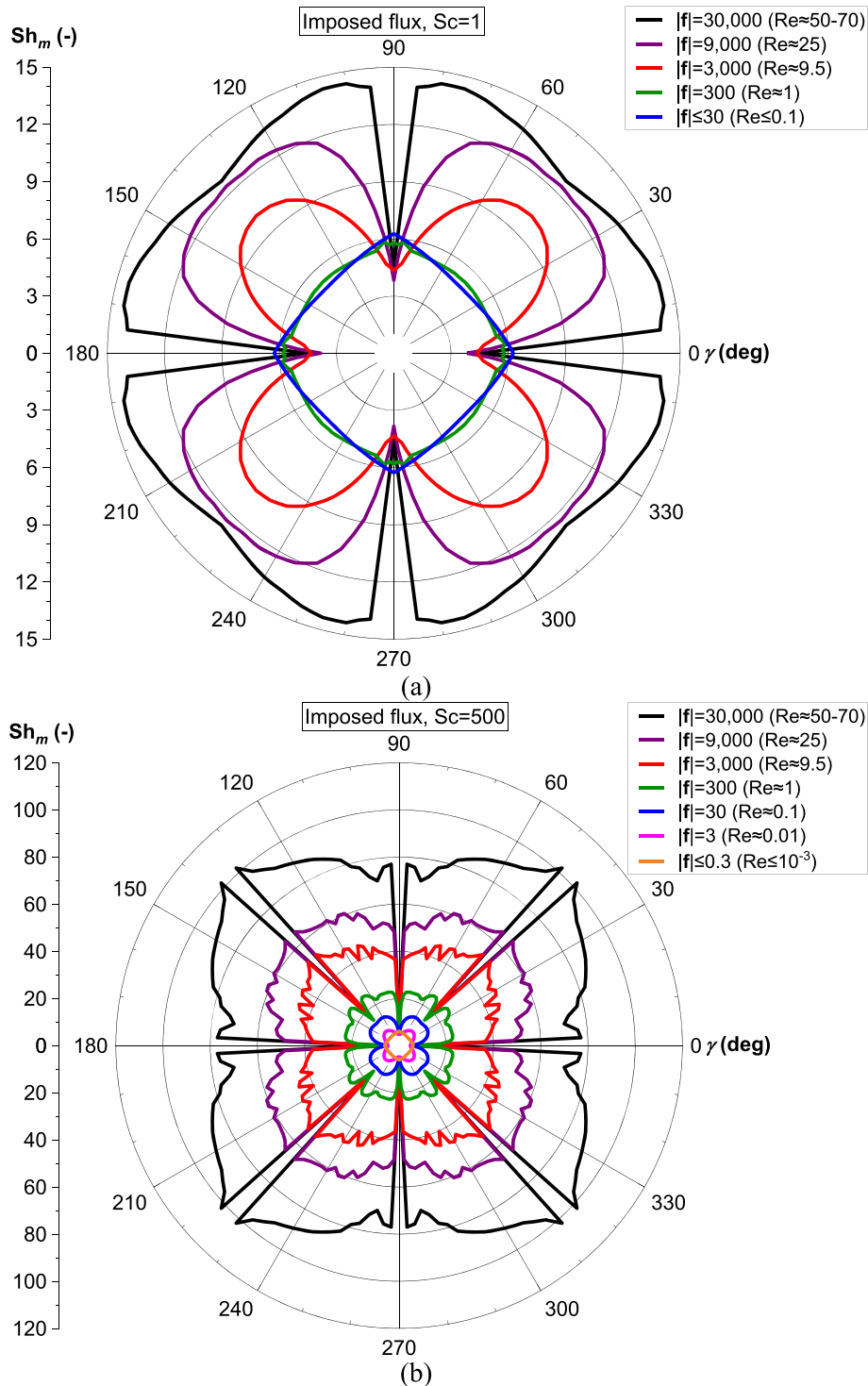


Fig. 10. Polar charts of the mean Sherwood number Sh_m as a function of the forcing term angle γ at different values of the dimensionless forcing term magnitude $|f|$ (uniform flux boundary conditions). (a) $Sc = 1$; (b) $Sc = 500$.

$f| \geq 0.3$, i.e. for $Re \geq \sim 10^{-3}$, and also the inversion between minima and maxima for $\gamma = i \cdot 90^\circ$ and $45^\circ + i \cdot 90^\circ$ occurs as soon as $|f|$ exceeds ~ 0.3 (i.e., Re exceeds $\sim 10^{-3}$).

The reason why the symmetry directions $\gamma = i \cdot 90^\circ$ and $\gamma = 45^\circ + i \cdot 90^\circ$ ($i = 0, 1, 2, 3$) are associated with minima of mass transfer at sufficiently high $|f|$ (i.e., Re) and Sc is partly clarified by Fig. 11. It compares color maps of the dimensionless concentration $\chi = (C - C_b)/(\overline{C_w} - C_b)$ (a quantity already used in Fig. 3) and superimposed velocity vector plots for a dimensionless forcing term $|f| = 9000$ (yielding $Re \approx 25$), a Schmidt number $Sc = 500$, uniform mass flux boundary conditions and three values of the forcing term angle γ : 0° (a), 30° (b) and 45° (c).

At the generic angle $\gamma = 30^\circ$, graph (b), the misalignment of the forcing term with the axes of geometrical symmetry causes an effective fluid mixing and leads to low values of concentration at the cylinder wall, corresponding to high values of the Sherwood number in virtue of Eqs. (11) and (12). When the forcing term (and, necessarily, also the mean flow) are aligned with the geometrical symmetry axes at $\gamma = 0^\circ$ or 45° , regions of stagnant flow arise both in front and behind a cylinder, mixing is poor, and regions of high concentration surround the cylinder, yielding low values of Sh_m .

A peculiar feature of Figs. 9 and 10 is the sharp dependence of Sh_m upon the forcing term angle γ in the proximity of the directions of geometrical symmetry at high $|f|$ and Sc . For example, in Fig. 10(b), for $|f| = 30,000$ and $Sc = 500$ (black line) a slight increase of γ from 42.5° to 45° is sufficient to cause the mean Sherwood number to fall steeply from ~ 103 to ~ 15 , whereas, in Fig. 10(a), for $|f| = 30,000$ and for $Sc = 1$ (black line), the same variation of γ leaves Sh_m practically unchanged at ~ 12 .

Fig. 12 purports to relate this behavior to that of the corresponding velocity and concentration distributions. Maps (a) and (b) show the

distribution of the velocity module $|u|$, normalized by $\langle u_s \rangle$, for $\gamma = 42.5^\circ$ and 45° , respectively, and $|f| = 30,000$ ($Re \approx 70$ at these values of the angle γ). Some streamlines are superimposed. It can be observed that the two distributions are practically identical, apart from minute differences in the impingement region.

The concentration distributions obtained for the same $|f|$ (i.e., Re) and the same angles γ for $Sc = 1$, shown in maps (c) and (d) using the previously defined dimensionless concentration $\chi = (C - C_b)/(\overline{C_w} - C_b)$, are also practically identical, which justifies the negligible variation of Sh_m between the two values of the angle γ observed in Fig. 10(a) (see ‘‘Supplementary Material’’, Figure S2(f)).

