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Two-dimensional mathematical model of the dynamic for the fluid and gases ( $CO_2$  and  $O_2$ ) concentrations in the pulmonary alveolar sacs

Modelo matemático de la dinámica bidimensional del flujo y concentraciones de gases  $(O_2 \ y \ CO_2)$  en los sacos alveolares pulmonares

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### Resumen

En este artículo simulamos la dinámica del transporte de  $CO_2$  en los sacos alveolares pulmonares. Usando el método Euleriano-Lagrangiano Arbitrario, se pudo controlar el movimiento del dominio para una respiración normal y forzada. El fluido de gas de ambiente inhalado y las concentraciones de  $CO_2$  fueron aproximadas por las ecuaciones de Navier-stokes y la ecuación de convección difusión, el stress paras diferentes maniobras fueron calculadas en tiempos iguales. La expansión para la maniobra normal y forzadas fueron representadas como el 9 y 90 % de la geometría inicial. Las diferencias de la cantidad de  $CO_2$  fue  $73x10^{-3}$  ml entre la respiración normal y forzada. El stress en la pared del saco alveolar cambió siguiendo el patrón del flujo inhalado a diferencia del stress para una maniobra forzada. Concluimos, que la cantidad de  $CO_2$  en el saco alveolar, depende del número de capilares en saco alveolar, además no se ve afectada por las maniobras forzadas.

Palabras clave. Dinámica del gas Alveolar, Arbitrary Lagrangian-Eulerian, Navier-Stokes equation.

## Abstract

We simulated the dynamics of  $CO_2$  transport in the alveolar sacs of the human lung. Using Arbitrary Lagrangian Eulerian (ALE) framework, we control the movement domain for a normal and fast maneuver. The fluid of room air inspired and  $CO_2$  concentrations were approximated by Navier-Stokes and convection diffusion equations; the stress-stretch in the wall for different volumes were quantified in equal time of respiration. The expansion for a normal and forced maneuver were represented as 9 and 90% to the initial geometry. The difference of the  $CO_2$  was  $73x10^{-3}$  ml between a normal and forced maneuver; the stress in the wall changed following the sinusoidal pattern as a flow in the normal inspiration. In conclusion, the amount of  $CO_2$  in the alveolar sacs, depends upon the number of capillaries in the wall and it is not affected by the expiratory fast maneuver.

Keywords. Alveolar gas dynamic, Arbitrary Lagrangian-Eulerian, Navier-Stokes equation.

1. Introduction. Caucha et al. (2010) [1] showed that the alveolar dilution of  $CO_2$  becomes more evident with the forced expiration and reveals the effect of  $CO_2$  diffusion from Residual Volume (RV) to Expiratory Reserve Volume (ERV) in the expired forced maneuver. We are interested in simulate the changes of  $CO_2$  concentration in the alveolar sacs, when it is filling with room air in a respiration.

The dynamic of the gas in the human lung was studied using one-dimensional mathematical model [2], this model used a geometry like a trumpet proposed by Weibel [3], with 23 bifurcations (generations) of the bronchial tree, starting from trachea (0<sup>th</sup>) to terminal bronchioles (23<sup>rd</sup>); this model was followed by Engel and Paiva [4, 5] considering the ideal gas condition in the alveolar zone, such as instantaneous homogeneity for the gas concentration in each respiration [6, 7]. After that, Swan et al. [8], and Federspiel et al. [9], analyzed the dispersion in the alveolar ducts, using the Navier-Stokes equation and convection-diffusion equation for the gas transport, those researches were made in the rigid domain, but the geometry of sacs move according to inspiration or expiration process.

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In this article, we made an analysis of the gas exchange and transport in the alveolar sac for a moving domain when it is submmited to Stress and stretch as a consequence of forced respiratory maneuver. The principal assumptions considered for this analysis were that sac has smooth alveolar deformation. As the geometry of the sac is small, we had especially cared to define the behavior in the boundary by the irregularity in the gas exchange and oscillation in the boundary. The fluid flow and CO<sub>2</sub> concentration in the alveolar sac is governed by the Navier-Stoke equation and transport equation on the moving domain, and transformed to the Arbitrary Lagrangian-Eulerian coordinate [10, 11].

