Proceedings of the ASME 2010 3rd Joint US-European Fluids Engineering Summer Meeting and 8th International Conference on Nanochannels, Microchannels, and Minichannels
FEDSM-ICNMM2010
August 1-5, 2010, Montreal, Canada

FEDSM-ICNMM2010-31093

Mixing Process in T-Shaped Micro-Mixers with Chaotic Advection: A Numerical Approach

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ABSTRACT
In this paper, a transient numerical model is presented to investigate the mixing phenomena in passive T-shaped barrier embedded micro-mixer (BEM) with rectangular cross-sections. The simulations are performed for two non-reactive miscible gases (i.e. oxygen and methanol). The compressibility and slip effects of the flow in the micro-channel are neglected. The model presented in this paper is used to numerically solve physical governing equations namely the continuity, momentum and specious transport equations. The equations are discritized using control volume numerical techniques. The distribution of the specious concentration within the domain is calculated. The Intensity factor is used as a criterion for mixing length. Also, the effects of the baffles' height and span on mixing efficiency and reducing the mixing length are studied. Having baffles in the channel can substantially decrease the mixing length.

KEYWORDS
T-shape Barrier Embedded Micro-mixer (BEM), numerical simulation, Intensity of segregation, non-reactive miscible gases, specious concentration

NOMENCLATURE
$\vec{\mathbf{V}}$ fluid velocity
$\mathbf{P}$ Pressure
$\boldsymbol{\rho}$ density
$\vec{\boldsymbol{g}}$ gravitational acceleration
$\overrightarrow{\boldsymbol{F_b}}$ body force
$\overleftrightarrow{\mathbf{T}}$ stress tensor
$\mathbf{D}$ mass diffusivity
$\mathbf{C}$ specious concentration
$\boldsymbol{g}$ gas
$\hat{\mathbf{n}}_{\perp}$ normal unit vector
$\hat{\boldsymbol{t}}_{\perp}$ tangential unit vector
$\boldsymbol{S}$ Baffles span
$\boldsymbol{H}$ Baffles height

INTRODUCTION
Mixing is a transport process for species, temperature, and phases to reduce in homogeneity. Micro mixing has recently drawn great attention because of low production cost, reduced reaction time, portability, the multiplicity of design [1-2], smaller reagent volumes, and shorter analysis time [3-4]. Mixers have diverse applications in chemical processing, polymer production, biotechnology, food engineering, pharmaceutical products [5], micro heat exchangers, micro reactors, lab-on-a-chips, medical applications [6] and micro total analysis systems [7].

The extremely large surface-to-volume ratio and short transport path in micro-mixers enhance heat and mass transfer dramatically [8]. In order to increase the mixing efficiency and reduce diffusion distance in micro-mixers, the contact surface between different fluids should be increased by controlling fluid flows within the channel. In addition, as the flow regime in micro channel is laminar, a mechanism which is called the "chaotic advection" is used to increase the mixing efficiency. Chaotic advection refers to the phenomenon which a simple Eulerian velocity field creates a chaotic response in the distribution of a Lagrangian marker [10].

Various numerical and experimental models have been proposed to study the chaotic mixing in micro channels. Lin et al. [9] analyzed the transient three-dimensional flow field and distribution of concentration within a planar serpentine channel. Kang et al. [10] investigated the effect of periodic and aperiodic sequences of mixing protocols on mixing performance in a barrier embedded micro-mixer. A staggered herringbone mixer was studied by Kee et al. [11] in which they used the particle tracking methods and numerical simulations to estimated the mixing length. Jeon et al. [12] simulated and analyzed a passive mixer in which they investigated the effect of various geometries on the mixing. Nguyen et al. [13] designed a Y-junction type micro-mixer with a square obstacle on the square-wave flow channel in order to enhance the mixing ability using the chaotic advection.