However, the concentration distributions obtained for the same $|f|$ (Re) and the same angles, but for $Sc = 500$, shown in maps (e) and (f) of Fig. 12, are completely different. The case $\gamma = 45^\circ$, map (f), exhibits a concentration distribution that does not differ much from that for $Sc = 1$, map (d). However, the small deviation of the angle γ from the symmetry direction (45°) to the near direction 42.5° , map (e), is sufficient to change this distribution completely, creating a region of very low concentration on one side of the cylinder and a region of only slightly higher concentration on the opposite side, with a drastic net reduction of the wall concentration and a corresponding drastic increase of Sh_m from ~ 15 to more than 100.

3.5. γ -averaged mean Sherwood number

In order to characterize in a synthetic way the overall mass transfer behavior of the bundle, one can define the γ -averaged mean Sherwood number $\{Sh_m\}$ as the average of the (γ -dependent) mean Sherwood number Sh_m over all possible directions γ of the forcing term F . Consistently, also for the other γ -dependent quantities Re (Reynolds

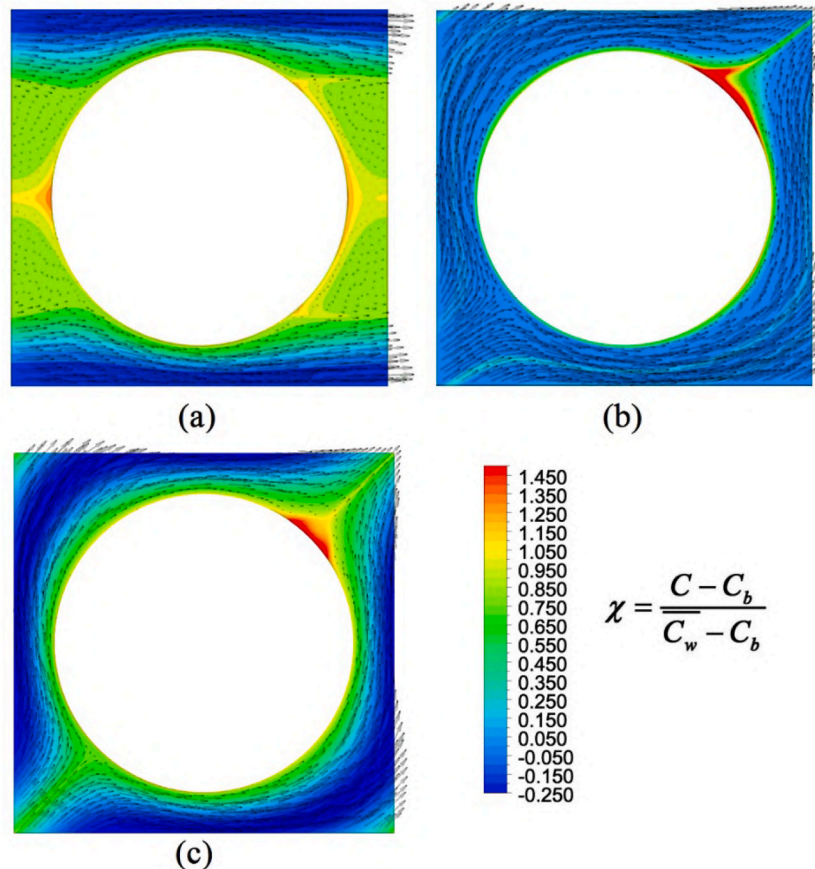


Fig. 11. Color maps of the dimensionless concentration $\chi = (C - C_b)/(\overline{C_w} - C_b)$ and superimposed velocity vector plots for a dimensionless forcing term magnitude $|f| = 9000$ (yielding $Re \approx 25$), $Sc = 500$, uniform flux boundary conditions and three values of the forcing term angle: (a) $\gamma = 0^\circ$; (b) $\gamma = 30^\circ$; (c) $\gamma = 45^\circ$.

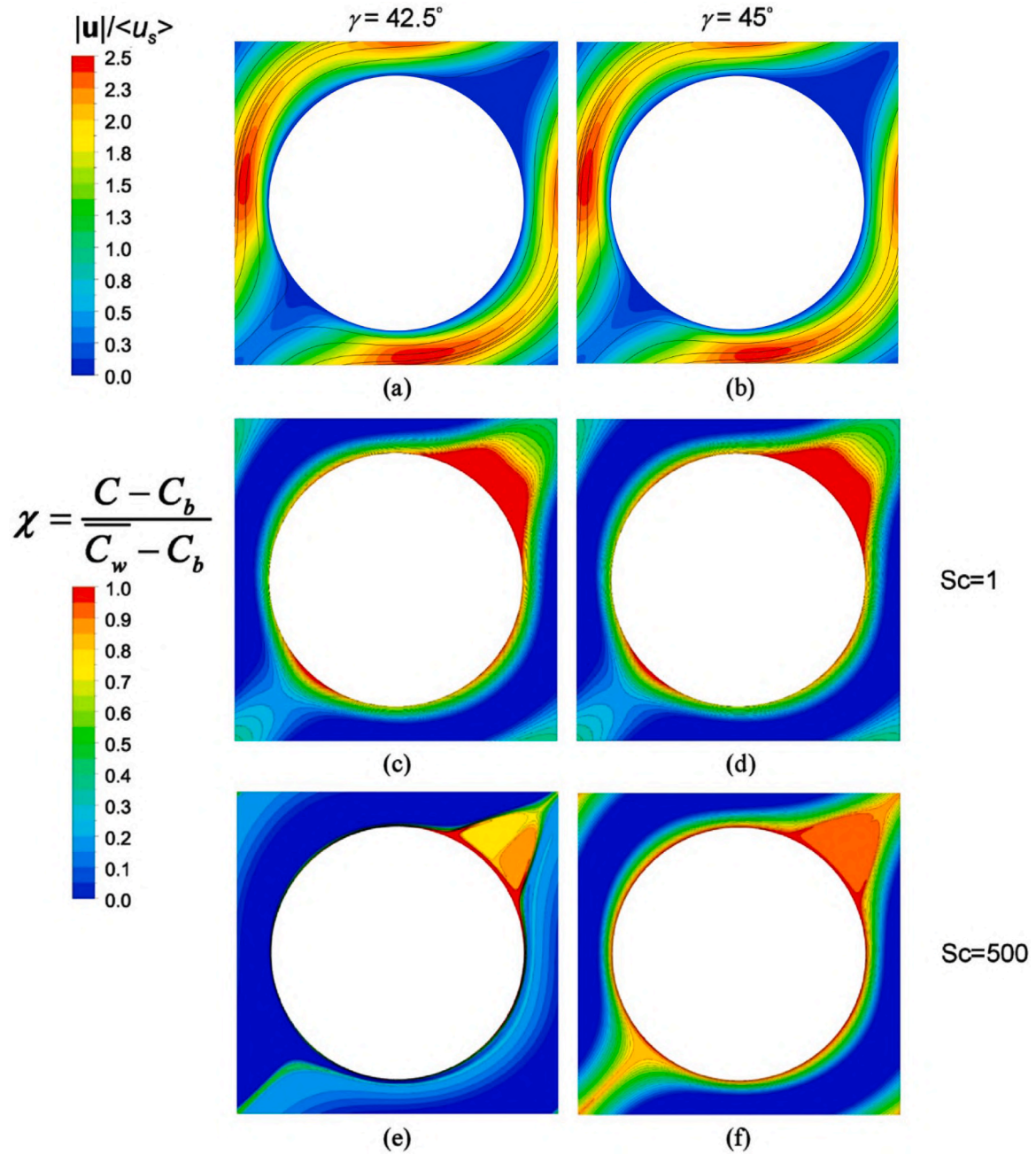


Fig. 12. Color maps of the dimensionless velocity module with superimposed streamlines (a, b) and of the dimensionless concentration $\chi = (C - C_b) / (\overline{C_w} - C_b)$ (c-f) for a dimensionless forcing term $|f| = 30,000$ ($Re \approx 70$) and uniform flux boundary conditions. Forcing term angle: $\gamma = 42.5^\circ$ (a, c, e); $\gamma = 45^\circ$ (b, d, f). Schmidt number: $Sc = 1$ (c, d); $Sc = 500$ (e, f).

