ON MULTICOMPONENT FLOWS: MECHANICAL MODELING AND FINITE ELEMENT SIMULATIONS

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Abstract. *The study of multicomponent systems finds a large scope of applications in engineering problems. They involve multi-phase problems, as porous media and gas-liquid interfaces; and single-phase problems, as gas and liquid mixtures. The main goal of this paper is the application of a finite element method to simulate flow problems involving incompressible mixtures. A mixture theory supported by continuum mechanics was employed to present the development of a mechanical modeling for multicomponent flows. This theory is based on classic conservation postulates, which were written for multicomponent systems. The mechanical modeling was summarized in a set of equations in terms of velocity, pressure and mass fraction fields. Those equations were approximated by a stabilized finite element method, for the classical Galerkin method does not have the ability of solving some flows of practical interest. That happens because: first, Galerkin approximation involves a mixed formulation where the compatibility of pressure and velocity subspaces is critical and demands the use of non-conventional finite elements; and second, it suffers from the asymmetric nature of advective terms – a numerical difficulty in the approximation of advective-dominated problems. The stabilized Galerkin/least-squares method (GLS) was able to overcome the numerical difficulties mentioned above. In this study the GLS formulation was applied to approximate generalized newtonian binary mixtures. Some results were compared with other authors showing good agreement. Those problems involved geometric and material non-linearities employing Carreau fluid model, opening the spectra for industrial applications in areas such as food, polymer, biological and environmental engineering.*

Keywords*. continuum mixture theory, finite elements in fluids*

1. Introduction

The objective of this study is to yield numerically stable and physically realistic approximations for mixture flow problems. For this, a stabilized finite element method shall be employed. Multicomponent flows find applications in many subjects in engineering. In petroleum engineering, modeling and simulation of mixture volumes, which arise between batch transfers of petroleum fractions in multiproduct pipelines, have been studied by Carvalho (2002), Rachid et al. (2002) and others. In environmental engineering, problems of liquid effluent dispersion in lakes and rivers represent multicomponent flows, with the prediction of spots and degrees of pollution are of high interest (Curran, 1981). In food industry, problems of in-line mixture of food colorants and additives, clean-in-place equipment, mixture tanks as homogenizers and bioreactors are also examples of multicomponent systems, in which modeling and computational simulation could be of great value (Geankoplis, 1995).

Initially in this paper, the development of a continuum mechanical modeling for multicomponent incompressible flows in a single phase is reviewed (Atkin & Craine 1976; Sampaio & Williams, 1979; Slattery, 1999). This modeling is able to describe a material body B consisting of N species, which might be undergoing an arbitrary number of homogeneous chemical reactions, and which might experiment a condition of stress distribution and answer to this condition as a generalized newtonian fluid. It is mathematically written as a boundary value problem, and in this study its variational formulation is approximated by a finite element method. The classical Galerkin finite element method suffers from two major difficulties when dealing with fluid problems. First, the need of satisfying Babuška-Brezzi condition (Babuška, 1973; Brezzi, 1974) in order to compatibilize velocity and pressure subspaces; and second, the inherent instability of central difference schemes in approximating advective dominated equations - in the case considered herein characterized by high Reynolds and mass Peclet numbers. Application of stabilized methods, such as Galerkin/least-squares (GLS) (Hughes et al., 1986; Hughes et al. 1989) is a useful tool to overcome the mentioned difficulties. The GLS method has the ability to circumvent Babuška-Brezzi condition and to generate stable approximations for highly advective flows preserving good accuracy properties (Franca et al., 1992). This is achieved by adding residual-based terms to the classic Galerkin formulation, retaining its weighted residual structure and not damaging its consistency (Hughes et al., 1986, Franca & Frey, 1992).

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2. Conservation and Constitutive Equations

In the view of continuum mechanics, each material body that forms the mixture is a continuum body, and the multicomponent body B is a superposition of the N single-component bodies $B_{(\alpha)}$. The study of kinematics of mixtures is based on the mapping $B_{(\alpha)}$ into Euclidean space E by the pair placement and volume fraction $(\boldsymbol{\chi}_{(\alpha)},\varphi_{(\alpha)})$, as follows (Sampaio & Williams, 1979):

$$\begin{aligned} &\boldsymbol{\chi}_{(\alpha)} : B_{(\alpha)} \times \Re^{+} \to E \\ &\varphi_{(\alpha)} : B_{(\alpha)} \times \Re^{+} \to [0,1], \end{aligned} \tag{1}$$

where the volume fraction is defined as the relation between the local volume of species α ($dV_{(\alpha)}$) and the local mixture volume (dV):

$$\varphi_{(\alpha)}(\mathbf{x}) = \frac{dV_{(\alpha)}}{dV} \tag{2}$$

Single-component material particles $P_{(\alpha)}$ are defined for each component, and their configuration is given by the position vector $\mathbf{x}$, as a consequence of the mapping of $B_{(\alpha)}$ into E:

$$\mathbf{x} = \boldsymbol{\chi}_{(\alpha)}(P_{(\alpha)}). \tag{3}$$

The family of deformations suffered from the material body, parameterized by the time t, from a reference configuration $\mathbf{X}_{(\alpha)}$, defines its motion (Truesdell & Toupin,1960; Slattery, 1999):

$$\mathbf{x} = \boldsymbol{\chi}_{\mathbf{X}(\alpha)}(\mathbf{X}_{(\alpha)}, t). \tag{4}$$