Numerous investigations have been proposed in order to study T-shape micro-mixers [14, 16-18]. Le and Hassan [19] simulated gas mixing in a T-shape micro-mixer numerically using the direct simulation Monte Carlo (DSMC) method. Soleymania et al. [20] proposed a dimensionless number to identify the flow regimes in liquid phase inside a T-shaped micro-mixer. They reported that the flow regimes in a T-shaped micro-mixer depend strongly on both the volume flow rates and the geometrical parameters of the mixer. Adeosun and Lawal [21] investigated the mixing performance in a multilaminated/elongational flow mixer and a T-junction micro-mixer in order to obtain concentration and the residence-time distribution.

Su et al. [22] investigated mass transfer characteristics of H2S absorption from gaseous mixture into methyldiethanolamine solution in a T-junction micro channel experimentally. The performance of most micro chemical devices strongly depends on the efficiency of mixing, especially when dealing with fast reactions, therefore is needed to enhance the efficiency of mixing.

Although the T-shapedd barrier embedded micro-mixer has a simple geometry, but its efficiency of mixing is significant as it uses the main concepts of mixing to generate the chaotic advection using stretching, folding and breaking the laminar flow.

In the present study, the mixing process for gaseous flow in T-shaped barrier embedded micro-mixer has been investigated in order to study the effect of baffles' height and span on the mixing efficiency, mixing length and time. The gases which are applied in this study are considered to be incompressible and miscible and the slip effect is negligible.

MATHEMATICAL MODEL

A schematic of micro-mixing process in a T-shaped channel is shown in Fig. 1. The mathematical model in this study is based on the following assumptions:

- The fluid flow is considered to be incompressible
- Knudsen number is less than 0.001, therefore, the slip effects of the gaseous flow in the micro-channel are negligible;
- The fluids are considered to be Newtonian and their flow to be laminar;
- The effect of surrounding gas is considered;

GOVERNING EQUATIONS

- Fluid Flow

The governing equations are the conservation of mass and momentum as follows:

$$\vec{\nabla}.\vec{V} = 0 \tag{1}$$

$$\frac{\partial \vec{V}}{\partial t} + \vec{\nabla}.\left(\vec{V}\vec{V}\right) = -\frac{1}{\rho}\vec{\nabla}\mathrm{P} + \frac{1}{\rho}\vec{\nabla}.\overleftrightarrow{\tau} + \vec{\mathrm{g}} + \frac{1}{\rho}\vec{F}_b \tag{2}$$

where $\vec{\mathrm{V}}$ is the fluid velocity, P, ρ are the pressure and density, $\vec{\mathrm{g}}$ is the gravitational acceleration, $\vec{\mathrm{F}}_{\mathrm{b}}$ is the body force, and $\overleftrightarrow{\tau}$ is stress tensor.

- Specious Transport

In order to predict the mixing efficiency, the specious transport equation should be solved as follows:

$$\frac{\partial C}{\partial t} + \vec{V}.\vec{\nabla}C = D\nabla^2\mathrm{C} \tag{3}$$

where D is the mass diffusivity and C is the specious concentration and it ranges from zero to one.

In addition, as the model is applied for the multiphase flow, the density, viscosity and mass diffusivity within the domain is estimated as follows[23]:

$$\rho = \mathrm{C}\rho_{\mathrm{g1}} + (1-\mathrm{C})\rho_{\mathrm{g2}} \tag{4}$$

$$\mu = \mathrm{C}\mu_{\mathrm{g1}} + (1-\mathrm{C})\mu_{\mathrm{g2}} \tag{5}$$

$$\mathrm{D} = \mathrm{C}\mathrm{D}_{\mathrm{g1}} + (1-\mathrm{C})\mathrm{D}_{\mathrm{g2}} \tag{6}$$

where the subscript g1 and g2 demonstrate the two distinct gases.