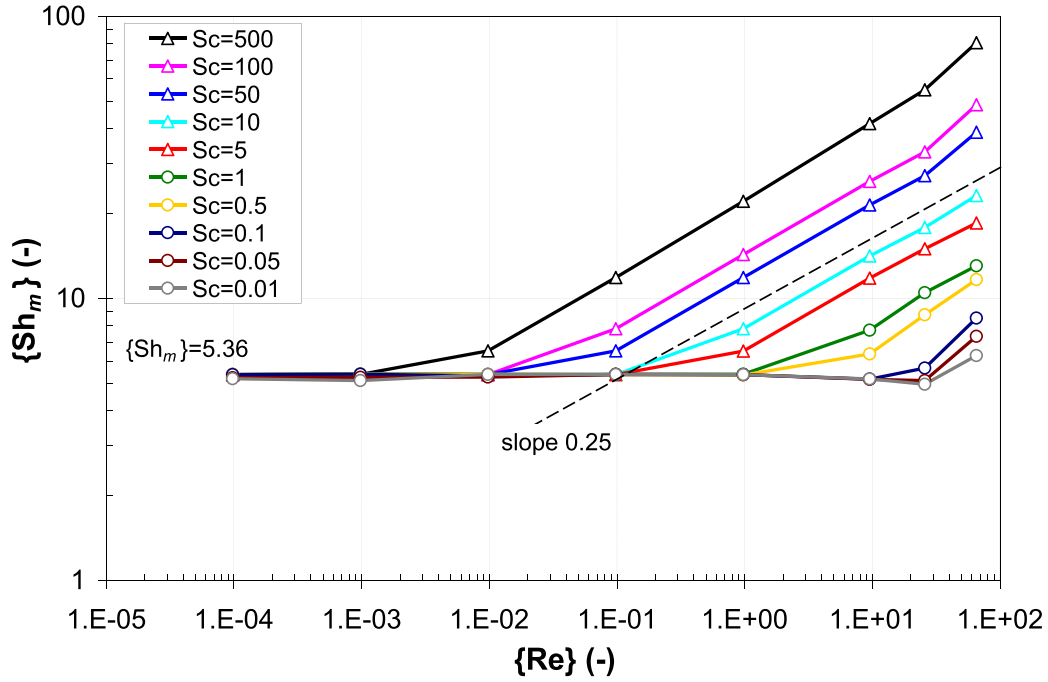


Fig. 13. $\{Sh_m\}$ as a function of $\{Re\}$ (see definitions in the text) at different Schmidt numbers for uniform flux boundary condition.

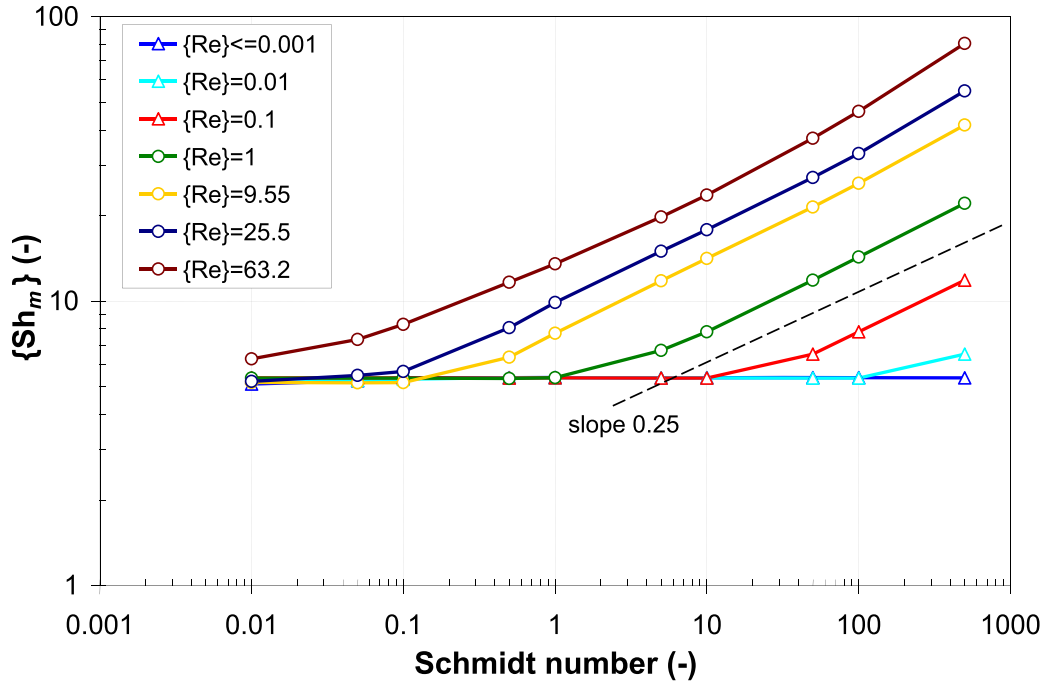


Fig. 14. $\{Sh_m\}$ as a function of the Schmidt number at different $\{Re\}$ (see definitions in the text) for uniform flux boundary condition.

number) and $Pe = ReSc$ (Péclet number) one can define angle-averaged values $\{Re\}$ and $\{Pe\}$ as averages over all possible directions of the forcing term F .

Fig. 13 shows $\{Sh_m\}$ as a function of $\{Re\}$ for all the values of Sc investigated and uniform flux boundary conditions. For each value of Sc , the corresponding $\{Sh_m\}$ versus $\{Re\}$ curve can be schematically divided into three regions: a *plateau* up to a certain, Sc -dependent, $\{Re\}$; a power-law dependence, characterized by an exponent close to 0.25, for large $\{Re\}$; and a connecting section in between. The limiting (angle-

averaged) Reynolds number at which each curve leaves the *plateau* decreases with the Schmidt number, from ~ 10 for $Sc = 0.1$ to ~ 1 for $Sc = 1$, ~ 0.1 for $Sc = 10$ and 0.01 for $Sc = 100$.

