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NUMERICAL STUDY OF SOLUTAL AND THERMAL INSTABILITIES IN MINI-CHANNELS FOR MEMBRANE-LESS APPLICATIONS

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ABSTRACT

Many industrial processes make extensive use of membranes to separate fluxes while allowing some of the constituent species to diffuse into each other. In recent years, high production and maintenance costs induced by fouling, poisoning and clogging of the membrane pores due to impurities have create conditions to study alternative way of making liquid and/or gaseous streams interact and diffuse without the presence of a physical barrier.

One of the possibilities is offered by the essentially laminar character of the flow in microfluidic devices that allows two or more different fluid streams to merge without mixing in a large range of experimental and industrial conditions. In this work, we will study, numerically, the case of two streams of different composition merging in a micro-channel. The upper and lower sides of the micro-channel are heated differentially and the inlet velocity of the streams is set independently in the range 0-1m/s. Simulations are carried out in 2D and 3D while fluids are chosen by considering their industrial importance and application. The main results are that the stability of the streams is very sensitive to the inlet conditions and that it is possible to modulate the mixing layer thickness by acting on thermal gradients, geometrical constraints and slip flow conditions.

INTRODUCTION

The possibility of having laminar flow in devices of mini and micrometric size has been exploited since decades especially in the bio-physical domain where different degree of mixing and/or separation of reactive, samples and fluxes was required. In recent years, a novel intriguing way of exploiting the essentially diffusive-dominated regimes characteristic of laminar flows in mini/micro devices was introduced in the pioneering works of Choban et alii [4][8], Burke[5], Ghangrekar[5]. The main point of their works was that, in many applications, the presence of membranes as physical barriers to separate interacting fluid streams is the limiting factor from both the economical and technical point of view. The costs of membranes , though constantly decreasing over years due to technological advances remain still high and, even more critical, it stands the problem of fouling, poisoning and clogging. Such aspects influence strongly the lifetime duration and maintenance costs and represents a real bottleneck in the market diffusion of membrane-based devices.

The idea followed of using laminar diffusive-driven regimes, typical of flows in micro-sized devices, as a possible alternative to by-pass membranes and to make fluid streams interact by simply make them flowing parallel to each other without the presence of a physical barrier, the so-called membrane-less devices.

By eliminating the physical barriers some problems are solved but many also arise due to the fact that differences in densities,

the presence of temperature gradients in addition to concentration ones, influences of physical boundaries of the micro-devices make the flow sensitive to disturbances that break-down the laminar character of the flow and eventually creates unwanted mixing and separation loss.
This situation is particularly critical in applications like fuel cells, reverse electro-dialysis systems or bio-reactors where a stable and robust diffusion-driven flow is required. The analysis of the effects of thermal and solutal perturbations is then critical.
In this paper, we studied numerically the flow patterns and the mixing degree of two fluids streams flowing in co-current direction in a mini-channel. The two streams interact in presence of a thermal gradient that is imposed parallel to the gravity vector. The density gradient is also parallel to the direction of the gravity vector resulting in a spectrum of cases where thermal and concentration gradients reinforce or oppose each others – see Figure 1.
To get some valuable information concerning the potentially unstable cases, we studied 2D and 3D cases where the thermal gradient is potentially unstable, i.e. parallel and directed in the direction of the gravity vector, and the concentration gradient is both stabilizing or destabilizing, i.e. the heavier fluids is the lower or upper stream respectively.

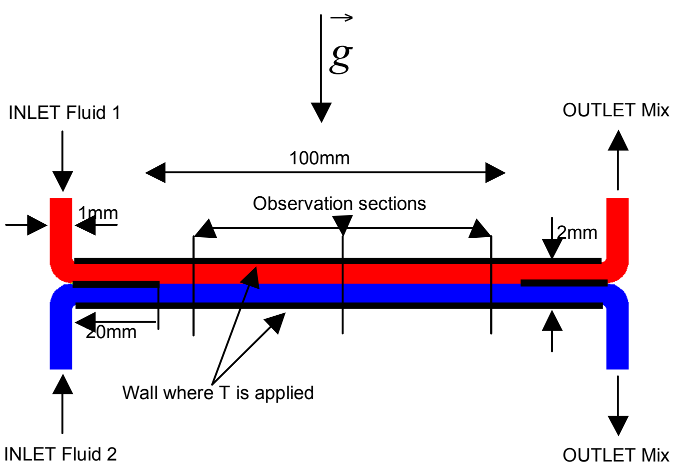

Figura 1 The geometrical section of the 3D domain used in calculation. The observation sections are at 2mm, 50mm and 100mm from the point where the two streams merge.

