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Mixing of binary fluids with composition-dependent viscosity in a T-shaped micro-device

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HIGHLIGHTS

- Laminar mixing in T-shaped micro-devices is studied by direct numerical simulation.
- The model mixture presents fluidity of mixing, Δf, both positive and negative.
- For negative Δf, no sudden increase of mixing efficiency at the engulfment.
- For positive or negligible Δf, strong mixing increase at the engulfment.

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ABSTRACT

The process of laminar mixing in a T-shaped micro-device is studied by direct numerical simulation for a model binary mixture, composed of two fluids having the same density and the same viscosity, yet presenting a strong fluidity of mixing effect, i.e. the viscosity of the mixture is a function of its composition. In all cases, the inlet streams remain separated up to a critical Reynolds number, corresponding to the transition from a vortex flow regime, with a double mirror symmetry, to an engulfment flow regime, with a point central symmetry. In the case of a positive fluidity of mixing, the onset of the engulfment regime is accompanied by a sharp increase of the degree of mixing, with the critical Re decreasing as the fluidity of mixing increases. On the contrary, when the fluid mixture has a larger viscosity than that of its pure components, a viscous layer forms at the confluence of the inlet flows, which tends to keep the two streams separated. Therefore, in this case, no sudden increase of the degree of mixing is observed at the onset of the engulfment regime.

1. Introduction

In a recent work, Orsi et al. (2013a) simulated the mixing process that follows the confluence of two fluids onto a T-junction, comparing the case where the two inlet fluids are both water with the case where one inlet fluid is water and the other is ethanol. In particular, it was shown that the degree of mixing increases sharply when the flow field turns from vortex to engulfment flow regimes, that is from a mirror symmetric morphology that keeps the two streams separated, to a point symmetric pattern, where fluid elements reach the opposite side of the mixing channels. Orsi et al. (2013a) observed that the symmetry breaking process, corresponding to the onset of the engulfment regime, occurs at $Re \approx 140$ in the water–water case, in agreement with several works in literature (see Engler et al., 2004; Bothe et al., 2006; Hoffmann et al., 2006; Galletti et al., 2012), whereas larger Re numbers (i.e., $Re = 230$) were needed to enhance mixing in the water–ethanol case. The reason of this mixing hindrance was ascribed to the fact that a water–ethanol mixture has a viscosity that is almost three times larger than that of water, so that at the confluence of the T-mixer, the two streams are separated by a viscous interfacial layer that hampers vortex formation and retards mixing.

Viscosity change due to mixing, however, is not the only possible cause of the above mentioned mixing hindrance. First of all, we should consider that the two pure fluids have different viscosities, i.e., ethanol is about 20% more viscous than water. This, however, by increasing the ethanol residence time, should enhance mixing. Then, there is the effect of density differences, which usually enhance fluid separation. In fact, the density of a water–ethanol mixture is a strong function of its composition: water is about 20% heavier than ethanol and, in addition, the volume of a water–ethanol mixture may be up to 5% smaller than the sum of the volumes that are initially occupied by its

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components. This latter, the so-called volume of mixing, effect was studied in a separate work by Orsi and Mauri (2013), showing that a volume sink at the confluence of the two fluid streams induces a velocity field heading towards the interface, but this effect is small and cannot be the cause of the above-mentioned suppression of mixing efficiency. As for the different densities of water and ethanol, Orsi et al. (2013a) concluded that this effect is important only at low Reynolds numbers, when the two fluids segregate vertically, but does not affect the strong variation of the degree of mixing that was observed. This point, however, deserves further investigations.

In this work, we want to corroborate the statement that the main cause of mixing reduction is the increase of the mixture viscosity upon mixing. To do that, we focus on the effect of the concentration-dependent viscosity, by totally eliminating any density changes and viscosity offset. Therefore, we consider a model binary mixture which, on one hand, has a constant density, while, on the other hand, has a viscosity that strongly depends on composition, although the two pure fluids have the same viscosity.

Our model of a composition-dependent mixture viscosity mirrors the thermodynamic description of a composition-dependent mixture volume. In fact, from multicomponent thermodynamics, we know that the density ρ (i.e., the inverse of the specific volume) of a binary mixture is related to the densities ρ_A and ρ_B of pure fluids A and B, respectively, through the following relation:

$$\frac{1}{\rho}=\frac{\phi}{\rho_A}+\frac{1-\phi}{\rho_B}+\Delta v_{mix}, \tag{1}$$

where ϕ is the mass fraction of component A. Here, we see that the difference between the specific volume of the mixture and the sum of the volumes of the pure components at constant temperature and pressure is the *volume of mixing*, Δv_{mix}, whose value is a function of the mixture composition. In particular, the so-called regular mixtures are characterized by $\Delta v_{mix}=0$, so that their volume is conserved. In this work, as mentioned above, we assume that $\rho_A=\rho_B=\rho_0$ and $\Delta v_{mix}=0$, so that $\rho=\rho_0$.