The article was structured by: in the section 2, we showed the equations for the fluid and gas transport, with their initial and boundary conditions. In section 3, we present the weak system equations in Arbitrary Lagrangian-Eulerian coordinates. In sections 4 we made the estimates in order to show the convergence of weak solution of the system; and 5, we present the numeric simulation and conclusion in the section 6.

**2. Mathematical Model.** The respiration consist in two process, inhalation and exhalation. The subject inhaled a mix of gases, could be room air or different mix as in Flores and Cruz (1999) [12], Sikand(1962) [13] and Milic-Emili(1966) [14], but always there are the fluid flow and gas tracer (gas of interest). For describing this dynamic we consider an equations system for the fluid flow (inhaled and exhaled process) and the gas transport equation for gas tracer (gas of interest), such as carbon dioxide (CO<sub>2</sub>) in this study.

The fluids considered for this analysis have a partial pressure outside (room air) and inside of the lung is practically constant (for example the Nitrogen), and moreover the temperature in the lung is constant. We simulated as an incompressible fluid as

(2.1) 
$$\begin{cases} \rho \partial_t u + \rho(u \cdot \nabla)u - div\sigma = 0 &, en \Omega(t), \\ div(u) = 0 &, en \Omega(t), \\ u = V^{dom} &, en \Gamma_{bl} \cup \Gamma_w, \\ \sigma \eta = 0 &, en \Gamma_{io}, \end{cases}$$

where:  $\Omega(t)$  is the domain representing the alveolar sac geometry, this domain changes as a function of time,  $V^{dom}$  (velocity of moving domain).

The boundary has three different parts such that:  $\Gamma_{bl}$  is the part for gas exchange between alveolar gas and the blood flow;  $\Gamma_w$  is the wall there is not exchange and  $\Gamma_{io}$  is the boundary where the inflow and outflow take place as a consequence of inhalation and exhalation.

For the incompressible fluid, the Cauchy tensor was

(2.2) 
$$\sigma = \rho \nu \nabla u - pI;$$

This is used in the system 2.1, where  $\rho$  is the fluid density, u velocity and p pressure.

In the model, we considered outside of the alveolar sac as approximate value Caucha et al. [15] and the boundary  $\Gamma_{io}$  such that do-nothing condition [16]. We considered the *inflow* and *outflow* velocity is known for  $\Gamma_{io}$  (by experiment), such that the moving domain was considered as a variable.

**2.1. Transport equation.** For the CO<sub>2</sub> transport, we have the convection-diffusion equation, such as:

(2.3) 
$$\begin{cases} \partial_t C + u \cdot \nabla C - D\Delta C = 0 &, en \Omega(t) \\ \partial_{\eta} C - \alpha_b (C_b - C) = 0 &, en \Gamma_{bl} \\ \partial_{\eta} C = 0 &, en \Gamma_w. \end{cases}$$

In the boundary  $\Gamma_{io}$ , we have the conditions for inflow and outflow

$$\begin{cases} C = C_{\rm ext} &, \ si \ v \cdot \eta < 0 \\ \partial_{\eta} C = 0 &, \ si \ v \cdot \eta > 0 \end{cases} en \Gamma_{io},$$

where, C is the gas concentration in the alveolar sac,  $C_{ext}$  initial condition in the boundary  $\Gamma_{io}$ ,  $C_b$  gas concentration in the pulmonary blood flow and u fluid velocity,  $\alpha_b$  constant of the gas solubility in the blood.

The Dirichlet condition, we include weakly in the variation formulation using Nitsche's method [17] such that

(2.5) 
$$\partial_{\eta} C - \gamma h^{-2} \mathcal{H}(v \cdot \eta) (C_{\text{ext}} - C) = 0, \ en \ \Gamma_{io},$$

where  $\gamma$  is a parameter (dimensionless), moreover  $h \to 0$  and  $\mathcal{H}$  is the unit step function defined as:

(2.6) 
$$\mathcal{H}(x) = \begin{cases} 1 & , x > 0 \\ 0 & , x \le 0. \end{cases}$$

The initial condition for the velocity and concentration were  $u(.,0) = v_o$ , and  $C(.,0) = C_o$ .