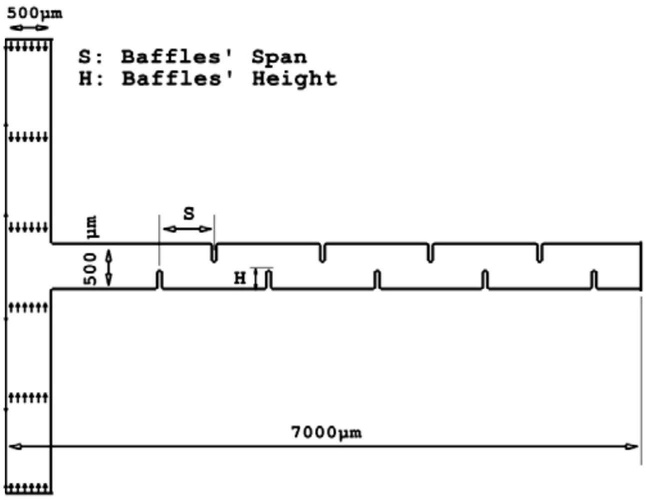

Figure 1: A SCHEMATIC OF MICRO MIXING PROCESS IN A T-SHAPED CHANNEL

In order to solve the governing equations, suitable boundary condition should be applied. The normal and tangential velocities should be zero at wall boundaries as follows:

$$\vec{V}.\hat{t}_{\perp} = 0 \tag{7}$$

$$\vec{V}.\hat{n}_{\perp} = 0 \tag{8}$$

Moreover, the impermeable wall condition should be applied to the concentration flied as follows:

$$\nabla C.\hat{n}_{\perp} = 0 \tag{9}$$

where $\hat{n}_{\perp}$ and $\hat{t}_{\perp}$ are the normal and tangential unit vectors, respectively. The velocity distribution is known for inlet boundaries and for outlet boundary condition, the velocity and pressure gradients should set to be zero as follows:

$$(\vec{\nabla}\vec{V}).\hat{n}_{\parallel} = 0 \tag{10}$$

$$(\vec{\nabla}\mathrm{P}).\hat{n}_{\parallel} = 0 \tag{11}$$

NUMERICAL SCHEME

The numerical scheme is based on the Eulerian frame of reference in the rectangular Cartesian coordinate. The fluid flow equations are discretized using a control volume approach based on staggered grid. The advection term in momentum equation is calculated using the second order-upwind van leer scheme [24].

A two-step projection method is used to solve for incompressible flow, with the Pressure Poisson Equation (PPE) solved via a robust incomplete Cholesky conjugate gradient (ICGG) technique [25].

The specious transport equation is discritized using a control volume approach. It is solved implicitly in order to calculate the specious concentration within the domain. The convective terms are discritized based on the upwind-second order scheme.

Time restrictions should be implemented to the terms which are derived explicitly (i.e. the convective and viscous terms in momentum equation).

In order to validate the model the results of simulations were verified with analytical solutions for simple geometries [26]. A mesh refinement study has also been performed in which the mesh size was progressively increased until no significant changes were observed in the results (number of cells per one millimeter corresponding to these mesh sizes was 10, 20, 40, 60, 80 cells). From this study, a mesh size corresponding to 40 cells per millimeter was found to be the optimum mesh with an error of less than 1% [26].

RESULTS AND DISCUSSION

The geometry of a T-shaped micro-mixer which is used in this paper is shown in figure 1. In order to increase the mixing efficiency and reducing the mixing length using chaotic mixing, some baffles are placed in the mixing channel. In the present study, the mixing process for gaseous flow of oxygen and methanol is simulated. The channel height and length is set to be 500µm and 7 mm. In addition, in order to evaluate the mixing efficiency, the area-weighted discrete intensity of segregation (I_d) is defined as follows:

$$I_d = \sqrt{\frac{1}{N}\frac{\sum_{j=1}^{N}(Cj-\bar{C})^2}{\bar{C}(1-\bar{C})}} \tag{12}$$

where $\bar{C}$ is the average specious concentration as follows:

$$\bar{C} = \frac{\sum_{j=1}^{N} Cj}{N} \tag{13}$$

where Cj is the specious concentration in each point of a cross section. The intensity of segregation demonstrates the deviation of local concentration from the ideal homogenous mixture. In a perfect mixing, $I_d = 0$, while $I_d = 1$ in a completely unmixed system [10]. The mixing length can be define as the span in which the $1 - I_d$ approaches to one. In addition, the amount of $1 - I_d$ is a criteria for mixing efficiency i.e. the more $1 - I_d$ approaches to one; the more efficiency would be obtained.