For different combinations of the thermal and concentration gradients, the study focused on the effects of the stream velocity on the separation ratio and on the thermal and concentration patterns along the channel length. Because the final goal is to develop an experimental setup devoted to the study of membraneless applications for energy harvesting, this study should be considered as a non-exhaustive, on-going contribution to the numerical modeling of this kind of applications.

NUMERICAL MODEL

To solve numerically the above-cited set of equations, the commercial software Fluent™ has been used together with the mesh generator Gambit™ to discretize the domain. Fluent belongs to the class of full Navier-Stokes equations solvers. It allows for dealing with very complex geometry as well as for adding custom made terms both in the set of boundary conditions and equations.
In our study, the evolution of a multi-component fluid flow in presence of temperature and concentration gradients parallel to the gravity vector has been studied for a 3D channel characterized by two 2,8mm long entries that are perpendicular to the channel axis. They join after a L-turn bend that is 20mm long. The outlets are symmetric to the inlets across the middle of the channel. The total length of the channel is 139,6mm while the distance where the liquids can interact is 100mm long. The width of the each inlet is 1 mm, so the width of the channel is 2mm. In the 3D model, the depth of the channel is also 2mm – see Figure 1.
For what concerns the velocity field, the two streams are injected with an even velocity varying in the 0-0.01 range. This assures that the flow itself is laminar in the channel and that instability patterns are exclusively due to the presence of thermal and concentration gradients and/or to the interaction of those gradients with the imposed flow.
From the usual definition of the Reynolds number

$$\mathrm{Re} = \frac{\rho \cdot \|\vec{v}\| \cdot D_H}{\mu}$$

where D_H is the hydraulic diameter of the channel, it is possible to infer that in the range of velocity studied the flow is everywhere laminar. As a matter of fact, the highest velocity tested is 0.01m/s to which corresponds a Re of about 30, far below the turbulent threshold.

The 3D model has been discretized with hexahedral volumes that assure for a better computational management of the concentration and thermal gradients. The total number of nodes composing the meshed geometry is 667,907 as shown in Figure 2.
All fluid properties are assumed to be independent from the temperature and concentration, except from the density which is computed as a linear function of both temperature and concentration - see table 1 in Annex.
The complete set of equations solved reads as follows:

Continuity:

$$\vec{\nabla} \cdot \vec{v} = 0$$

Momentum:

$$\rho \frac{d\vec{v}}{dt} = \mu \Delta \vec{v} - \vec{\nabla} p - \rho g w \vec{j}$$

Species without chemical reactions:

$$\frac{\partial}{\partial t}\left(\rho \mathrm{Y}_i\right)+\vec{\nabla}\cdot\left(\rho\vec{v}\mathrm{Y}_i\right)=-\vec{\nabla}\cdot\vec{J}_i$$

Where: $\mathrm{Y}_i=\frac{\rho_i}{\rho}$

Where the index i =1,2 identifies the two fluids, ρ is the density, μ is the dynamic viscosity, p the pressure.

Despite the relative importance that the thermal diffusion process can have in similar cases, the only mass diffusion contribution has been computed and the relative coefficient considered constant. The associated diffusive flux is evaluated as:

$$\vec{J}_i=-\rho D_{i,m}\vec{\nabla}\mathrm{Y}_i$$

Here, $D_{i,m}$ is the binary diffusion coefficient.

The general form of the energy conservation equation is expressed in a multi-component flow as:

$$\frac{\partial}{\partial t}\left(\rho E\right)+\nabla\cdot\left(\vec{v}\left(\rho E+p\right)\right)=\nabla.\left[\lambda\nabla T-\sum_i h_i\vec{J}_i+\left(\overline{\overline{\tau}}\cdot\vec{v}\right)\right]+S_h$$

Where $S_h=0$ since there is no chemical reaction,

$\sum_i h_i\vec{J}_i=0$ since the effect of enthalpy transport due to species diffusion is negligible,

$\overline{\overline{\tau}}\cdot\vec{v}=0$ since the viscous heating is negligible.