3. Model in ALE coordinates. Considering  $\Omega(t)$  as the domain that represent the Eulerian movement of the fluid as a consequence of inflation and deflation of the alveolar sac by the respiratory cycle, and  $\hat{\Omega}_o$  the reference system that represent the rest (Functional residual capacity or residual volume of the lung).

To Control the moving domain, we add an arbitrary fixed domain  $\hat{W}$ , and could take  $\hat{W} = \hat{\Omega}_o$  without considering some physical meaning. As  $\hat{W}$  is fixed in the time, there is exist an invertible map  $\hat{T}_w(t) \colon \hat{W} \to \Omega(t)$  with gradient  $\hat{F}_w := \nabla \hat{T}_w$  and Jacobian  $\hat{J}_w = \det(\hat{F}_w)$ , which  $F_w$  and  $J_w$  have the properties of deformation of Lagrangian gradient , the Lagrangian particle  $\hat{x} \in \hat{\Omega}_0$ , the Eulerian path  $x(\hat{x},t) \in \Omega(t)$  and  $\hat{x}_w \in \hat{W}$  with  $\hat{T}_w(\hat{x}_w,t) = x = \hat{T}(\hat{x},t)$ ; we must consider the difference between the velocity  $\partial_t \hat{T}_w$  (velocity of movement of the reference system) and the physic velocity  $\hat{V}$  [18, 19, 20].

The weak form of Equation system 2.1 and 2.3 are transformed to ALE coordinate [18], such that the variables of interest are  $\hat{v}$ ,  $\hat{p}$  and  $\hat{C}$ .

The weak form of the problem in ALE coordinates is giving by : Find  $\hat{v} \in \hat{\mathcal{V}}(\hat{\Omega})$ ,  $\hat{p} \in \hat{\mathcal{L}}(\hat{\Omega})$  and  $\hat{C} \in \mathcal{H}$  such that

$$\begin{cases} \rho(\hat{J}(\partial_t \hat{v} + \hat{F}^{-1}(\hat{v} - \partial_t \hat{T}) \cdot \hat{\nabla})\hat{v}, \hat{\phi})_{\hat{\Omega}} + (\hat{J}\hat{\sigma}\hat{F}^{-T}, \hat{\nabla}\hat{\phi})_{\hat{\Omega}} &= 0, \ \forall \hat{\phi} \in \hat{\mathcal{V}} \\ (\hat{\operatorname{div}}(\hat{J}\hat{F}^{-1}\hat{v}), \hat{\xi})_{\hat{\Omega}} &= 0, \ \forall \hat{\xi} \in \hat{\mathcal{L}} \\ (\hat{J}(\partial_t \hat{C} + (\hat{F}^{-1}(\hat{v} - \partial_t \hat{T}) \cdot \hat{\nabla})\hat{C}), \hat{\psi}) + (D\hat{J}\hat{F}^{-T}\hat{\nabla}\hat{C}, \hat{\nabla}\hat{\psi}) - (\alpha(c_b - \hat{C}), \hat{\psi})_{\hat{\Gamma}_{bl}} \\ + (\gamma h^{-2}\mathcal{H}(\hat{v} \cdot \eta)(c_{ext} - \hat{C}), \hat{\psi})_{\Gamma_{to}} &= 0, \ \forall \hat{\psi} \in \hat{\mathcal{X}}, \end{cases}$$

where the domain  $\hat{\Omega}$  is fixed and the test spaces are defined as

$$\hat{\mathcal{V}}_{\hat{\Omega}} := \left(\overline{C_0^{\infty}(\hat{\Omega}, \partial \hat{\Omega} \setminus_{\hat{\Gamma}_{bl} \cup \hat{\Gamma}_{w}})}^{\|\cdot\|_{H_0^1}}\right)^2, \quad \hat{\mathcal{L}}_{\hat{\Omega}} = \overline{C_0^{\infty}(\hat{\Omega})}^{\|\cdot\|_{L^2}}, \quad \hat{\mathcal{X}} = \overline{C_0^{\infty}(\hat{\Omega})}^{\|\cdot\|_{H^1}}.$$

where  $\|.\|_{H_0^1}$ ,  $\|.\|_{L^2}$  and  $\|.\|_{H^1}$  are the norm in the usual Sobolev,  $L^2$  and Hilbert Space, respectively. The Cauchy tensor in the reference domain is

$$\hat{\sigma} := -\hat{P}I + \rho\nu(\hat{\nabla}\hat{v}\hat{F}^{-1}).$$

- **4. Estimates for the weak solution of the fluid velocity and gas concentrations.** For this section we following the classical idea to prove the existence and uniqueness of weak solution for the Navier-Stokes equations described by Temam [21] but in ALE coordinates.
- **4.1. Estimates for the fluid velocity**  $\hat{u}$ **.** Taking a Navier-Stokes equations in ALE coordinates (3.1), we have the following definition.