For the same uniform mass flux boundary conditions, Fig. 14 shows $\{Sh_m\}$ as a function of Sc for all values of $\{Re\}$ investigated. It can be observed that, for sufficiently high Sc , $\{Sh_m\}$ increases with Sc approximately following a power law with an exponent similar to that found for the Reynolds number dependence (~ 0.25 , Fig. 13). Each curve departs from the low-Schmidt number *plateau* at a value of Sc that, for example,

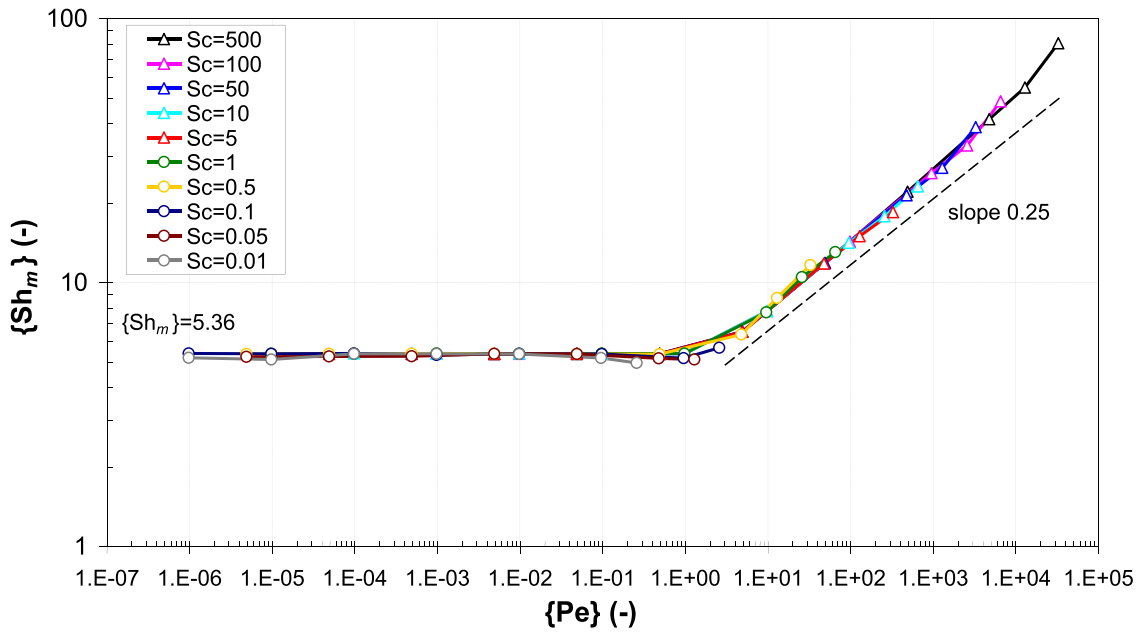


Fig. 15. $\{Sh_m\}$ as a function of $\{Pe\}$ (see definitions in the text) at different Schmidt numbers for uniform flux boundary conditions.

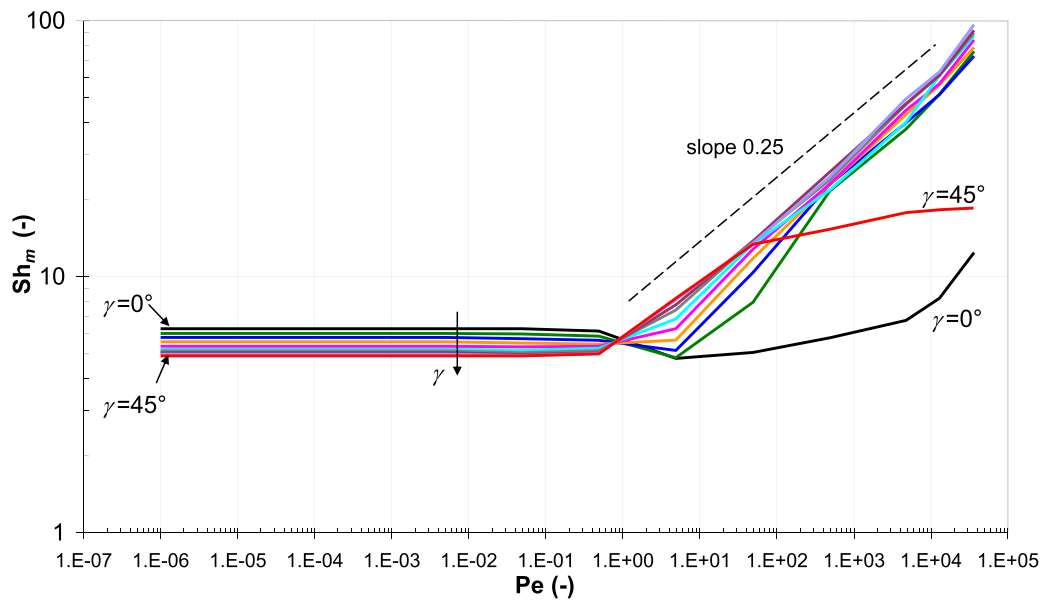


Fig. 16. Mean Sherwood number Sh_m as a function of the Péclet number Pe for different forcing term angles γ in the range $0^\circ - 45^\circ$ ($Sc = 500$, uniform flux boundary condition).

is ~ 100 at $\{Re\} = 0.01$ and 0.1 at $\{Re\} = 10$.

This behavior implies that $\{Sh_m\}$ can actually be expressed as a function of $\{Pe\}$ only. This is actually done in Fig. 15, which collects all the results obtained for different values of $|f|$ (and thus of $\{Re\}$) and Sc .

The results in Fig. 15 can be approximated with good accuracy up to $\{Pe\} \approx 10^4$ by the simple two-region piecewise correlation:

$$\{Sh_m\} = 5.36 \quad (\{Pe\} \leq 2) \quad (13.a)$$

$$\{Sh_m\} = 5.36(\{Pe\}/2)^{0.25} \quad (2 < \{Pe\} < 10^4) \quad (13.b)$$

Note, however, that Eqs. (13) are subjected to the further restriction $\{Re\} < \sim 100$ because no simulation was conducted beyond this value.

For Péclet numbers larger than $\sim 10^4$ (corresponding, for example, to Reynolds numbers larger than ~ 20 if $Sc = 500$) $\{Sh_m\}$ tends to increase

with a slope larger than 0.25.

3.6. Combined effects of the Péclet number and the forcing term angle on Sh_m

Fig. 16 shows the mean Sherwood number Sh_m as a function of the Péclet number Pe for $Sc = 500$ and all forcing term angles γ tested (here, neither Pe nor Sh_m are averaged over γ). The step between different values of γ is 5° .