In the case of incompressible flow of several species, the total energy E is defined as the following expression:

$$E=\sum_i \mathrm{Y}_i\int_{T_0}^{T}c_{p_i}dT+\frac{v^2}{2}$$

Boundary conditions:

At the inlets, velocity is imposed and pressure calculated from the Bernoulli condition. In the frame of the present calculations, the flow velocity ranges from 0 to 0.01m/s

Outflow boundary condition is applied at the outlet section of the channel. This condition consists in imposing that no diffusion flux exists in the direction normal to the outlet section. As a result, Fluent extrapolates the outflow conditions from within the domain.

At the wall the no-slip boundary conditions is applied as well as the condition of no-diffusion flux.

$$\vec{v}=0$$

$$\vec{\nabla}Y_i=0$$

The temperature of the lower wall and the upper wall are alternatively fixed to T_w = 275K and T_w = 325K.

$$y=0 \quad and \quad y=h$$

$$T=T_{wall}$$

The average temperature at the beginning of the calculations is set to T_0= 300K.

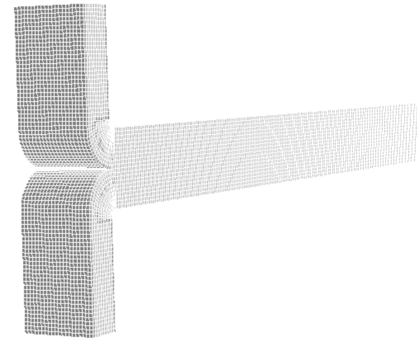

Figura 2 - The mesh for the 3D geometry studied.

RESULTS

The main parameter used to evaluate the degree of mixing of the two interacting streams is the standard deviation of the mass fraction N_i of one of the interacting species σ_c :

$$\sqrt{\frac{\sum_{i=1}^{n}\left(x-x_0\right)^2}{n}}$$

Where x is the cell value of the selected variables at each facet, x_0 is the mean of x

$$x_0=\frac{\sum_{i=1}^{n}x}{n}$$

and n is the total number of facets.

Given this definition, the case where the two streams occupy half of the channel height, correspond to a σ_c = 0.5. As long as the streams mix, the variance is supposed to decrease because the number of facets where the mass fraction is different from the average mass fraction decreases.

In simulations where the thermal gradient is present, the thermal gradient has been set to 2.5K/mm. If we consider the Rayleigh number as a stability parameter respect to thermal perturbations:

$$Ra=\frac{g\cdot\beta\cdot c_p.\lambda}{\mu}\left(\Delta T\cdot w^3\right)$$

where ΔT is temperature difference applied between the upper and lower walls of the channel, and w is the width of the channel, β the volumetric expansion, in the present case where w=2mm and β of the order of 10^{-3}, Ra~5370 far above the theoretical threshold .

The thermal gradient is supposed to generate convection patterns of the Bénard type in absence of stabilizing contributions.

Figure 3 reports the standard deviation of the mass fraction in the three observation sections (see Figure 1) for the case where both the thermal gradient and the concentration gradient are stabilizing and there is no velocity at the inlets. In that case, the diminution of the σ_c is due essentially to the diffusion at the interface between the two fluids.

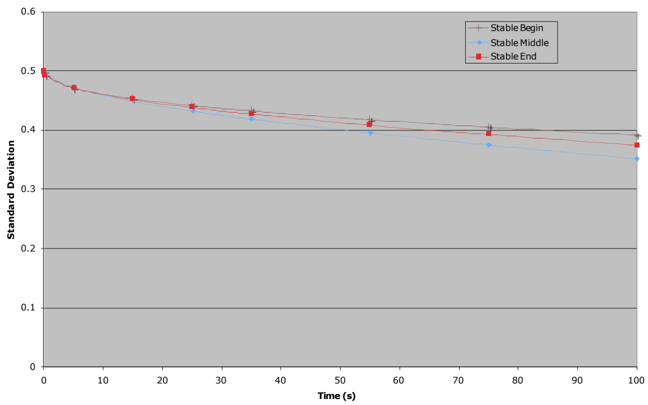

Figure 3 - The standard deviation in the case of a stabilizing temperature and concentration gradient

Figure 4, 5 and 6 show the temporal distribution of the standard deviation in the case where the both the thermal gradients and the concentration gradient are destabilizing or absent, for the three observation sections.