DEFINITION 1. We say that  $\hat{u}$  is a weak solution of the system (3.1), if satisfy the following formulation

$$\rho(\hat{J}(\partial_t \hat{u} + (\hat{F}^{-1}(\hat{u} - \partial_t \hat{T}) \cdot \hat{\nabla})\hat{u}, \hat{\phi})_{\hat{L}^2(\hat{\Omega})} + (\hat{J}\rho\nu(\hat{\nabla}\hat{u}\hat{F}^{-1}), \hat{\nabla}\hat{\phi})_{\hat{L}^2(\hat{\Omega})} = 0, \quad \forall \hat{\phi} \in \hat{\mathcal{V}}$$

in sense of distribution in (0,T); such that

$$\int_0^T \rho(\hat{J}(\partial_t \hat{u} + (\hat{F}^{-1}(\hat{u} - \partial_t \hat{T}) \cdot \hat{\nabla})\hat{u}, \hat{\phi})_{\hat{\mathcal{L}}^2(\hat{\Omega})} \psi \, dt + \int_0^T (\hat{J}\rho\nu(\hat{\nabla}\hat{u}\hat{F}^{-1}), \hat{\nabla}\hat{\phi})_{\hat{\mathcal{L}}^2(\hat{\Omega})} \psi \, dt = 0, \qquad \forall \, \psi \in C_0^\infty(0, T; \mathbb{R}).$$

Utilizing the condition of the function of free divergence [22], the ALE system (3.1) is equivalent to

$$\rho(\hat{J}(\partial_t \hat{u} + (\hat{F}^{-1}(\hat{u} - \partial_t \hat{T}) \cdot \hat{\nabla})\hat{u}, \hat{\phi}) + (\hat{J}\rho\nu(\hat{\nabla}\hat{u}\hat{F}^{-1}), \hat{\nabla}\hat{\phi}) = 0, \quad \forall \hat{\phi} \in \hat{\mathcal{V}}.$$

As  $\mathcal{H}^1_0(\hat{\Omega}) \hookrightarrow \hat{\mathcal{L}}^2(\hat{\Omega})$  is dense and continuous, we considered a base of  $\hat{\mathcal{L}}^2(\hat{\Omega})$  formed by elements of  $\mathcal{H}^1_0(\hat{\Omega})$  and use the Galerkin's method, such that, we take

$$\hat{u}_m = \sum_{j=1}^m \alpha_j(t)\hat{w}_j$$

as lineal combination of elements  $\hat{w}_j \in H^1_0$ , where  $\alpha_j(t)$  are the scalar function and depend of the time t. For  $m \geq 1$ , replacing  $\hat{u}$  in the equation (4.1) by  $\hat{u}_m$ , we have a system of ordinary differential equations, that applying Peano's theorem [23], exist  $T = T_m$  and an unique solution in  $[0, T_m]$ ; this show a local existence of solution of Galerkin's approximation.

**4.1.1.** Energy equation. In this section, we show the convergence of the weak solution and the terms that control the energy dissipation for the fluid.