In addition, two dimensionless parameters which determine the flow regime in micro-mixers are the Reynolds number and Schmidt number as follows:

$$Re = \frac{V D_{\mathrm{h}}}{\upsilon} \tag{14}$$

$$Sc = \frac{\upsilon}{D} \tag{15}$$

where υ, V and D_{h} are the kinematic viscosity, inlet velocity and the hydraulic diameter of the channel, respectively.

The Reynolds number is often low therefore, turbulence is not possible in micro-mixers and the flow pattern is dominated by viscous effect. The main transport phenomena in micro-mixers are the convection and molecular diffusion. Convection is caused by fluid motion, while the molecular diffusion is caused by the motion of the molecules which is characterized by the molecular diffusion coefficient. This kind of response is called chaotic advection and it takes place in laminar flow regime. In addition, the Schmidt number shows the ratio of the viscous effect to the molecular diffusion effect.

In the present study, the Reynolds number is as the order of 70 therefore is flow regime is laminar and the Schmidt number is about 1 which shows that both viscous and molecular diffusion effects are dominant.

Figure 2 depicts a sample transient simulation of a typical T-shaped BEM with following parameters:

Inlet velocity	=	2 m/s
Baffles' Height	=	200 µm
Baffles' Span	=	400 µm
Baffles' Width	=	50 µm

As shown in this figure, the distribution of spacious concentration within the domain is calculated where C=1 shows the methanol and C=0 corresponds to the oxygen. Both convection and diffusion mechanisms exist in this case, however, as the velocity increases, the convection effect becomes more dominant than the diffusion mechanism. The effect of baffles in the channel is to generate the chaotic advection using stretching, folding and breaking the laminar low.

Figure 3 depicts the effect of baffles' span (400, 600 and 800 µm) on the mixing length. As shown in this figure, in order to obtain a proper efficiency, the mixing length increases with the baffles' span. However, the mixing takes place in a longer time to become steady as the span increases.

The effect of the baffles' height (0, 100 and 200 µm) on the mixing length is shown in Fig 4. As seen in the figure, the mixing length reduces as the baffles' height increases. However, the steady state duration increases with baffles' height. In case of having no baffle in the mixing channel, a good mixing would not take place within the channel.

The influence of inlet velocity (1, 2 and 3 m/s) on the mixing length is studied in Fig 5. The mixing length increases as the inlet velocity increases. However, when the velocity is low, it takes more time to become the steady state.

The main effect of the baffles is to create a velocity perpendicular to the main flow stream; therefore, the convective term (in spacious transport equation) thrives.

CONCLUSIONS

A transient numerical model is developed to simulate the flow pattern and specious concentration in a T-shaped barrier embedded micro-mixer. The physical governing equations (i.e. continuity, momentum, and specious transport equations) are discretized using a control volume scheme. A two step projection method is used to solve the fluid flow. The second order-upwind numerical scheme is applied to derive the convective terms. In order to evaluate the mixing efficiency and mixing length, the definition of intensity of segregation is used. In the present study, the flow pattern is laminar and the effects of advection and molecular diffusion are considered. The simulations show that as the baffles' span increases, the mixing length increases, however, the prefect mixing takes place in longer time and length which is not favorable. Moreover, as the baffles' height increases the mixing length decreases but it takes longer time to become steady. In addition, the mixing length increases while the steady state time decrease as the inlet velocity increases.