For $Pe < \sim 1$ and all angles γ , Sh_m is independent of Pe , consistently with the low-Péclet number plateau observed in Fig. 15 for the γ -averaged mean Sherwood number $\{Sh_m\}$. In this region, the influence of the angle γ is moderate, with the highest Sh_m being attained for $\gamma = 0^\circ$ and the lowest for $\gamma = 45^\circ$, consistently with the diamond-shape exhibited by

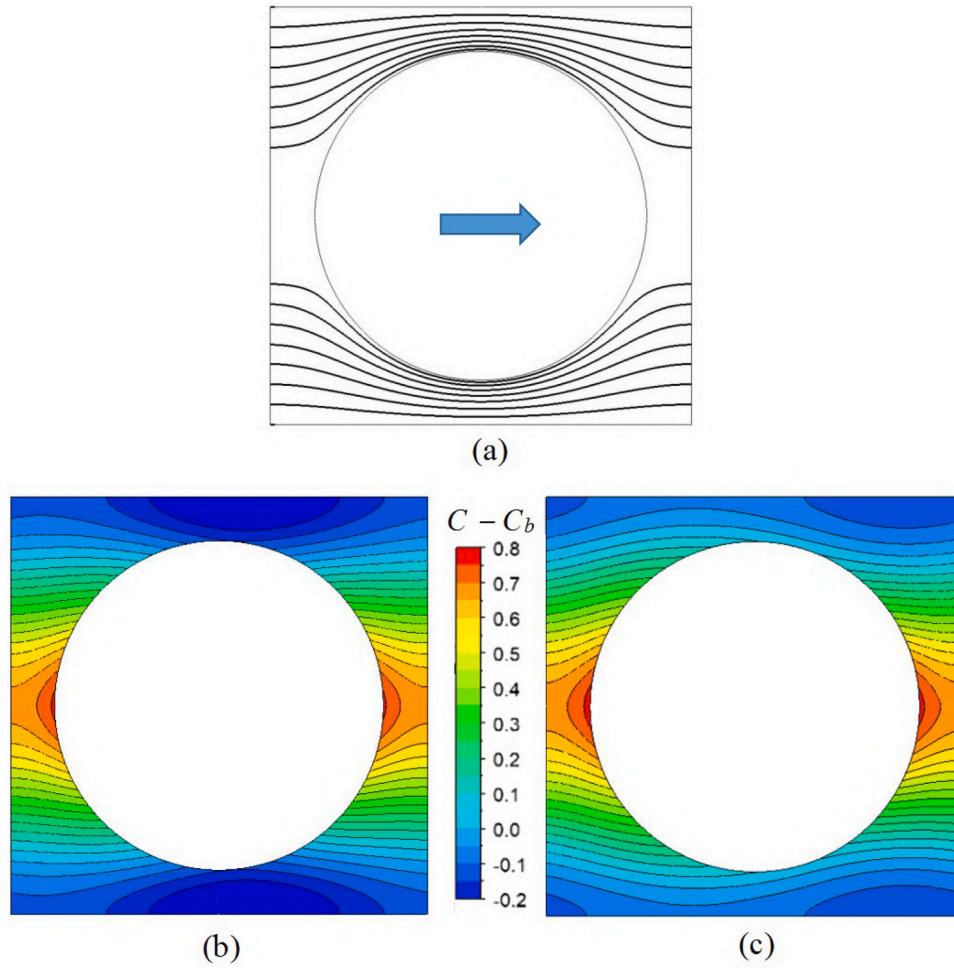


Fig. 17. Flow and concentration fields for $Sc = 500$, $\gamma = 0^\circ$, uniform flux boundary conditions and two values of the forcing term magnitude $|f|$. (a) Flow field, self-similar in the two cases, visualized by streamlines; the arrow indicates the forcing term (and mean flow) direction; (b) color map of the quantity $C - C_b$ for $|f| = 0.3$ (yielding $Re = 10^{-3}$, $Pe = 0.5$); (c) color map of $C - C_b$ for $|f| = 3$ (yielding $Re = 10^{-2}$, $Pe = 5$).

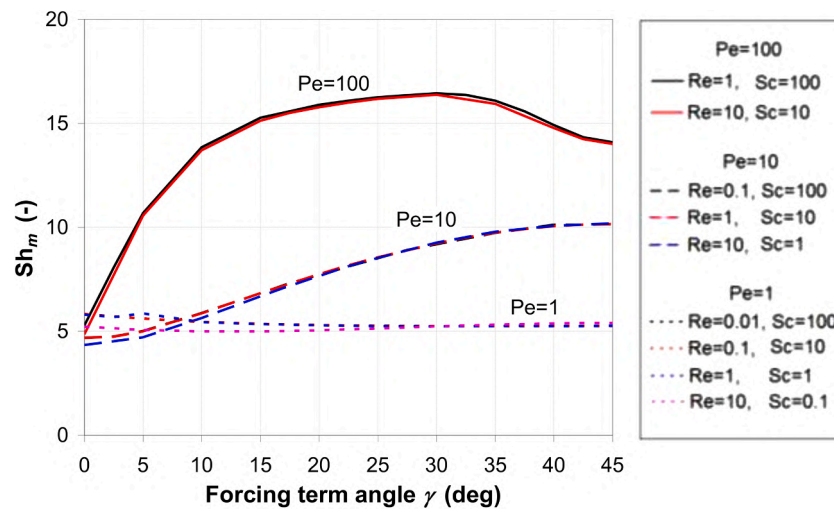


Fig. 18. Behavior of the mean Sherwood number Sh_m as a function of the forcing term angle γ for three values of Pe obtained by different combinations of Re and Sc (uniform flux boundary conditions). Solid lines: $Pe = 100$; broken lines: $Pe = 10$; dotted lines: $Pe = 1$.

the polar charts in Figs. 9 and 10 for very low values of $|f|$ (Re) and Sc .

However, for $Pe > \sim 1$, Sh_m starts to vary with Pe . The curves for $5^\circ \leq \gamma \leq 40^\circ$ are close to one another and, for sufficiently high Pe , follow a power law of exponent ~ 0.25 as the angle-averaged mean Sherwood number $\{Sh_m\}$ in Fig. 15, while the curves for $\gamma = 0^\circ$ and 45° (directions of geometrical symmetry) follow a different trend, much less dependent on Pe and lying (for sufficiently high Pe) below all other curves. In this range, the curve for $\gamma = 0^\circ$, associated with the steep minimum in the polar charts, is the lowest.

When Pe exceeds ~ 1 , the Sh_m curves reverse their hierarchy, in correspondence with the inversion from minima to maxima and vice versa between the values attained at the limiting angles of 0° and 45° , already observed in the polar charts of Figs. 9 and 10.

A striking feature of Fig. 16 is that, in a narrow interval of Péclet numbers (1 - 10), the curves for angles $\gamma \leq 15^\circ$ decrease with Pe . A decrease of the Sherwood (or Nusselt) number as the Reynolds or Péclet numbers increase is indeed uncommon and counter-intuitive, but it is well possible in the presence of relatively complex geometries, such as interacting obstacles. Consider, for example, the curve reporting the mean Sherwood number Sh_m as a function of the Péclet number Pe for $\gamma = 0^\circ$. It exhibits a marked decrease as Pe increases from $Pe = 0.5$ (corresponding to $Re = 10^{-3}$) to $Pe = 5$ ($Re = 10^{-2}$). In Fig. 17, the corresponding flow field is represented in the form of streamlines in graph (a), and is almost perfectly self-similar for the two Reynolds number cases, since they both lie well within the Darcyan regime. Of course, velocities increase ten times between the two cases.

Consider now the corresponding concentration distributions reported in Fig. 17, graphs (b) and (c). The quantity shown is the difference $\Delta C = C - C_b$ between the local and bulk concentrations (values are in mol m^{-3} and were obtained for a uniform wall mass flux of $10^{-5} \text{ mol m}^{-2} \text{ s}^{-1}$). For $Re = 10^{-3}$, graph (b), the distribution is that typical of creeping flow and is mainly determined by diffusion, as indicated by the almost symmetric shape of the iso ΔC lines with respect to the vertical midline (geometric symmetry line). By increasing the Reynolds number to $Re = 10^{-2}$, graph (c), the larger relative importance of advection with respect to diffusion causes the low- ΔC (blue) regions to be shifted downstream. As a consequence, large portions of the cylinder wall are now in contact with flow regions at higher concentration, and the circumferentially-averaged concentration difference at the wall, $\bar{C}_w - C_b$, increases. In virtue of Eq. (12), this causes a significant decrease of the mean Sherwood number Sh_m (namely, from ~ 5.7 to ~ 4.5).