Considering  $\phi_m = \hat{u}_m$  and replacing in the equation (4.1), we have

(4.3) 
$$\rho(\hat{J}(\partial_t \hat{u}_m + (\hat{F}^{-1}(\hat{u}_m - \partial_t \hat{T}) \cdot \hat{\nabla})\hat{u}_m), \hat{u}_m) + (\hat{J}\rho\nu(\hat{\nabla}\hat{u}_m \hat{F}^{-1}), \hat{\nabla}\hat{u}_m) = 0.$$

This equation calling *energy equation* gives a priori estimates, showing a candidate to be a weak solution. The next lemma shows the convergence of the weak solution

LEMMA 1. Given the energy equation (4.3) then we have the convergence for the Galerkin's approximation

$$\hat{u}_m \stackrel{*}{\rightharpoonup} \hat{u} \text{ in } \hat{\mathcal{L}}^{\infty}(0, T; \hat{\mathcal{L}}^2(\hat{\Omega})),$$

(4.5) 
$$\hat{u}_m \rightharpoonup \hat{u} \text{ in } \hat{\mathcal{L}}^2(0, T; H_0^1(\hat{\Omega})).$$

Proof Skipping technical steps here, we have the inequality for the energy equation, such as

$$\partial_t \|\hat{u}_m\|_{\hat{\mathcal{L}}^2(\hat{\Omega})}^2 + (2\lambda\nu \|\hat{F}^{-1}\|_{L^\infty} + \|\hat{F}^{-1}\|_{L^\infty} \|\mathrm{div}(\partial_t \hat{T})\|_{\hat{\mathcal{L}}^\infty(\hat{\Omega})} \big) \|\hat{u}_m\|_{\hat{\mathcal{L}}^2(\hat{\Omega})}^2 \leq 0,$$

applying the Grönwall's lemma, we have that

From (4.6) follow the Galerkin approximation  $\hat{u}_m$  exist globally in the time; that is  $T_m = \infty$ . Additionally, we observe that the dissipation of the initial energy is a function of the viscosity and domain deformation. Furthermore, we have that

(4.7) 
$$\{u_m\}$$
 is bounded in  $\hat{\mathcal{L}}^{\infty}(0,T;\hat{\mathcal{L}}^2(\hat{\Omega}))$ .

Integrating from 0 to T the equation (4.6), we have

(4.8) 
$$\int_0^T |\hat{\nabla} \hat{u}_m|_{\hat{\mathcal{L}}^2(\hat{\Omega})}^2 ds \le \frac{1}{2\nu \|\hat{F}^{-1}\|_{L^{\infty}}} \|\hat{u}_m(0)\|_{\hat{\mathcal{L}}^2(\hat{\Omega})}^2$$

and we have that

(4.9) 
$$\{\hat{u}_m\} \text{ is bounded in } \hat{\mathcal{L}}^2(0,T;H_0^1(\hat{\Omega})),$$

Now, from (4.7), (4.9) and diagonalization argument, exist  $\hat{u}$ , such that  $\hat{u}_m \stackrel{*}{\rightharpoonup} \hat{u}$  in  $\hat{\mathcal{L}}^\infty(0,T;\hat{\mathcal{L}}^2(\hat{\Omega}))$  and  $\hat{u}_m \rightharpoonup u$  in  $\hat{\mathcal{L}}^2(0,T;\mathcal{H}^1_0(\hat{\Omega}))$ , respectively. As a consequence of nonlinearity, the weak convergences are not sufficient to take the limit to the approximate formulation. Then, we need a strong convergence of  $\{\hat{u}_m\}$ ; for this process, we used the Fréchet-Kolmogorov theorem [24], and conclude that  $\{\hat{u}_m\}$  is pre-compact in  $\hat{\mathcal{L}}^2(0,T;\hat{\mathcal{L}}^2(\hat{\Omega}))$ , as a consequence there is a subsequence  $\hat{u}_{mk} \to \hat{u}$  in  $\hat{\mathcal{L}}^2(0,T;\hat{\mathcal{L}}^2(\hat{\Omega}))$  strongly. We can propose the theorem of existence for the weak solution of the fluid equation in ALE coordinates.