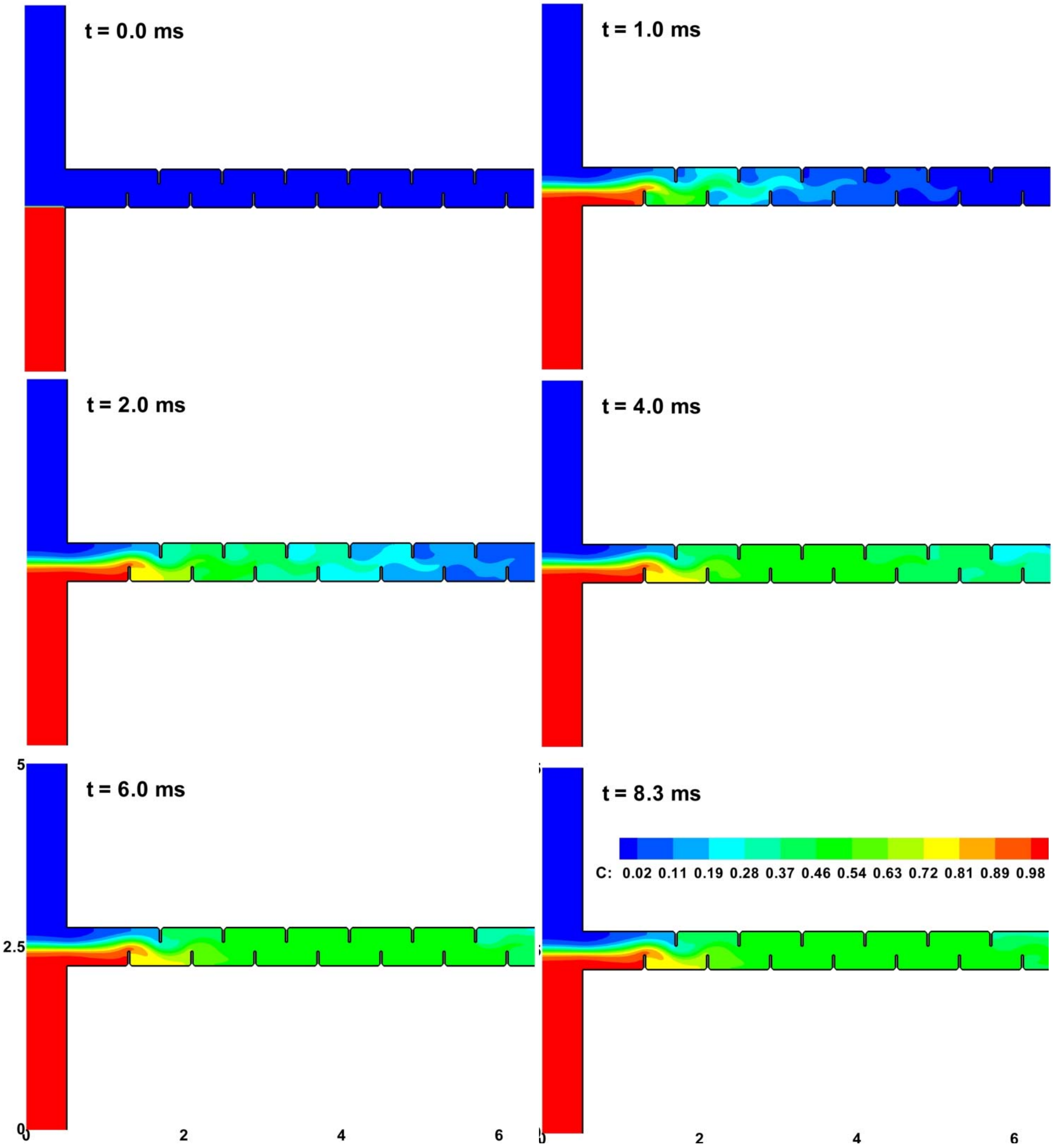

Figure 2: A MODEL RESULTS FOR THE DISTRIBUTION OF THE SPECIOUS TRANSPORT DURING THE MIXING PROCESS IN A T-SHAPED BARRIER EMBEDDED MICRO-MIXER