Many different mixing rules can be found in the literature to evaluate the viscosity of a mixture starting from that of its pure components (see Laliberté, 2007). Considering that viscosity represents the resistance of a fluid against the diffusive transport of momentum, and that in fluid mixtures these resistances are in parallel (Ottino and Chella, 1983), the viscosity μ of a binary mixture can be related to the viscosities of pure fluids A and B, μ_A and μ_B, respectively, through the following relation, which is similar to the density one:

$$\frac{1}{\mu}=\frac{\phi}{\mu_A}+\frac{1-\phi}{\mu_B}+\Delta f_{mix}, \tag{2}$$

where Δf_{mix} is the fluidity of mixing, that accounts for the non-ideality of the mixture. This term is particularly important; for example, a mixture of ethanol and water at 20 °C with $0.3<\phi<0.6$ has a viscosity which is almost three times that of pure water (Simmonds, 1919). Similar behavior is observed for many aqueous mixtures of organic solvents, such as acetone, methanol, propanol and acetic acid (see Dizechi and Marschall, 1982; Wang et al., 2004; Laliberté, 2007) and propylene-carbonate/acetone (Jain and Singh, 2004). On the other hand, the fluidity of mixing can also be positive, as for example in the cases of 1,2-dichloroethane/carbon-tetrachloride (Zhang and Ha, 1997), octan-2-ol/n-tetradecane or octan-2-ol/n-octane (Mahajan and Mirgane, 2013), ethanol/methylacetate (González et al., 2007).

Here, since our objective is to investigate the effect of the fluidity of mixing Δf_{mix} alone, we eliminate any viscosity offset by assuming that the two pure fluids have the same viscosity, i.e. $\mu_A=\mu_B=\mu_0$. In addition, we assume for the viscosity of the mixture the following simple, quadratic expression:

$$\mu(\phi)=\mu_0[1+4(\alpha-1)\phi(1-\phi)], \tag{3}$$

where α expresses the ratio between the viscosity of a 50–50% mixture and that of a pure fluid species. Three cases will be considered, namely $\alpha=3$, $\alpha=\frac{1}{3}$ and $\alpha=1$. The former, $\alpha=3$ case, presents a negative fluidity of mixing and corresponds, indicatively, to a water–ethanol mixture, where the effects due to density changes, together with those due to the different viscosities of the two pure species, have been eliminated. The second case, with $\alpha=\frac{1}{3}$, presents a positive fluidity of mixing and corresponds approximately to octan-2-ol/n-tetradecane (Mahajan and Mirgane, 2013); finally, the $\alpha=1$ case, corresponds to two identical fluids.

In the present work, we will determine the velocity and concentration fields resulting from the confluence of the model fluid mixtures at a T-junction.

2. Problem description

2.1. The governing equations

Consider two fluids at the same temperature and density, converging onto a T junction. Assuming that the heat of mixing and the volume of mixing are negligible, so that the process can be modeled to be isothermal and isovolumetric, at steady state the governing equations are

$$\rho_0\mathbf{v}\cdot\nabla\mathbf{v}+\nabla P=\nabla\cdot[\mu(\phi)(\nabla\mathbf{v}+(\nabla\mathbf{v})^T)], \tag{4}$$

$$\nabla\cdot\mathbf{v}=0, \tag{5}$$

$$\mathbf{v}\cdot\nabla\phi=D\nabla^2\phi, \tag{6}$$

where $\mathbf{v}$ is the solenoidal velocity field, P is the dynamic pressure, ϕ the mass (and volume) fraction of, say, component A of the binary mixture, and D is the molecular diffusivity, while the T superscript indicates the transpose of a tensor. If the two fluids are identical, we can imagine adding a very small amount of contaminant, i.e. a dye, to one of the fluids (which therefore continue to have the same physical properties) and therefore, in this case, ϕ indicates the (normalized) dye mass fraction. The characteristics of the velocity and concentration fields can be described through the Reynolds and Peclet numbers,

$$Re=\frac{\rho_0 Ud}{\mu_0},\quad Pe=\frac{Ud}{D}=Re\,Sc,\quad Sc=\frac{\mu_0}{\rho_0 D}, \tag{7}$$

where Sc is the Schmidt number, U is the mean velocity, while the characteristic fluid length d is assumed to be the hydraulic diameter, i.e.,

$$d=\frac{2WH}{W+H}, \tag{8}$$

where W and H are the mixing channel width and height, respectively (see Fig. 1).

Finally, as mentioned above, we assume that the process is isothermal, therefore neglecting the temperature change due to the heat of mixing. As shown in Orsi et al. (2013a) in the water–ethanol case, this hypothesis is verified, as the effect of the heat of mixing consists of a small temperature decrease along the mixing channel, which amounts to a negligible change in the properties (i.e. density and viscosity) of the mixture.

2.2. Geometry and numerical model

The geometric setting of our simulation consists of the T-shaped micro-device shown in Fig. 1. The mixing channel has