THEOREM 2. Given the system (3.1) that describe the conservation and mass for the fluid, then, exist a weak solution, in sense of (1), in the spaces

$$\hat{u} \in \hat{\mathcal{L}}^{\infty}(0,T;\hat{\mathcal{L}}^2(\hat{\Omega})) \cap \hat{\mathcal{L}}^2(0,T;\mathcal{H}_0^1(\hat{\Omega})) \cap \hat{\mathcal{L}}^2(0,T;\hat{\mathcal{L}}^2(\hat{\Omega})).$$

Proof Now, we pass to limit to the weak form (4.3), for that, taking  $\hat{w} = \hat{w}_j$  where  $\hat{w}_j \in Span\{\hat{w}_1, \hat{w}_2, \cdots, \hat{w}_m\}$  and multiplying the equation by  $\phi \in \mathcal{C}_0^{\infty}(0,T)$  and integrating from 0 to T. And utilizing the Stokes's theorem [23], we have that

$$(4.10) \quad -\frac{1}{2} \int_0^T (\hat{u}_m, \hat{w}_j) \frac{d\phi}{dt} dt + \nu \int_0^T (\hat{\nabla} \hat{u}_m \hat{F}^{-1}, \hat{\nabla} \hat{w}_j) \phi dt + int_0^T ((\hat{F}^{-1} (\hat{u}_m - \partial_t \hat{T}) \cdot \hat{\nabla}) \hat{u}_m, \hat{w}_j) \phi dt = 0$$

then, using the lemmas (1), and strong convergence, we have that  $\{\hat{u}_m\}$  converge in time to  $\hat{u}$  defined in the theorem (2).

**4.1.2.** Uniqueness for the velocity. Given  $\hat{u}_1, \hat{u}_2$  weak solutions of the equation (4.1), then we define  $\hat{w} = \hat{u}_1 - \hat{u}_2 \in \hat{\mathcal{V}}(\hat{\Omega})$ . Then,  $\hat{w}$  is a weak solution and using the equation (4.6), we have that  $\hat{u}_1 = \hat{u}_2$  for  $t \to \infty$ .

**4.2. Estimates for the weak solution of the gas concentrations.** For the system (3.1), we made an analysis in the same way that analysis of fluid velocity, considering the result given by theorem 2.

DEFINITION 2. We say that  $\hat{C}$  is a weak solution for the system (3.1) if it satisfy the next weak formulation

$$(\hat{J}(\partial_t \hat{C} + (\hat{F}^{-1}(\hat{v} - \partial_t T) \cdot \hat{\nabla})C), \hat{\psi}) + (D\hat{J}\hat{F}^{-T}\hat{\nabla}\hat{C}, \hat{\nabla}\hat{\psi}) - (\alpha(c_b - \hat{C}), \hat{\psi})_{\Gamma_{bl}} + (\rho h^{-2}\mathcal{H}(v \cdot \eta)(C_{ext} - \hat{C}), \hat{\psi}) = 0, \quad \forall \hat{\psi} \in \hat{\mathcal{X}},$$

in the sense of distribution in (0,T), such that

$$\int_0^T (\hat{J}(\partial_t \hat{C} + (\hat{F}^{-1}(\hat{v} - \partial_t T) \cdot \hat{\nabla})C), \hat{\psi})\phi \, dt + \int_0^T (D\hat{J}\hat{F}^{-T}\hat{\nabla}\hat{C}, \hat{\nabla}\hat{\psi})\phi \, dt - \int_0^T (\alpha(c_b - \hat{C}), \hat{\psi})_{\Gamma_{bl}}\phi \, dt + \int_0^T (\rho h^{-2}\mathcal{H}(v \cdot \eta)(C_{ext} - \hat{C}), \hat{\psi})\phi \, dt = 0, \quad \forall \, \phi \in C_0^{\infty}(0, T; \mathbb{R}).$$

From the equation in the ALE coordinates, we have

$$\hat{J}(\hat{J}(\hat{\partial}_t \hat{C} + (\hat{F}^{-1}(\hat{v} - \partial_t T) \cdot \hat{\nabla})C), \hat{\psi}) + (D\hat{J}\hat{F}^{-T}\hat{\nabla}\hat{C}, \hat{\nabla}\hat{\psi}) - (\alpha(c_b - \hat{C}), \hat{\psi})_{\Gamma_{bl}} + (\rho h^{-2}\mathcal{H}(v \cdot \eta)(C_{ext} - \hat{C}), \hat{\psi}) = 0;$$

given the Faedo-Galerkin's approximation

(4.12) 
$$\hat{C}_m = \sum_{j=1}^m \alpha_j(t)\hat{w}_j, \quad \hat{C}_m \in \mathcal{X}_m$$

for the equation (4.11) with spaces  $V_m = span\{\hat{w}_1, \hat{w}_2, \cdots, \hat{w}_m\}$ ,  $\hat{w}_i \in \mathcal{H}^1(\hat{\Omega})$  and  $\mathcal{X}_m \subset \hat{\mathcal{L}}^2$ , and  $\alpha_j(t)$  scalar functions depending on the time.