The velocity and acceleration fields are defined for each component by the first and second time derivatives of the placement. In the Eulerean point of view, these fields are described as functions of a fixed position in space:

$$\begin{aligned} &\mathbf{u}_{(\alpha)} = \mathbf{u}_{(\alpha)}(\mathbf{x}, t), \\ &\mathbf{a}_{(\alpha)} = \mathbf{a}_{(\alpha)}(\mathbf{x}, t). \end{aligned} \tag{5}$$

For the single-component bodies $B_{(1)}$, $B_{(2)}$,..., $B_{(N)}$ are given motions whose trajectories may overlap, which requires that (Sampaio & Williams, 1979)

$$\sum_{\alpha=1}^{N} \varphi_{(\alpha)} = 1. \tag{6}$$

It is useful to describe the dynamic relations in terms of mass variables, such as mass fractions, which are non-dimensional. The mass density of species α is denoted as $\rho_{(\alpha)}$, and is defined as the relation between the mass density of α (in a point at the mixture) and the mass density of the mixture itself (in that point). The mass density of species α in respect to mixture's mass density in a position $\mathbf{x}$ is called mass fraction of α, and denoted by $\omega_{(\alpha)}$:

$$\omega_{(\alpha)}(\mathbf{x}) = \frac{\rho_{(\alpha)}(\mathbf{x})}{\rho(\mathbf{x})}, \tag{7}$$

with ρ representing the density of the multicomponent body. When considering the theory of superposing the N single-material bodies $B_{(\alpha)}$, the following intuitive relation is usually postulated (Atkin & Craine 1976):

$$\rho(\mathbf{x}) = \sum_{\alpha=1}^{N} \rho_{(\alpha)}(\mathbf{x}), \tag{8}$$

and consequently, from Eq.(7) one achieves that

$$\sum_{\alpha=1}^{N} \omega_{(\alpha)}(\mathbf{x}) = 1. \tag{9}$$

In studying the phenomena of flow in a multicomponent system, it is important to define a velocity for the mixture. The mass averaged velocity, mixture velocity or bulk velocity is defined as:

$$\mathbf{u} = \frac{1}{\rho}\sum_{\alpha=1}^{N}\rho_{(\alpha)}\mathbf{u}_{(\alpha)} = \sum_{\alpha=1}^{N}\omega_{(\alpha)}\mathbf{u}_{(\alpha)}. \tag{10}$$

The relative velocity for α with respect to bulk velocity is $(\mathbf{u}_{(\alpha)}-\mathbf{u})$. The N relative velocities are related to one another, as follows from Eqs. (8) and (10), by:

$$\sum_{\alpha}^{N}\rho_{(\alpha)}(\mathbf{u}_{(\alpha)} - \mathbf{u}) = 0. \tag{11}$$

Thus, the definition of bulk velocity ensures that the sum of the mass flux of all diffusive movements is null. The mass flux of α with respect to bulk velocity, called relative mass flux, denoted by $\mathbf{j}_{(\alpha)}$, is defined as:

$$\begin{aligned}\mathbf{j}_{(\alpha)} &\equiv \rho_{(\alpha)}(\mathbf{u}_{(\alpha)} - \mathbf{u}) \\ &= \rho\,\omega_{(\alpha)}(\mathbf{u}_{(\alpha)} - \mathbf{u}),\end{aligned} \tag{12}$$

and it follows from Eq. (11) that:

$$\sum_{\alpha=1}^{N}\mathbf{j}_{(\alpha)} = 0. \tag{13}$$

Each single component body is characterized by its relevant physical properties, determined in its pure state as in the single continuum theory, and also by a volume fraction field from the mapping in E. Other quantities that describe its dynamic state, such as velocity, pressure, external forces and tension distribution are also defined for each single-component body. The physical properties and dynamic state of the mixture as a whole depend on each component's physical properties, volume fraction distribution and dynamic state, and also by the physical-chemistry interactions among them. The mathematical relations describing these dependencies shall be determined theoretically or empirically (references in Atkin & Craine, 1976; Cao et al., 1992; Martins et al., 2001).

As in engineering applications there is a major interest in obtaining results for velocity and pressure fields for the mixture as a whole (bulk velocity and bulk pressure), a mechanical model must be developed in terms of these bulk variables, and also in terms of each component volume or mass fraction field. Thus, the model presented herein consists of two equations (for bulk velocity and bulk pressure) plus N-1 equations for a mixture of N components, that allow the solution of N-1 mass fraction fields, plus Eq. (6) or Eq. (9). These equations are derived from conservation principles (Gurtin, 1981; Slattery, 1999)explored in sequence, for the multicomponent body B that occupies the region of volume Ω of frontier Γ.

Principle of mass conservation for a multicomponent body *B*: The mass of a body does not change with time. This is written as:

$$\frac{d}{dt}\int_{\Omega}\rho d\Omega = 0. \tag{14}$$

Applying Reynolds transport theorem (Gurtin, 1981), the differential mass conservation equation for the mixture is obtained:

$$\frac{\partial\rho}{\partial t} + \mathrm{div}(\rho\mathbf{u}) = 0. \tag{15}$$

Principle of mass conservation for a single-component body $B_{(\alpha)}$: The time rate of change of species α in a region Ω of B is equal to the rate in which this species is produced or consumed by chemical reactions. In the case of a single-phase, this principle is written as

$$\frac{d}{dt}\int_{\Omega}\rho_{(\alpha)}d\Omega = \int_{\Omega}r_{(\alpha)}d\Omega\ . \tag{16}$$

where $r_{(\alpha)}$ denotes the rate of production of α by homogeneous chemical reactions per unit volume. Applying Reynolds transport theorem (Truesdell & Toupin,1960) to Eq. (16), results:

$$\int_{\Omega}\left(\frac{d_{(\alpha)}\rho_{(\alpha)}}{dt}+\rho_{(\alpha)}\,\mathrm{div}\,\mathbf{u}_{(\alpha)}-r_{(\alpha)}\right)d\Omega=0. \tag{17}$$