Although this phenomenon has been demonstrated here for a specific forcing term angle γ ($\gamma = 0^\circ$), it is clear that, when averages of Sh_m are performed over all possible values of γ to obtain the γ -averaged mean

Sherwood number $\{Sh_m\}$, a slight decrease of this quantity with Re (or Pe) can still persist, as (barely) visible for some values of Sc in Fig. 15.

Fig. 18 reports the behavior of the mean Sherwood number Sh_m as a function of the forcing term angle γ for three values of Pe , obtained by different combinations of Re and Sc for uniform mass flux boundary conditions. This figure is a further confirmation that the dependence on Pe accounts for almost all the variation in the mean Sherwood number Sh_m , while, for any given Pe , the Reynolds and Schmidt numbers play only a minor role.

4. Conclusions

Accurate and grid-independent numerical predictions were obtained for laminar, steady and fully developed cross flow with mass transfer past an infinite square array of cylindrical rods. For a fixed bundle porosity of 0.5 the Reynolds and Schmidt number and the orientation of a forcing term (representing a driving pressure gradient) were made to vary in a broad range, and their influence on local and overall mass transfer was investigated by using the well-established unit cell approach. Both uniform mass flux and uniform concentration conditions at the cylinder-fluid interface were considered.

In regard to the local Sherwood number Sh_{loc} , for both uniform concentration and uniform mass flux boundary conditions, polar charts of Sh_{loc} along the cylinder periphery were obtained for different orientations of the forcing term, Reynolds numbers, and Schmidt numbers. For the orientation $\gamma = 0^\circ$ (corresponding to in-line tube banks) the present results were in good agreement with previous numerical heat transfer predictions by Antonopoulos [21]. For the same orientation, deep local minima of Sh_{loc} were predicted both at the front stagnation point and at the opposite location downstream of each cylinder. However, for other orientations, and in particular for $\gamma = 45^\circ$ (corresponding to staggered tube banks), a local maximum of Sh_{loc} was predicted at the front stagnation point, and a local minimum at the opposite downstream location. These features were in qualitative agreement with previous works [21,49].

In regard to the mean (i.e., circumferentially averaged) Sherwood number Sh_m , a large section of the present study was devoted to the prediction of its dependence on the forcing term angle γ (which, discounting minor hydrodynamic anisotropies of the lattice, is close to the direction of the superficially-averaged velocity). This issue is generally omitted in the literature, which, as recalled above, mostly concentrates on the two values $\gamma = 0^\circ$ and 45° , corresponding to in-line and staggered rod arrangements. A complex dependence of Sh_m on γ was observed, which became increasingly strong and affected also by the Schmidt

number as the Reynolds number increased.

A striking feature of the results is that, for sufficiently high Reynolds and Schmidt numbers, profiles of Sh_m as a function of γ exhibit deep minima when $\gamma = i \cdot 90^\circ$ and only slightly less deep minima when $\gamma = 45^\circ + i \cdot 90^\circ$ ($i = 0, 1, 2, 3$), i.e. when the forcing term is aligned with one of the eight axes of geometrical symmetry of the square lattice, while all intermediate directions exhibit larger values of Sh_m . It is odd that these minimum-transfer directions (i) are just those that have received most attention in the literature, (ii) are the subject of most existing heat or mass transfer correlations, (iii) and are most frequently chosen in actual equipment. Of course, in real life equipment the inevitable irregularities of a bundle, slight asymmetries or time oscillations of inlet velocity profiles, and other sources of noise, will smooth out what appear as sharp deep minima in the computational results. However, the fact probably remains that, especially in arrays of rigid tubes (as opposed, for example, to flexible hollow fibers), other choices of the orientation of forcing term and mean flow might allow higher mean values of mass or heat transfer coefficients.

In the Appendix, the present results for Sh_m at $\gamma = 0^\circ$ and 45° are compared with different literature correlations (most of which developed for heat transfer) for in-line and staggered tube banks (identified here with the orientations $\gamma = 0^\circ$ and $\gamma = 45^\circ$, respectively). Only few of these correlations can be applied to Reynolds numbers $< 10^2$, and thus to the range investigated here. In the limited region of overlapping, the quantitative agreement in Sh_m , at least for intermediate and high Schmidt / Prandtl numbers, is acceptable for some correlations [50,51], much less for others [23,26]. However, all published correlations overestimate the exponents n , m in the power-law dependence $Sh_m \sim Re^n Sc^m$, adopting for n values between 0.4 and 0.6 and for m values close to 1/3, whereas both exponents appear to be close to 0.25 for $Re < 100$ on the basis of the present simulations. This suggests that the extrapolation of correlations based on data for $Re > 100$ to much lower Reynolds numbers, including the creeping flow range $Re < 1$, is not justified. Moreover, simple power-law correlations such as those proposed in most of the literature [22,23,26,27,50] are necessarily bound to fail in the low- Re range since they (unphysically) predict $Sh_m \rightarrow 0$ for $Re \rightarrow 0$. Correlations containing a constant additive term, e.g. those presented by Gamrat et al. [51] or Eqs. (13.a) and (13.b) proposed in this paper, are by far preferable.

The average of the mean Sherwood number Sh_m with respect to the forcing term angle γ was also considered. This quantity, denoted as

$\{Sh_m\}$, is usually neglected in the literature but can be of importance in some contexts. An example is a square-lattice rod bundle filling a cylindrical sleeve and invested by a radial cross flow, so that each unit cell has its own flow attack angle. The present results showed that $\{Sh_m\}$ can be expressed as a function of the Péclet number only and exhibits a plateau for values of the Péclet numbers $< \sim 2$ and a power-law increase of exponent ~ 0.25 for larger values.

Finally, the influence of the boundary conditions (uniform flux versus uniform concentration) was investigated. They were found significantly to affect the angular distribution of the local mass transfer coefficient (local Sherwood number Sh_{loc}), but much less its azimuthally-averaged value (mean Sherwood number Sh_m) and even less its γ -averaged values $\{Sh_m\}$.

CRediT authorship contribution statement

N. Cancilla: Writing – original draft, Visualization, Validation, Software, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **M. Ciofalo:** Writing – review & editing, Validation, Supervision, Software, Methodology, Formal analysis, Data curation, Conceptualization. **A. Tamburini:** Writing – review & editing, Validation, Supervision, Resources, Project administration, Data curation, Conceptualization. **G. Micale:** Writing – review & editing, Supervision, Resources, Project administration, Funding acquisition, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

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Appendix. comparison with literature heat transfer correlations for flow across tube banks

As mentioned in the Introduction, in the past, experimental correlations for the shell-side mass transfer past fiber bundles were proposed by several authors [7–11]. However, in most cases these correlations are not comparable with the results of the present study (regarding regular square arrays of cylinders and fully developed mass transfer conditions) because:

- are obtained for randomly arranged distributions of cylinders (e.g., gas-liquid hollow fiber contactors);
- are often of difficult interpretation due to an ambiguous or missing definition of quantities such as the porosity and the Reynolds number;
- apply to the entry region of the geometry with developing concentration and velocity profiles.