Evaluating (4.12) in the elements of the base  $\hat{w}_k$ , we have a system of ordinary differential equation in t; then with Peano's theorem [23], exist  $T = T_m$  and an unique solution [0, T].

**4.2.1.** Energy equation for the gas concentration. Using the approximation  $\hat{C}_m$ , we have

(4.13) 
$$\hat{J}(\partial_{t}\hat{C}_{m}, \hat{C}_{m}) + (D\hat{J}\hat{F}^{-T}\hat{\nabla}\hat{C}_{m}, \hat{\nabla}\hat{C}_{m}) + \hat{J}(\hat{F}^{-1}(\hat{v} - \partial_{t}\hat{T}) \cdot \hat{\nabla})\hat{C}_{m}, \hat{C}_{m}) - \langle \alpha_{b}(c_{b} - \hat{C}_{m}), \hat{C}_{m}\rangle_{\mathcal{H}^{-1/2}(\Gamma_{b,t})} + \langle \gamma h^{-2}\mathcal{H}(C_{ext} - \hat{C}_{m}), \hat{C}_{m}\rangle_{\mathcal{H}^{-1/2}(\Gamma_{b,t})} = 0;$$

with this equation, we be able to make the estimates; those give us a weak solution defined in (2).

The lemma gives us the spaces of convergence for the weak solution for the gas concentration

LEMMA 3. From the equation (4.13), we have the next convergences for the Faedo-Galerkin's approximation

$$\hat{C}_m \stackrel{*}{\rightharpoonup} \hat{C} \quad \text{in } \hat{\mathcal{L}}^{\infty}(0, T; \hat{\mathcal{L}}^2(\hat{\Omega})),$$

$$\hat{C}_m \stackrel{}{\rightharpoonup} \hat{C} \quad \text{in } \hat{\mathcal{L}}^2(0, T; \mathcal{H}^1(\hat{\Omega})).$$

Proof We skip the technical details and show the principal results.

Defining the terms  $a: = (|D|\hat{J}||\hat{F}^{-T}||_{\hat{L}^{\infty}} - (\alpha_b + |\gamma h^{-2}\mathcal{H}|))$ 

and 
$$b \colon = \left(C(\alpha_b, c_b) + |\gamma h^{-2} \mathcal{H} c_{ext}|\right), \theta = \left(-\lambda \frac{a}{\hat{j}} + \|\hat{F}^{-1}\|_{\hat{\mathcal{L}}^{\infty}} \|\operatorname{div}(\partial_t \hat{T})\|_{\hat{\mathcal{L}}^{\infty}}\right)$$
 and  $\hbar = \frac{b^2}{\hat{\jmath}a}$ , we have

$$\partial_t \|\hat{C}_m\|^2 + \theta \|\hat{C}_m\|_{\hat{\mathcal{L}}^2}^2 \le \hbar;$$

using the Grönwall's inequality [21], we have

$$\|\hat{C}_m\|_{\hat{\mathcal{L}}^2}^2 \le (\|\hat{C}_m(0) + \frac{\hbar}{\theta}\|) exp(-\theta t).$$

We see that  $\hat{C}_m$  is uniform limited in  $\hat{\mathcal{L}}^{\infty}(0,T;\hat{\mathcal{L}}^2(\hat{\Omega}))$ , as it is not depend of m and t, then we say that

$$(4.14) \qquad \qquad \hat{C}_m \stackrel{*}{\rightharpoonup} \hat{C} \quad \text{in } \hat{\mathcal{L}}^{\infty}(0, T; \hat{\mathcal{L}}^2(\hat{\Omega})).$$

Now, integrating the inequality from 0 to T, we have

$$\int_0^T \|\hat{\nabla} \hat{C}_m\|_{\hat{\mathcal{L}}^2}^2 dt \le \frac{2}{|\lambda a|} \left[ \hat{J} \|\hat{C}_m(0)\|_{\hat{\mathcal{L}}^2}^2 + \frac{b^2}{2a} T \right]$$