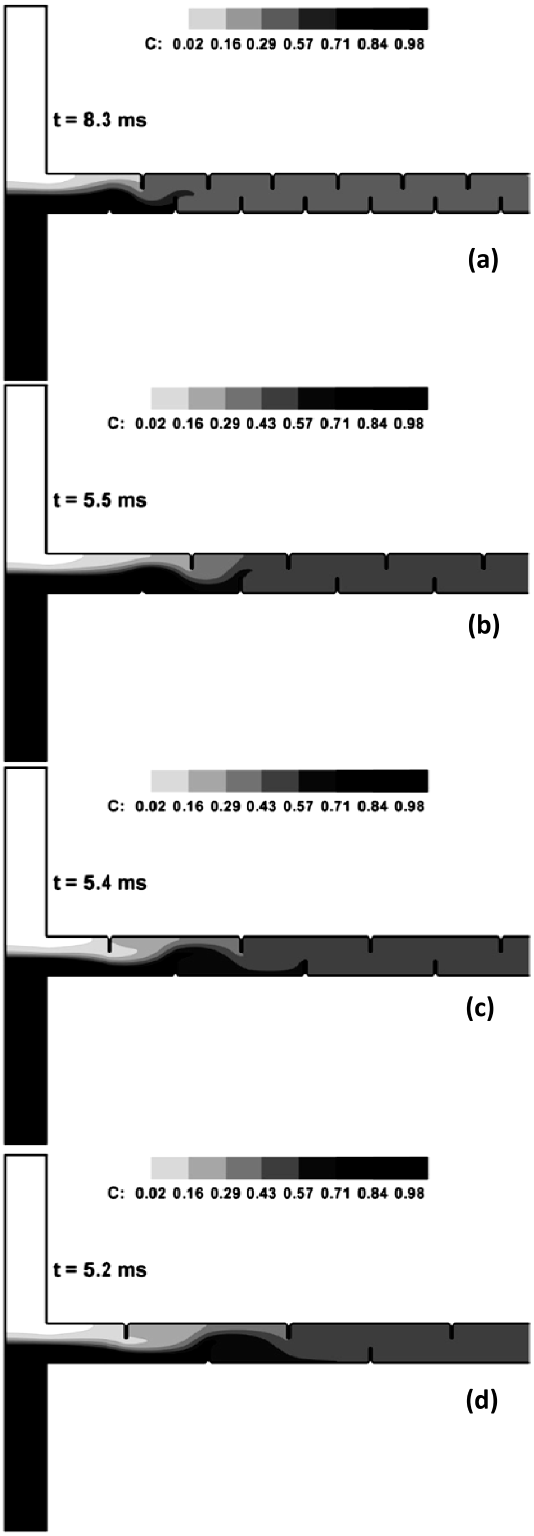

Figure 3: THE DISTRIBUTION OF SPECIOUS CONCENTRATION FOR DIFFERENT BAFFLES' SPAN:
a) S=400µm b) S=600µm c) S=800µm d) S=1000µm