With a localization argument (Gurtin, 1981), the differential mass balance for species α is derived:

$$\frac{d_{(\alpha)}\rho_{(\alpha)}}{dt}+\rho_{(\alpha)}\,\mathrm{div}\,\mathbf{u}_{(\alpha)}=r_{(\alpha)}. \tag{18}$$

In terms of relative mass flux (Eq. (12)) and mass fractions, for an incompressible system Eq. (18) results in:

$$\rho\frac{d_{(u)}\omega_{(\alpha)}}{dt}+\mathrm{div}\,\mathbf{j}_{(\alpha)}=r_{(\alpha)}. \tag{19}$$

where $d_{(u)}(\cdot)/dt$ represents the multicomponent material derivative, the time derivative following a material particle with the bulk velocity.

Principle of momentum conservation for a single-component body $B_{(\alpha)}$: The rate of change of linear momentum of a material volume relative to an inertial frame of reference is equal to the resultant force on the volume. In this case, body forces are denoted by $\mathbf{f}_{(\alpha)}$ (force per unit mass of α). Contact forces are represented by the partial stress vector $\mathbf{t}_{(\alpha)}(\mathbf{n}, \mathbf{x}, t)$, defined over Γ. In addition, the effects of interactions between mixture constituents must be considered (Atkin & Craine, 1976). The momentum supplied to α due to chemical reactions with other constituents is denoted by $\mathbf{J}_{(\alpha)}$, and the momentum supplied to α due to other interactions, such as the relative motion between the constituents because of a diffusive force, is denoted by $\mathbf{p}_{(\alpha)}$. The postulate is mathematically written as:

$$\frac{d}{dt}\int_{\Omega}\rho_{(\alpha)}(\mathbf{x},t)\,\mathbf{u}_{(\alpha)}(\mathbf{x},t)\,d\Omega=\int_{\Omega}r_{(\alpha)}(\mathbf{x},t)\,\mathbf{J}_{(\alpha)}(\mathbf{x},t)d\Omega+\int_{\Omega}(\rho_{(\alpha)}(\mathbf{x},t)\,\mathbf{f}_{(\alpha)}(\mathbf{x},t)+\mathbf{p}_{(\alpha)}(\mathbf{x},t))d\Omega+\int_{\Gamma}\mathbf{t}_{(\alpha)}(\mathbf{n},\mathbf{x},t)d\Gamma. \tag{20}$$

Applying Reynolds transport theorem (Gurtin, 1981) to Eq. (20), results:

$$\int_{\Omega}\rho_{(\alpha)}\left(\frac{d_{(\alpha)}\mathbf{u}_{(\alpha)}}{dt}-\mathbf{f}_{(\alpha)}\right)+r_{(\alpha)}\mathbf{J}_{(\alpha)}-\mathbf{p}_{(\alpha)}d\Omega=\int_{\Gamma}\mathbf{t}_{(\alpha)}d\Gamma. \tag{21}$$

Following Cauchy's hypothesis for a single-component body (Gurtin, 1981), there may be established the existence of a partial stress tensor $\mathbf{T}_{(\alpha)}$ associated with species α, such that:

$$\mathbf{t}_{(\alpha)}(\mathbf{n})=\mathbf{T}_{(\alpha)}\mathbf{n}. \tag{22}$$

Green's transformation (Slattery, 1999) and localization theorem (Gurtin, 1981) are employed to transform the integral formulation in the differential form of the momentum conservation for species α:

$$\rho_{(\alpha)}\frac{d_{(\alpha)}\mathbf{u}_{(\alpha)}}{dt}=\mathrm{div}\,\mathbf{T}_{(\alpha)}+\mathbf{p}_{(\alpha)}-r_{(\alpha)}(\mathbf{u}_{(\alpha)}-\mathbf{J}_{(\alpha)})+\rho_{(\alpha)}\mathbf{f}_{(\alpha)}. \tag{23}$$

To postulate the momentum balance for the mixture as a whole, the following hypothesis have been assumed, according to Atkin & Craine (1976):

$$\begin{aligned}&\mathbf{f}=\frac{1}{\rho}\sum_{\alpha=1}^{N}\rho_{(\alpha)}\mathbf{f}_{(\alpha)},\\&\mathbf{T}^{*}=\sum_{\alpha=1}^{N}\mathbf{T}_{(\alpha)},\\&\sum_{\alpha=1}^{N}(\mathbf{p}_{(\alpha)}+r_{(\alpha)}\mathbf{J}_{(\alpha)})=0,\end{aligned} \tag{24}$$

where $\mathbf{f}$ is the total external body force per unit mass acting on the mixture, $\mathbf{T}^*$ is the total stress tensor, and the last relation accounts for the fact that the sum of all momentum interactions by chemical reactions and relative motions is null. A summation for the N species in Eq. (23) results:

$$\sum_{N} \rho_{(\alpha)} \frac{d_{(\alpha)}\mathbf{u}_{(\alpha)}}{dt} = \operatorname{div}\mathbf{T}^{*} + \rho\mathbf{f}, \tag{25}$$

which is approximated by:

$$\rho\dot{\mathbf{u}} = \operatorname{div}\mathbf{T} + \rho\mathbf{f} \tag{26}$$

where **T** a stress tensor that is the total stress tensor plus the apparent stress that arises from diffusion (Atkin & Craine, 1976). Equation (25) then represents the First Cauchy's law written for a multicomponent material body. As **T** is taken to be symmetric, then the moment of momentum conservation is also satisfied (Gurtin, 1981; Atkin & Craine, 1976).