The subject of this paper is obviously connected with one of the most classic topics in heat transfer research, namely, heat transfer in tube banks. Early research in this field is reviewed, for example, by Beale and Spalding [46].

Restricting our attention on fully developed cross flow in square lattices, most of the existing results regard two flow attack angles only: $\gamma = 0^\circ$ (“in line” configuration), and $\gamma = 90^\circ$ (“staggered” configuration). Note that, for symmetry reasons, along these two directions the mean velocity is aligned with the forcing term, or driving pressure gradient, even in the case of an anisotropic hydraulic permeability, so that flow attack angle and forcing term angle coincide.

In regard to the mean Nusselt number, results are usually presented in the form of correlations expressing the circumferentially averaged Nusselt number (corresponding to the quantity defined in this paper as Sh_m) as a function of the lattice configuration, the Prandtl number (corresponding to

the Schmidt number in mass transfer problems) and the Reynolds number.

In the literature on tube banks in cross flow, the Reynolds number is usually defined as

$$Re_{max} = \frac{\rho u_{max} d}{\mu} \quad (A.1)$$

in which u_{max} is the mean velocity in the narrowest section of the tube array. The relation between Re_{max} and the Reynolds number Re as defined by Eq. (7) on the basis of the superficial velocity is (see Fig. 2):

$$Re = Re_{max} \left(1 - \frac{d}{L} \right) \quad (A.2)$$

or, in terms of the lattice porosity ε , Eq. (6):

$$Re = Re_{max} \left[1 - \sqrt{\frac{4}{\pi} (1 - \varepsilon)} \right] \quad (A.3)$$

For $\varepsilon = 0.5$ ($d/L \approx 0.8$), Eq. (A.2) or Eq. (A.3) yield $Re \approx 0.2 \cdot Re_{max}$. Note that proposed correlations, even if they do not explicitly contain the porosity ε , yet implicitly account for this quantity via the dependence of Re_{max} on the pitch-to-diameter ratio for any given Re .

Perhaps the most famous of these correlations is that proposed by Colburn [22] for the staggered arrangement, which, for $\varepsilon = 0.5$ ($Re_{max} \approx Re/0.2$ as discussed above), can be expressed in the present notation as

$$Nu = 0.866 \cdot Re^{0.6} Pr^{1/3} \quad (400 \leq Re \leq 8,000) \quad (A.4)$$

However, its range of applicability regards transitional and turbulent flows and is far from that ($Re < 100$) considered in the present study (although Colburn's paper itself contains hypothetical charts in which the same correlation is boldly extrapolated to Reynolds numbers as low as 1).

During the years, Colburn's correlation has been extended to lower Reynolds numbers and different tube arrangements (in-line, rectangular or triangular lattices), generalized to account for the variation of the fluid properties, and variously modified on the basis of new experimental results. For example, a modified form of Colburn's correlation, with slightly different exponents and the constant accounting for the lattice geometry, was proposed by Hausen [52], but also this was based on data mostly obtained for high Re (> 1000).

In the low-Reynolds number range, several authors report that the dependence of Nu upon Re follows a power law of exponent less than at high Re . Khan et al. [27], on the basis of a semi-analytical approach, proposed for $Re > 10$ a correlation which, for square lattices with $\varepsilon = 0.5$, can be written in the present notation as:

$$Nu = 0.841 \cdot Re^{1/2} Pr^{1/3} \quad (\text{in-line}) \quad (A.5.a)$$

$$Nu = 1.291 \cdot Re^{1/2} Pr^{1/3} \quad (\text{staggered}) \quad (A.5.b)$$

For $2 \leq Re \leq 20$, on the basis of data from Bergelin et al. [53] and other authors, obtained with fluids of different Prandtl numbers, Zukauskas [23, 26] proposed

$$Nu = 0.8 \cdot Re^{0.4} Pr^{0.36} (Pr_b/Pr_w)^{0.25} \quad (\text{in-line}) \quad (A.6.a)$$

$$Nu = 0.9 \cdot Re^{0.4} Pr^{0.36} (Pr_b/Pr_w)^{0.25} \quad (\text{staggered}) \quad (A.6.b)$$

in which the term in parentheses accounts for the variation of the Prandtl number between the bulk fluid (subscript "b") and the wall (subscript "w").

Le Clair and Hamielec [50], based on numerical calculations, proposed for $10 \leq Re \leq 100$ a porosity-dependent correlation which, for $\varepsilon = 0.5$, can be written

$$Nu = 1.87 \cdot Re^{0.418} Pr^{1/3} \quad (A.7)$$

(authors' model does not explicitly distinguish in-line from staggered arrangements). Mandhani et al. [49] reported a fair agreement of their own computational results with the above correlation in the range $Re = 10$ – 100 .

Note, however, that, despite the fact that the power-law correlations Eq. (A.5) through Eq. (A.7) are claimed by their authors to be applicable to low Reynolds numbers, the lack of a constant additive term actually makes them poorly apt to predict Nu_m or Sh_m at very low Re , since for physical reasons these quantities must necessarily tend to a finite value $\neq 0$ as $Re \rightarrow 0$. Correlations including such an additive term were proposed, for example, by Gamrat et al. [51] for banks of square bars in cross flow, based on computational results obtained for $0.001 \leq Re \leq 100$; for a porosity ε of 0.5 they can be written

$$Nu = 8.87 + 0.312 \cdot Re^{0.5} Pr^{0.2} \quad (\text{in-line}) \quad (A.8.a)$$

$$Nu = 8.87 + 0.904 \cdot Re^{0.5} Pr^{0.3} \quad (\text{staggered}) \quad (A.8.b)$$

A comparison of the present results for Sh_m with some of the above correlations for Nu_m is reported in Fig. A.1(a)–(c) for three values of the Schmidt or Prandtl number: 0.05, chart (a), representative of heat transfer to liquid metals; 5, chart (b), representative of heat transfer to water and other liquids; and 500, chart (c), representative of many mass transfer processes in water. The values of Sh_m for $\gamma = 0^\circ$ and 45° and the angle-averaged values $\{Sh_m\}$, are reported. The correlation obtained for $\{Sh_m\}$ in this paper, Eqs. (13), is graphically undistinguishable from the "raw" CFD results and was not reported to avoid line clogging.