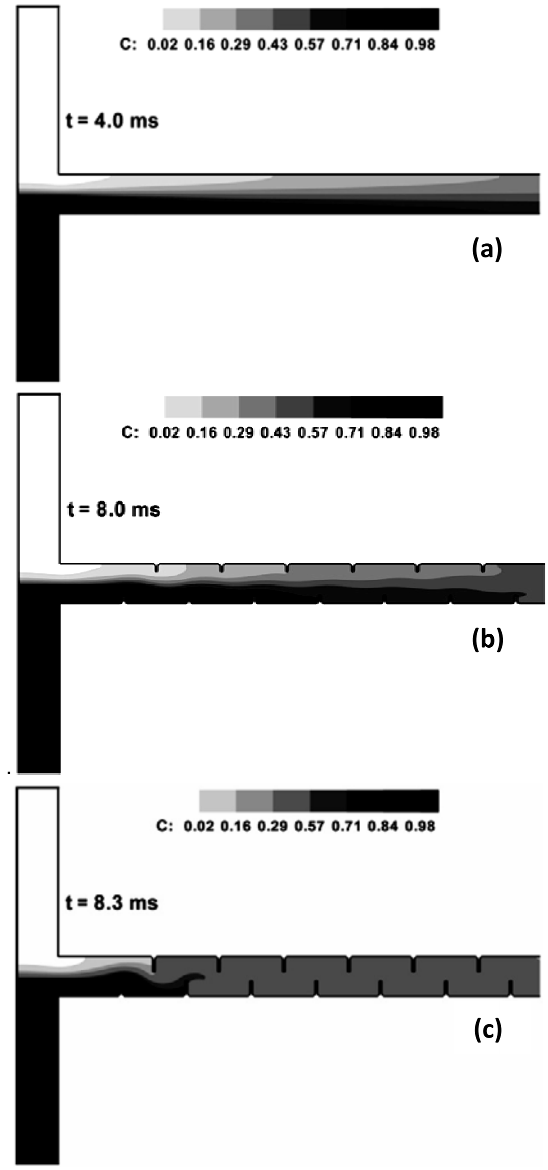

Figure 4: THE DISTRIBUTION OF SPECIOUS CONCENTRATION FOR DIFFERENT BAFFLES' HEIGHT:
a) H=0µm b) H=100µm c) H=200µm

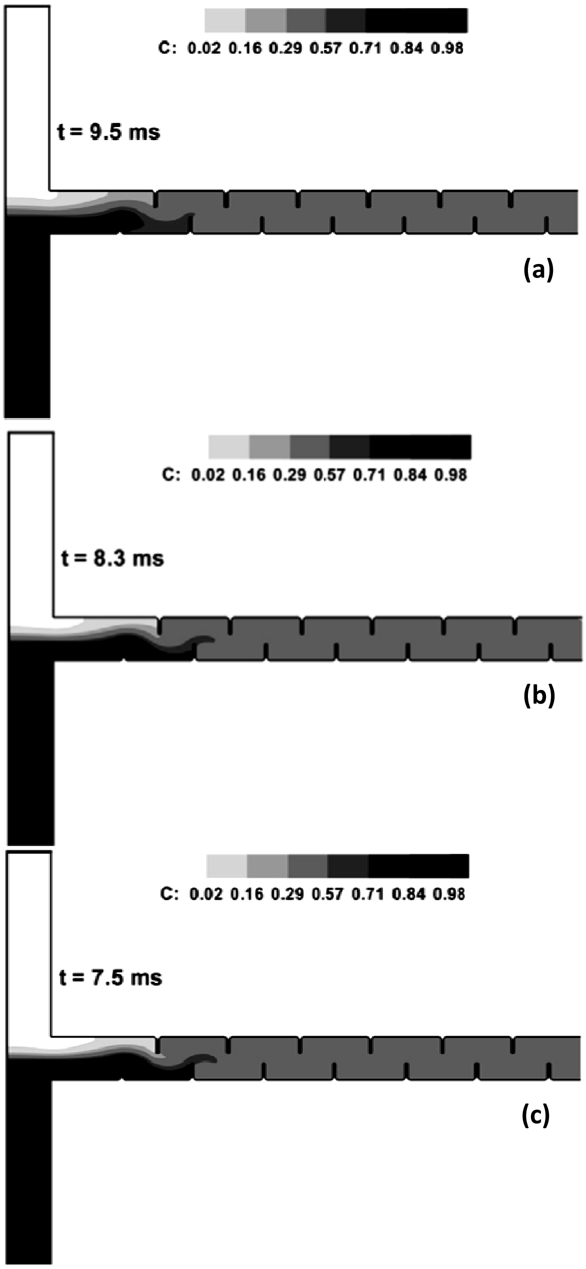

Figure 5: THE DISTRIBUTION OF SPECIOUS CONCENTRATION FOR DIFFERENT INLET VELOCITY:
a) V= 1m/s b) V= 2m/s c) V= 3m/s

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