Material behavior, constitutive equations for $\mathbf{j}_{(\alpha)}$:

A classic discussion on the diffusion in multicomponent systems is given by Curtiss, referred by Slattery (1999). This author has worked on the context of the Chapman-Enskog solution for Boltzmann equation to get to an expression for $\mathbf{j}_{(\alpha)}$. This expression resumes the dependence of $\mathbf{j}_{(\alpha)}$ on thermal effects, pressure, external forces and concentration gradients. In binary mixtures, Curtiss equation is reduced to a form that can be represented as:

$$\mathbf{j}_{(\alpha)} = \mathbf{j}_{(\alpha)}^{(o)} + \mathbf{j}_{(\alpha)}^{(P)} + \mathbf{j}_{(\alpha)}^{(f)} + \mathbf{j}_{(\alpha)}^{(T)}. \tag{27}$$

The fist term, $\mathbf{j}_{(\alpha)}^{(o)}$, represents the ordinary diffusion, caused by concentration gradients. The other terms represent the diffusion forces by other phenomena, such as mentioned before: $\mathbf{j}_{(\alpha)}^{(P)}$ for pressure effects, $\mathbf{j}_{(\alpha)}^{(f)}$ the effects of external forces and $\mathbf{j}_{(\alpha)}^{(T)}$ the thermal effects. These last three terms can be neglected in most common cases (Slattery, 1999). Fundamentally, the term of ordinary diffusion is a function of each component's concentration gradient. In addition, it may be a function of parameters such as the molar mass and other chemical properties of each component, and also by mixture properties and characteristics, which represents the object of study for many researchers (Bird, 1960). In this work, the term of ordinary diffusion is taken as the Fick's Law (Slattery, 1999; Bird, 1960), as follows:

$$\mathbf{j}_{(\alpha)}^{(o)} = -\rho D_{(\alpha\beta)} \nabla \omega_{(\alpha)}, \tag{28}$$

where the mass diffusivity coefficient $D_{(\alpha\beta)}$ accounts for the dependence of $\mathbf{j}_{(\alpha)}^{(o)}$ on parameters as cited above.

Material behavior, constitutive equations for T: The First Cauchy's Law (Eq. (25)) is a conservation law that describes the dynamical conditions of any material body. The specific material behavior is given by the way in which **T** depends on the motion and deformation suffered by the body. This dependence is described by constitutive equations. Fore a single-component body, one single constitutive equation is necessary to describe its behavior, while for a multicomponent body, it may be necessary to have more information in order to describe the mixture's material behavior in any concentration of its constituents. The materials considered herein are those that present a generalized newtonian behavior, which means a linear relation between **T** and the rate of deformation tensor **D** (the symmetric part of velocity gradient tensor). The models for this behavior are largely applied in describing viscometric flows, where there is the absence of normal stresses or elastic effects (Bird et al., 1987). For a generalized newtonian fluid, a constitutive equation for **T** is given by:

$$\mathbf{T} = -p\mathbf{I} + 2\eta(\dot{\gamma})\mathbf{D}. \tag{29}$$

The function $\eta(\dot{\gamma})$ is dependent on the model employed to describe the fluid, and $\dot{\gamma}$ is the magnitude of tensor **D** (Slattery, 1999). The apparent viscosity for a generalized newtonian fluid defined as:

$$\eta_{ap} = \frac{(1/2\ \operatorname{tr}\mathbf{S})^{1/2}}{(2\operatorname{tr}\mathbf{D})^{1/2}} = \frac{\mathcal{T}}{\dot{\gamma}}, \tag{30}$$

where $\mathcal{T}$ represents the shear stress. Generalized newtonian models are only applicable to shear flows (without normal stresses).

The constitutive equation known as Carreau model is used to describe the behavior of blood and many polymer solutions. For this model, the apparent viscosity is given by the relation:

$$\eta_{ap} = \eta^{*}\left(\tilde{\eta} + \left[1 + \left(\mathrm{W}\tilde{\dot{\gamma}}\right)^{2}\right]^{(n-1)/2}\right), \tag{31}$$

where the parameters have been changed to a non dimensional form (Franceschini, 2001) as suggested by Tran-Canh & Tran-Cong (2002):

$$\eta^* = \eta_0 - \eta_\infty; \quad \tilde{\eta} = \frac{\eta_\infty}{\eta^*}; \quad \tilde{\gamma} = \frac{\gamma}{\mathbf{u}_\infty / L}; \quad \mathrm{W} = \lambda\left(\frac{\mathbf{u}_\infty}{L}\right). \tag{32}$$

The parameter η^* is used to characterize the Reynolds number of the flow. In most practical cases, the parameter n in this model is less than one. In those cases, the fluid is named shear thinning, and its apparent viscosity decreases as the shear stress increases.