It is worthy to note that when no velocity at the inlet is present – lines red and green, the mixing of the two streams is always strong, by taking into account that the σ_c changes in less than 10 seconds from 0.5 to ~ 0.1 and then continue to constantly decrease.

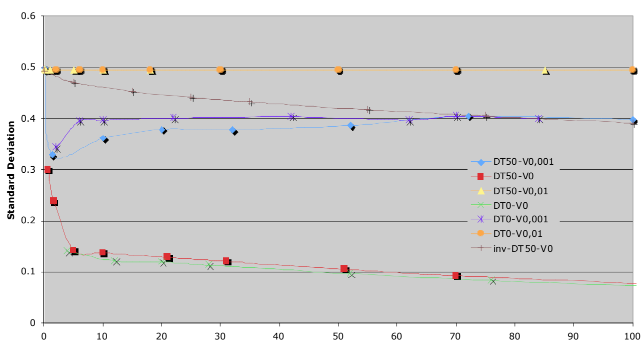

Figure 4 The computed standard deviation for the section at the beginning of the channel

For velocities at the inlets of the order of 1mm/s – violet and blue lines, the mixing is less pronounced that in the previous case, but the standard deviation seems to stabilize around a value of 0.2-0.3 with a pronounced degradation of the separation as long as the streams flow along the channel, as expected.

Brown and yellow lines refers to the case where the velocity at the inlet is of 0.01m/s. in that case it is possible to observe that the mixing is strongly reduced with a standard deviation of the order of 0.4 all along the channel length.

It is interesting to note that in the cases where the velocity is present, the standard deviation firstly decrease in time and then increases again. This is due to the fact that the curve concerns the cases where the concentration gradient is destabilizing.

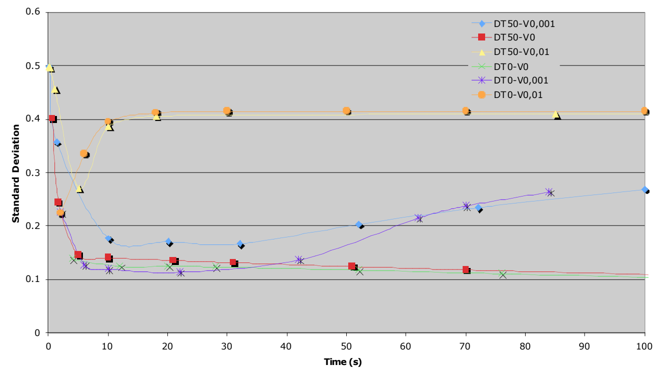

Figure 5 The computed standard deviation for the section at the middle of the channel

This means that at first the heavier fluid sink down and occupy the place of the lighter in the evolution of the system, i.e. there is an inversion of the density streams and then the velocity of the streams stabilizes the layer respect to the case of absence of flow.

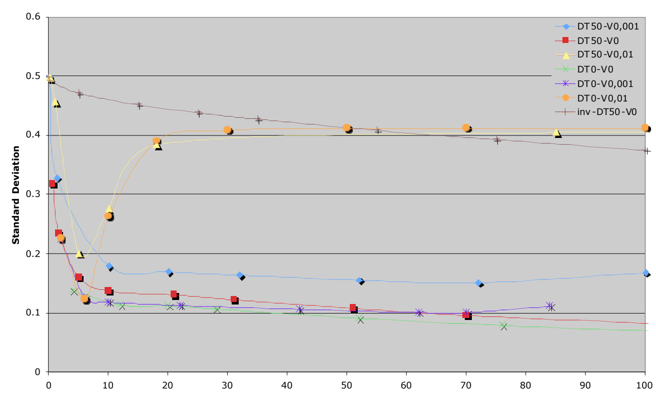

Figure 6 The computed standard deviation for the section at the outlet of the channel