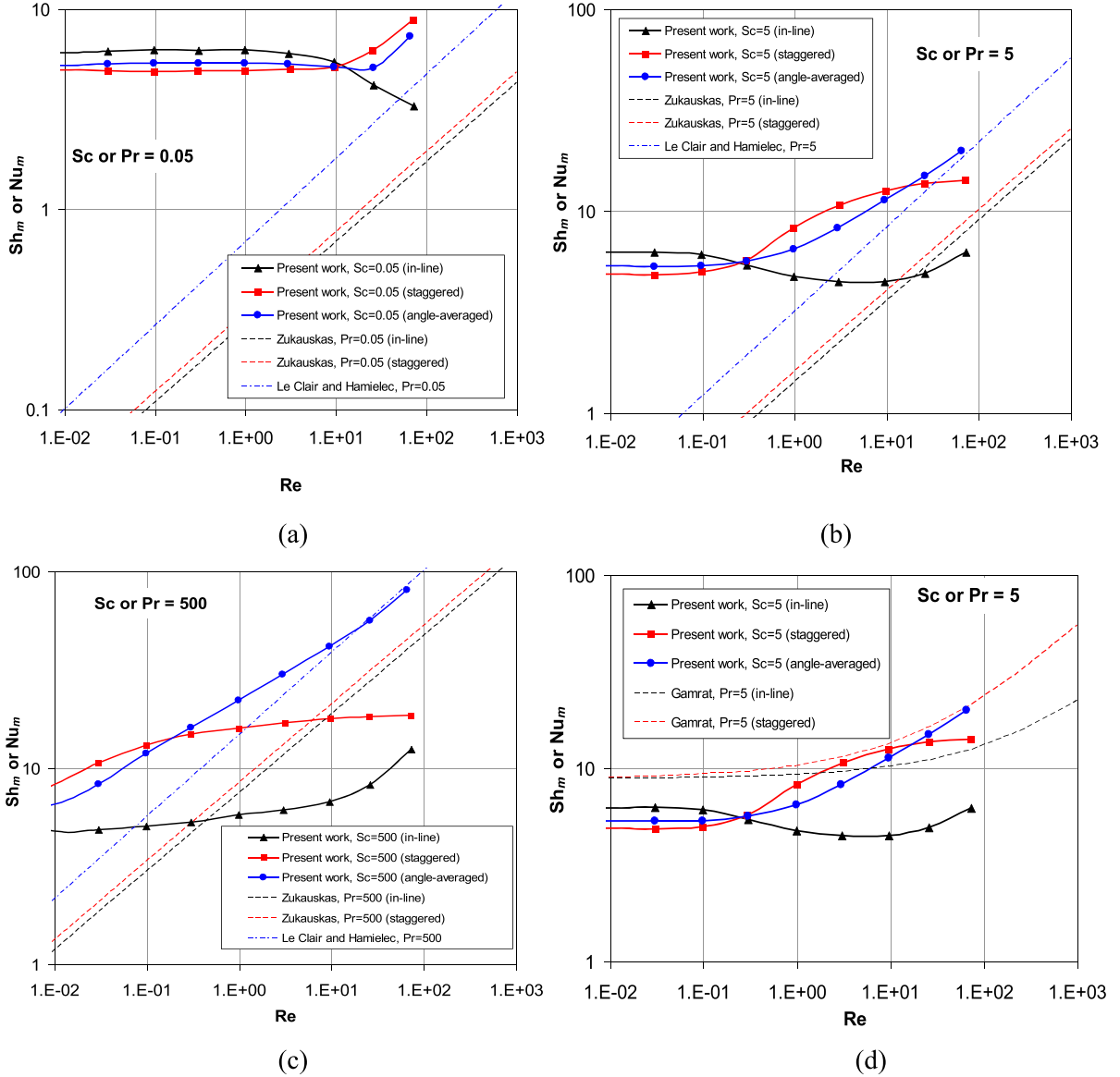


Fig. A.1. Comparison of the present CFD results for Sh_m (symbols and solid lines) with literature correlations [26,50] for Nu_m (broken lines) at three values of the Prandtl (Schmidt) number: (a) $Pr = 0.05$; (b, d) $Pr = 5$; (c) $Pr = 500$. Graph (d) reports a further comparison with correlations in [51] for Sc (Pr) = 5.

- I. Let us first consider the overall levels of Sh_m or Nu_m and their dependence on Re and Sc or Pr , independent of the flow orientation (i.e. in-line or staggered). To this purpose, let us focus on the present angle-averaged results ($\{Sh_m\}$) and compare them with the correlation proposed by Le Clair and Hamielec [50], which does not distinguish between the two orientations, and with those by Zukauskas [26], which exhibit only a small difference between the in-line and the staggered orientation. It is clear that:
 - i. all correlations are completely inadequate for the lowest Schmidt / Prandtl number (0.05), Fig. A.1(a), which is not surprising since they eventually rest on experimental data obtained using air, water or oil as the working fluid;
 - ii. for Sc (Pr) = 5 and 500, Figs. A.1(b) and A.1(c), in the limited range $Re = 10 - 100$ (highest Reynolds numbers simulated in the present study) $\{Sh_m\}$ results are fairly close to the correlation of Le Clair and Hamielec [50]; the power-law exponent, however, is significantly lower (~ 0.25 against 0.418). The graphs suggest that a better agreement might be obtained at higher Re , provided the predicted trend is not affected by unsteadiness phenomena. The correlations by Zukauskas [23,26] underpredict the results by a factor of ~ 2 . Of course, the left $\{Sh_m\}$ plateau, predicted by CFD for $Sc = 5$ at $Re < \sim 0.1$ and for $Sc = 500$ at lower Re , not included in the graph, is not matched by the power-law correlations.

The last graph, Fig. A.1(d), drawn separately for readability purposes, compares for Pr (Sc) = 5 the present predictions with the correlations proposed by Gamrat et al. [51] for banks of square bars. It is clear that, despite quantitative discrepancies in the plateau region (expected also because of the different geometries considered), at least the correlations including an additive term can qualitatively capture the overall trend of the curves over a relatively large interval of low Reynolds numbers.

- I. Let us now consider the orientation-dependent values of Sh_m or Nu_m ($\gamma = 0^\circ$, identified here with the “in-line” orientation, or $\gamma = 45^\circ$, identified here with the “staggered” orientation). As also Fig. 16 shows, the Sh_m versus Pe curves predicted for these two orientations (corresponding to axes of symmetry of the lattice) behave differently from those obtained at any intermediate orientations: they do not follow a power-law trend, increase

slowly with Re (or even decrease in some interval) and, for sufficiently high Re and Sc (i.e., $Pe > \sim 100$) they lie below all other curves. As discussed at length in Section 3.3, the reason is that for these two orientations large stagnation regions are formed both upstream and downstream of each rod, yielding high concentrations over its surface and thus low values not only of the local Sh (Sh_{loc}), but also of the mean Sh (Sh_m). This explains the deep minima appearing in polar charts of Sh_m versus γ for these orientations, see e.g. Fig. 9.

Now, none of these features is reflected in the heat transfer correlations for the “in-line” and “staggered” configurations reported in Fig. A.1, and, in particular, in the corresponding power-law exponents, which are way too high. A possible explanation is that the present computational results assume the mean flow to be precisely directed along a given direction (including, in particular, the two symmetry directions $\gamma = 0^\circ$ and 45° or their periodic copies). However, this is only an ideal condition, easily implemented in a numerical simulation but not in the laboratory. In any real experiment the direction of the mean flow can be imposed only approximately and is presumably affected, even under low-Re conditions, by fluctuations and uncertainties. Therefore, what existing correlations really express is the value that Nu_m or Sh_m exhibit when the flow direction lies in a certain interval of directions around $\gamma = 0^\circ$ (for the “in-line” configuration) or 45° (for the “staggered” configuration). As Figs. 9 and 12 and the relevant discussion show, at sufficiently high Péclet numbers a small deflection from one of the symmetry directions destroys the thick and stagnant high-concentration or high-temperature layer around a rod and causes a drastic increase of the Sherwood or Nusselt number.

Data availability

Data will be made available on request.

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