3. Finite element approximation

As a consequence of the conservation equations described above, the mechanical modeling for multicomponent flows is described as a boundary-value problem. In the case of a generalized newtonian fluid mixture in isochoric motion with $\mathbf{j}_{(\alpha)}$ given by Fick's law (Eq. (28)) is given by:

$$\begin{aligned}
&\frac{\partial \mathbf{u}}{\partial t} + (\nabla \mathbf{u})\mathbf{u} + \nabla p - 2\,\mathrm{Re}^{-1}\,\mathrm{div}\,\mathbf{D}(\mathbf{u}) - \mathrm{Fr}^{-2} = 0 \qquad \text{in } \Omega \times (0, t_\infty) \\
&\mathrm{div}\,\mathbf{u} = 0 \qquad \text{in } \Omega \times (0, t_\infty) \\
&\frac{\partial \omega_{(\alpha)}}{\partial t} + \nabla \omega_{(\alpha)} \cdot \mathbf{u} - \mathrm{Pe}_m^{-1}\,\mathrm{div}\,\nabla \omega_{(\alpha)} - R_{(\alpha)} = 0 \qquad \text{in } \Omega \times (0, t_\infty)
\end{aligned} \tag{33}$$

subjected to the following boundary conditions:

$$\begin{aligned}
&\mathbf{u} = \mathbf{u}_g && \text{on } \Gamma_g \times (0, t_\infty), \\
&\omega_{(\alpha)} = \omega_{(\alpha)g} && \text{on } \Gamma_g \times (0, t_\infty);
\end{aligned} \tag{34}$$

$$\begin{aligned}
&\mathbf{T}\mathbf{n} = \mathbf{t}_h && \text{on } \Gamma_h \times (0, t_\infty), \\
&\mathbf{j}_{(\alpha)} \cdot \mathbf{n} = j_{(\alpha)h} && \text{on } \Gamma_h \times (0, t_\infty);
\end{aligned} \tag{35}$$

where $\mathbf{u}$ is the bulk velocity, p is the bulk pressure, Fr is the Froude number, that represents external forces, $\mathbf{D}(\mathbf{u})$ is the symmetric part of the tensor velocity gradient, $\omega_{(\alpha)}$ is the mass fraction field for the species α, $R_{(\alpha)}$ is the mass generation rate for species α, $\mathbf{u}_g$ and $\omega_{(\alpha)g}$ are prescribed velocity and mass fraction fields (Dirichlet boundary conditions), $\mathbf{t}_h$ and $j_{(\alpha)h}$ are prescribed tension and mass flux (Neumann boundary conditions). The non dimensional Reynolds and mass Peclet numbers are given by:

$$\mathrm{Re} = \frac{\rho \mathbf{u} L}{\eta}, \quad \mathrm{Pe}_m = \frac{\mathbf{u} L}{D_{(\alpha m)}}; \tag{36}$$

where ρ and η are mixture's density and viscosity, L is a characteristic length, $D_{(\alpha m)}$ is the effective diffusivity of species α in the mixture. The third equation in Eq. (33) is solved N-1 times for a mixture of N components.

The magnitude of Reynolds number gives the relative importance of the advection term over the diffusivity term, in the process of momentum transport. The magnitude of mass Peclet number also gives the relative importance of the advection term over the diffusivity term, but for the process of mass transfer of species α.

A variational formulation of Eqs. (33) is approximated by a stabilized finite element method, namely GLS. The use of a stabilization technique is necessary because of the highly advective character of the equations in problems of interest (high Re and Pe_m), and also because the bilinear finite element Q1 does not satisfy Babuška-Brezzi condition (Babuška, 1973; Brezzi, 1974). The approximation is performed over the partition C_h of the closed domain $\bar{\Omega}$, consisting of convex quadrilateral Q1 elements in $\Re^{nsd=2}$. The usual spaces of functions (Ciarlet, 1978) are employed to define the finite element subspaces to approximate the velocity field ($\mathbf{V}_h$), the pressure field (P_h) and the scalar field mass fraction (W_h) (Franca et al., 1992):

$$\mathbf{V}_h = \{\mathbf{v} \in H_0^1(\Omega)^{nsd} \,\big|\, \mathbf{v}_{|K} \in R_k(K)^{nsd}, K \in \Omega_K\} \tag{37}$$

$$P_h = \{p \in C^0(\Omega) \cap L_0^2(\Omega) \,\big|\, p_{|K} \in R_l(K), K \in \Omega_K\} \tag{38}$$

$$W_h = \left\{w \in H_0^1(\Omega) \,\middle|\, w_{|K} \in R_k(K), K \in \Omega_K\right\} \tag{39}$$

and also for the fields prescribed over Γ_g:

$$\mathbf{V}_h^g = \{\mathbf{v}(\cdot,t) \in H^1(\Omega)^{nsd}, t \in [0,t_\infty] \,\big|\, \mathbf{v}_{|K} \in R_k(K)^{nsd}, K \in \Omega_K, \mathbf{v}(\cdot,t) = \mathbf{u}_g \text{ on } \Gamma_g\} \tag{40}$$

$$W_h^g = \left\{ w(\cdot,t) \in H^1(\Omega), t \in [0,t_\infty] \,\big|\, w_{|K} \in R_k(K), K \in \Omega_K, w(\cdot,t) = \omega_{(\alpha)_g} \text{ on } \Gamma_g \right\} \tag{41}$$

where R_k, R_l denote the polynomial spaces of degrees k and l, respectively. Finally, $(\cdot\,,\,\cdot)$ and $\|\cdot\|$ represent the L^2-inner product and norm in Ω, and $(\cdot\,,\,\cdot)_K$ and $\|\cdot\|_{0,K}$ denote the L^2 -inner product and norm in the element domain K, respectively.