Figure 7 shows the mass fraction distribution in the middle section of the channel for increasing velocities at the inlets. It is clear that for increasing velocity (left to right in the picture) the mixing is reduced. This effect is even more clearly shown in Figure 8 that reports the temporal evolution of the mass fraction profile in the middle section of the channel for different velocities and in the case the denser fluid represents the upper current. It is possible to observe that when the velocity increases from ~1mm/sec to ~ 1cm/sec, the inversion of the density profile induced by the gravity is not only quicker but sharper. In this latter case, the final stage is a co-current flow of the two stream with no or negligible mixing.

CONCLUSIONS

Numerical simulations performed has shown that when in a channel two streams interact without the presence of a physical separation barrier like a membranes, the system become more sensitive to thermal and solutal perturbations. More specifically, when both temperature and concentration gradient are destabilizing respect to the gravitational equilibrium, the mixing of the concurrent streams is unavoidable. In those cases, the presence of a velocity field – or of a pressure gradient in the direction of the channel length – can be strongly beneficial.

This paper should be considered as a partial and non-exhaustive contribution to the study of membrane-less systems. A more complete analysis of the full spectra of stability issues is under investigations.

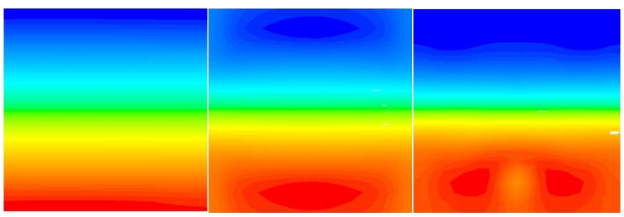

Figure 7 The mass fraction distribution in the middle section of the channel for V=0m/s, V=0.001m/s and V=0.01m/s when no temperature gradient is imposed

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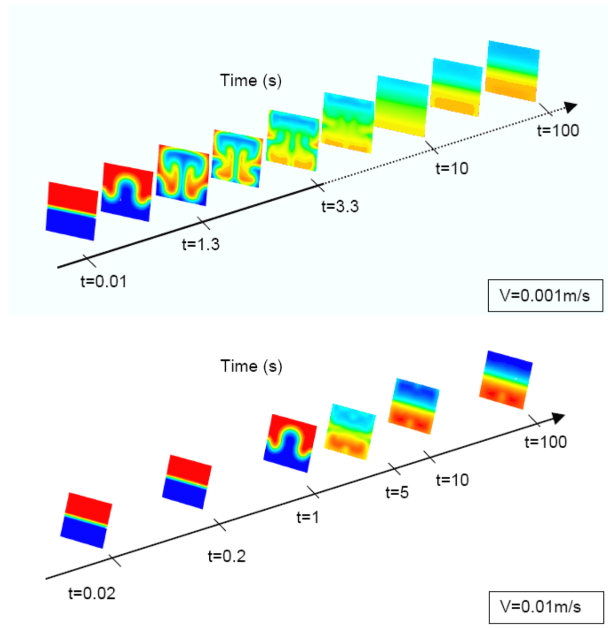

Figure 8 Contour of mass fraction of the co-current species (heavier fluid occupies the upper phase) in the central section of the channel. The increase in the inlet velocity is clearly beneficial.

ANNEX A

TABLE 1 – MODEL PARAMETER USED IN COMPUTATIONS

	Symbol	Unity	Fluid 1	Fluid 2	Mixture
Density	ρ	$kg.m^{-3}$	1060.188-0,2066274T	1110.829-0.28693T	Volume weighted mixing law
Specific heat	c_p	$J.kg^{-1}.K^{-1}$	1482	3903	Mixing law
Thermal conductivity	λ	$W.m^{-1}.K^{-1}$	0.6	0.596	Mass weighted mixing law
Viscosity	μ	$kg.m^{-1}.s^{-1}$	0.001003	0.001008	Mass weighted mixing law
Mass Diffusivity	$D_{i,m}$	$m^2.s^{-1}$	10^{-9}	10^{-9}	