The functions $\mathbf{u}$, p and $\omega_{(\alpha)}$ are approximated by functions $\mathbf{u}^h$, p^h and $\omega_{(\alpha)}{}^h$, in which h is referred to the association of these functions with a the partition or mesh C_h, parameterized by a characteristic length h. The finite element approximation for model in presented previously, using a GLS stabilized method, is given by:

Find the triple $(\mathbf{u}^h, p^h, \omega_{(\alpha)}{}^h) \in \mathbf{V}_h$, x P_h x W_h such as:

$$B(\mathbf{u}^h, p^h, \omega_{(\alpha)}^h; \mathbf{v}, q, w) = F(\mathbf{v}, q, w), \quad (\mathbf{v}, q, w) \in \mathbf{V}_h \times P_h \times W_h; \tag{42}$$

where

$$\begin{aligned} B(\mathbf{u}^h, p^h, \omega_{(\alpha)}^h; \mathbf{v}, q, w) = & \left(\frac{\partial \mathbf{u}}{\partial t}, \mathbf{v}\right) + \left([\nabla \mathbf{u}]\mathbf{u}, \mathbf{v}\right) + (2\nu \mathbf{D}(\mathbf{u}), \mathbf{D}(\mathbf{v})) - (\nabla \cdot \mathbf{v}, p) \\ & - (\nabla \cdot \mathbf{u}, q) + \left(\frac{\partial \omega_{(\alpha)}}{\partial t}, w\right) + \left(\nabla \omega_{(\alpha)} \cdot \mathbf{u}, w\right) - \left(D_{\alpha\beta} \nabla \omega_{(\alpha)}, \nabla w\right) \\ & + \sum_{K \in C_h} \left(\frac{\partial \mathbf{u}}{\partial t} + [\nabla \mathbf{u}]\mathbf{u} + \nabla p - 2\nu \nabla \cdot \mathbf{D}(\mathbf{u}), \tau(\mathrm{Re}_K)([\nabla \mathbf{v}]\mathbf{u} - 2\nu \nabla \cdot \mathbf{D}(\mathbf{v}) - \nabla q) \right)_K \\ & + \sum_{K \in C_h} \left(\frac{\partial \omega_{(\alpha)}}{\partial t} + \nabla \omega_{(\alpha)} \cdot \mathbf{u} - D_{\alpha\beta} \nabla^2 \omega_{(\alpha)}, \sigma(\mathrm{Pe}_K^m)(\nabla w \cdot \mathbf{u} - D_{\alpha\beta} \nabla^2 w) \right)_K \end{aligned} \tag{43}$$

and

$$\begin{aligned} F(\mathbf{v}, q, w) = & (\mathbf{f}, \mathbf{v}) + (\mathbf{t}_h, \mathbf{v})_{\Gamma_h} + \left(R_{(\alpha)}, w\right) + (j_{(\alpha)h}, w)_{\Gamma_h} \\ & + \sum_{K \in C_h} (\mathbf{f}, \tau(\mathrm{Re}_K)([\nabla \mathbf{v}]\mathbf{u} - 2\nu \nabla \cdot \mathbf{D}(\mathbf{v}) - \nabla q))_K \\ & + \sum_{K \in C_h} (R_{(\alpha)}, \sigma(\mathrm{Pe}_K^m)(\nabla w \cdot \mathbf{u} - D_{\alpha\beta} \nabla^2 w))_K \end{aligned} \tag{44}$$

where the terms before the sums are original terms in Galerkin formulation, and the terms within the sums correspond to added stabilized terms, that are evaluated elementwise. The stability parameter for the velocity-pressure terms is given as in Franca et al. (1992):

$$\tau(\mathrm{Re}_K) = \frac{h_K}{2|\mathbf{u}|_p} \xi(\mathrm{Re}_K); \tag{45}$$

where

$$\xi(\mathrm{Re}_K) = \begin{cases} \mathrm{Re}_K, 0 \le \mathrm{Re}_K < 1 \\ 1\ , \mathrm{Re}_K \ge 1 \end{cases}, \tag{46}$$

$$\mathrm{Re}_K = \frac{m_k |\mathbf{u}|_p h_K}{4\nu}, \tag{47}$$

$$m_k = \min\left\{\frac{1}{3}, 2\tilde{C}_k\right\}. \tag{48}$$

The parameter $\tilde{C}_k$ derives from inverse estimate (Franca & Frey, 1992). Its value corresponds to $\tilde{C}_k = \infty$ for a 2-D bilinear (Q1) element. The p corresponds to the norm type employed to calculate the velocity norm, usually p=2, corresponding to the Euclidean norm (Franca & Frey, 1992).

For advection-diffusion terms, the stability parameter used was that suggested by Franca & Frey (1992):

$$\sigma\left(\mathrm{Pe}_K^m\right)=\frac{h_K}{2\left|\mathbf{u}\right|_p}\xi\left(\mathrm{Pe}_K^m\right); \tag{49}$$

where $\mathrm{Pe}^m{}_K(x)$ is the element K mass Peclet number, as follows:

$$\begin{aligned}&\mathrm{Pe}_K^m=\frac{m_k\left|\mathbf{u}\right|_p h_K}{2D},\\ &\xi\left(\mathrm{Pe}_K^m\right)=\begin{cases}\mathrm{Pe}_K^m, & 0\le \mathrm{Pe}_K^m\le 1\\ 1, & \mathrm{Pe}_K^m\ge 1.\end{cases}\end{aligned} \tag{50}$$

The functions $\mathbf{u}^h$, p^h $\omega_{(\alpha)}{}^h$ e w are substituted by finite element expansions, resulting in an algebraic system of equations such as:

$$\begin{aligned}&[\mathbf{M}+\mathbf{M}_\tau^\nu]\mathbf{a}+\mathbf{N}(\mathbf{u})+\mathbf{N}_\tau^\nu(\mathbf{u})+[\mathbf{K}+\mathbf{K}_\tau^\nu]\mathbf{u}+[\mathbf{G}+\mathbf{G}_\tau^\nu]\mathbf{p}=\mathbf{F}+\mathbf{F}_\tau\\ &[\mathbf{M}_\tau^q]\mathbf{a}+\mathbf{N}_\tau^\nu(\mathbf{u})+[\mathbf{G}^T+\mathbf{K}_\tau^q]\mathbf{u}+[\mathbf{G}_\tau^q]\mathbf{p}=\mathbf{E}_\tau\\ &[\bar{\mathbf{M}}+\bar{\mathbf{M}}_\sigma]\dot{\boldsymbol{\omega}}_{(\alpha)}+[\bar{\mathbf{N}}(\mathbf{u})+\bar{\mathbf{N}}_\sigma(\mathbf{u})]\dot{\boldsymbol{\omega}}_{(\alpha)}+[\bar{\mathbf{K}}+\bar{\mathbf{K}}_\sigma]\dot{\boldsymbol{\omega}}_{(\alpha)}=\bar{\mathbf{F}}+\bar{\mathbf{F}}_\sigma\end{aligned} \tag{51}$$

where $\mathbf{u}$, p and $\boldsymbol{\omega}_{(\alpha)}$ are the degrees of freedom for $\mathbf{u}^h$, p^h and $\omega_{(\alpha)}{}^h$, respectively, $\mathbf{a}$ is the vector of degrees of freedom for the transient term $\partial\mathbf{u}^h/\partial t$, $\dot{\boldsymbol{\omega}}_{(\alpha)}$ is the vector of degrees of freedom for the transient term $\partial\omega_{(\alpha)}{}^h/\partial t$. The matrices [**M**], [**K**], [**G**] arise from the transient, viscous and pressure terms, respectively, and [$\bar{\mathbf{M}}$], [$\bar{\mathbf{K}}$] arise from the transient and diffusive terms. **N**(**u**) and $\bar{\mathbf{N}}(\mathbf{u})$ arise from the advective transport terms. The matrices on the right-hand-side are the font terms, and all the other matrices correspond to the stabilized terms. The time integration algorithm is based on Hughes et al. (1979), and is a predictor/corrector scheme for the pressure-velocity problem.

4. Numerical results

In this section, some numerical results for the finite element approximation (Eq. (42)) for Eqs. (33) are presented. The analyzed problem is the axial injection of a fluid (species 1) into another (species 2) flowing over a backward facing step. The bulk properties were considered constant, the constitutive equations for a Carreau fluid were employed, and the mass diffusion was assumed to be governed by Fick's Law with a constant mass diffusion coefficient. The pertinent boundary conditions are non slippery walls, constant mass fraction for species 1 equals to 1.0 in the entrance region, free traction and freestream mass flux for species 1 at the outflow boundary. The problem is transient, as it is supposed that in the instant t_0, pure component 1 is injected over component 2. The geometry is showed on Fig. (1). The Reynolds number, calculated using bulk properties and characteristic length D=H-h=0.5m, was equal to 100.

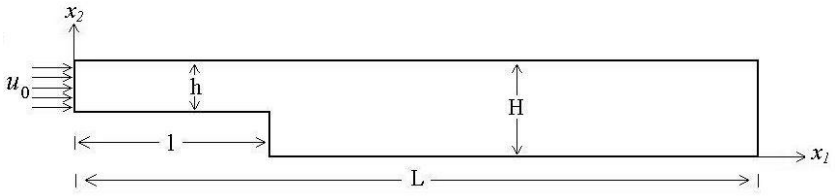

Figure 1: Problem statement

Three orders of magnitude for mass Peclet number were tested: Pe_m=0.5E+02, Pe_m=0.5E+03, Pe_m=0.5E+04. The mean velocity in the entrance of the channel u_0 was set to 1m/s. The finite element mesh consisted of 4600 Q1/Q1 elements. For Pe_m=0.5E+04, the maximum mesh mass Peclet number occurs in the regions of maximum velocity (**u**=1.5u_0), in the center of the channel, as follows:

$$\mathrm{Pe}_K^m=\frac{\left|\mathbf{u}\right|_p h}{2D_{12}}\approx 2.12\mathrm{E}+02 \tag{52}$$

The time evolution is showed based on the non-dimensional time parameter t*,

$$t^* = \frac{tu_0}{(H-h)} \tag{53}$$

The following pictures show the mass fraction evolution over the flat channel. Figure (2) depicts time evolution for Pe_m=0.5E+02 (diffusive case) and Fig. (3) shows the results for Pe_m=0.5E+04 (advective dominated case).

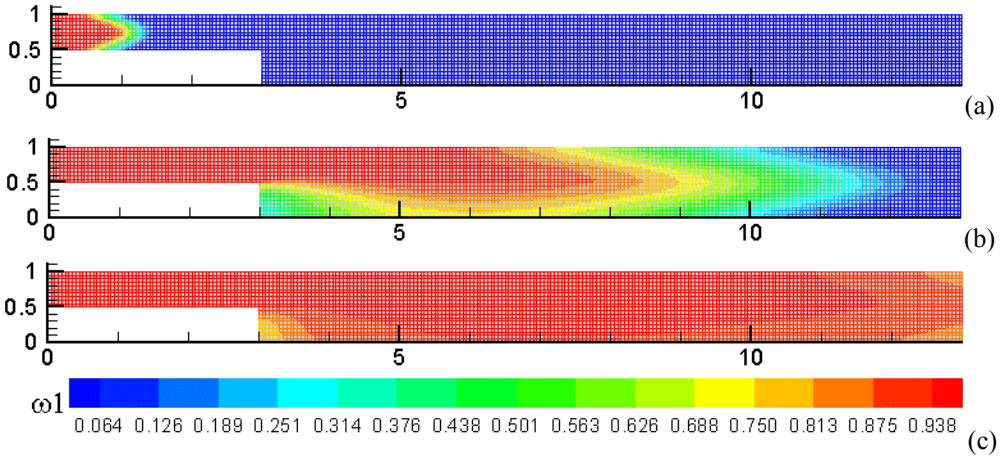

Figure 2: Results for Pe_m=0.5E+02. Time steps: (a) t^*=2, (b) t^*=30, (c) t^*=60.

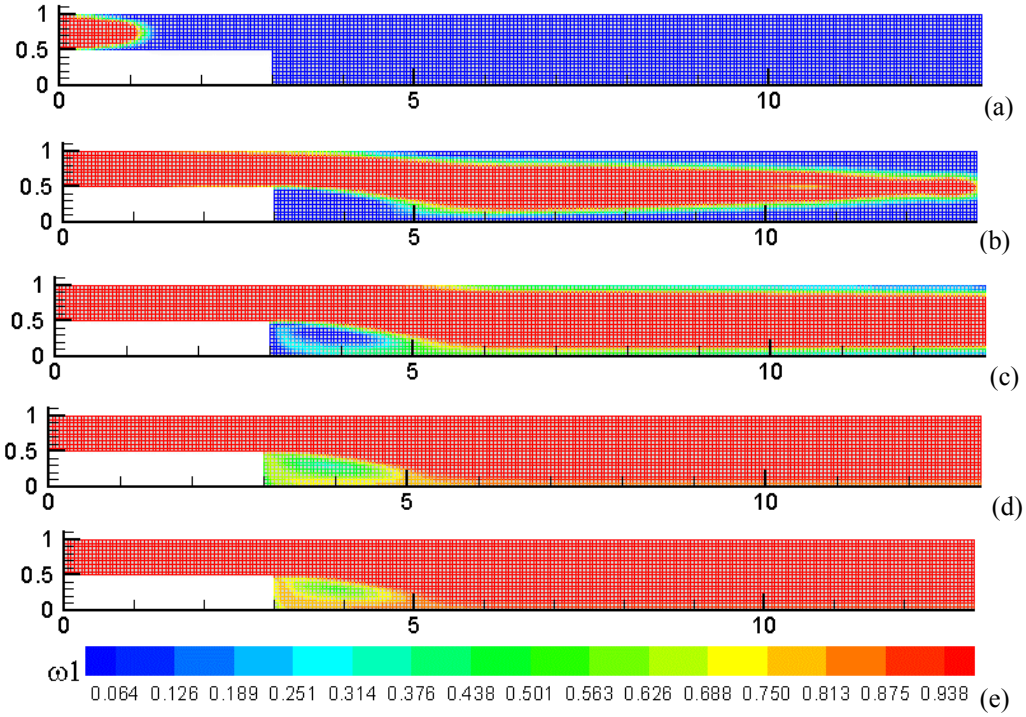

Figure 3: Result for Pe_m=0.5E+04. Time steps: (a) t^*=2, (b) t^*=60, (c) t^*=150, (d) t^*=290, (e) t^*=420.

The figures show the feature of the GLS method to stabilize advective dominated problems. The mixture length is shorter for the diffusive case Pe_m=0.5E+02 with component 2 not retained in the recirculation zone and in the momentum boundary layer. In the case Pe_m=0.5E+04, a longer period of time was necessary to homogenize the mixture. Because of the low diffusive character of the mixture, component 2 is retained in the region of recirculation and in the momentum boundary layer, forming a mass boundary layer in the channel. Real liquid mixtures usually present very low diffusive characteristics (Geankoplis, 1995) tending to behave more like the flow illustrated in Fig. (3).

5. Final remarks

This article presented the mechanical modeling for multicomponent incompressible flows, which was developed based in the conservation laws of continuum mechanics. The modeling is based on the assumption that a

multicomponent system behaves as a superposition of *N* continuous single-component bodies. The resulting boundary value problem was approximated by the GLS finite element method.

Numerical results concerning a problem of axial injection were analyzed. Three orders of magnitude for mass Peclet number were tested, from Pe_m=0.5E+02 to Pe_m=0.5E+04. The GLS method showed good stability properties. The mixture length was shorter for the diffusive case. In the advective case, a species was retained in regions of recirculation and momentum boundary layer, forming a mass boundary layer, which prevented total homogenization. This case represents more closely the real behavior of mixture flows of liquids, where mass diffusivities are usually very low.

As this work is still in progress, some other characteristics of multicomponent flows shall be approached. Among them, there are the use of more general constitutive assumptions for the diffusing mixture, and the study of the flow behavior with variable physical properties.

6. Acknowledgement

The authors F. Franceschini and S. Frey gratefully acknowledge the financial support provided by the agencies CAPES and CNPq (grant 350747/93-8), respectively.

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