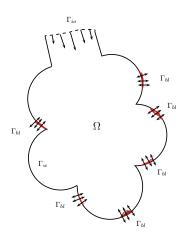


FIGURA 5.1. Geometry of alveolar Sac

then,  $\hat{C}_m$  is limited in  $\hat{\mathcal{L}}^2(0,T;\mathcal{H}^1(\hat{\Omega}))$  , for each T, then

$$(4.15) \qquad \qquad \hat{C}_m \rightharpoonup \hat{C} \text{ in } \hat{\mathcal{L}}^2(0,T;\mathcal{H}^1(\hat{\Omega})).$$

Using the Fréchet-Kolmogorov theorem [24], we have that  $\hat{C}_m$  is pre-compact in  $\hat{\mathcal{L}}^2(0,T;\hat{\mathcal{L}}^2(\hat{\Omega}))$ . Now, we have the theorem for the existence of the concentrations.

THEOREM 4. Given the system (3.1) in which we have the gas transport equation, then exist and a weak solution defined by (2) in the spaces:

$$\hat{C} \in \hat{\mathcal{L}}^{\infty}(0,T;\hat{\mathcal{L}}^2(\hat{\Omega})) \cap \hat{\mathcal{L}}^2(0,T;\mathcal{H}^1(\hat{\Omega})) \cap \hat{\mathcal{L}}^2(0,T;\hat{\mathcal{L}}^2(\hat{\Omega})).$$

- **5. Simulation.** Considering the differences from the apex and base of the lung (see Millic-Emili [14]), we are interesting in simulated the dynamic in the base of the lung, because is the place that has more ventilation and perfusion in a normal breath [1].
- **5.1. Parameters for simulations.** We studied alveolar sacs in the base region for two different generations in the Weibel's generations [3] of the lung. We considered the density constant for all generation  $\rho = 1.21x10^{-6}gr/mm^3$  [25],

Generation	kinematic viscosity	Reynolds number
19	3.0813	0.08
23	85.88	$7x10^{-3}$

Those values were taken from Sznitman [26].

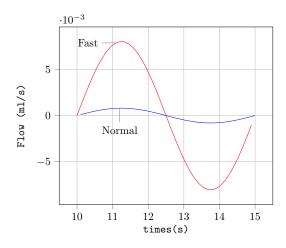
Using Finite Element Method, we have the results for a normal and fast maneuvers. The parameters for finite element methods were : Number of iterations 50 for each global refine, 5 global refine and step of time  $\delta t=0,1$ ; also the extreme deformation was  $\gamma=0,9$  and, the tolerance for linear system and nonlinear system was 1.e-8; those approximations were made using Gascoing3D [27].

The initial  $CO_2$  concentration in the alveolar sac was considered constant 0.04302 [1]. We have considered the alveolar sac deformation as a sinusoidal function.

## **5.1.1. Numerical results.** The figure 5.1, shows the alveolar sac with five sources of $CO_2$ gas.

The figure (5.2) shows the two different flow in the alveolar sac when the wall  $\partial\Omega$  is moving, for a normal and forced maneuver. This movement makes that the pressure changed and as a consequence permit that the gas flow enter.

The distribution for inflow in the alveolar sac for the fast maneuver is showed in figure (5.3), in the left side shows the flow in the middle of time for inspiration and the figure of right side shows the maximal inflations for the alveolar sac.



 $FIGURA\ 5.2.\ Gas\ flow\ simulation\ for\ a\ normal\ and\ forced\ maneuver$ 

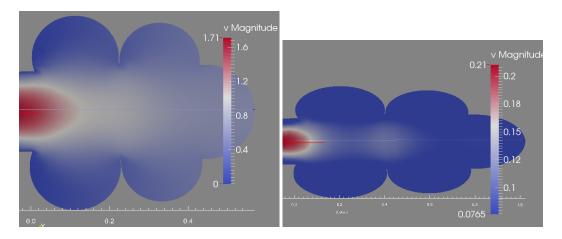


FIGURA 5.3. Inflow in the alveolar  $Sac\ 2D$ 

Those curves in the figure (5.4) were taken in line straight down the middle in the alveolar sac, showing the fluid velocity in the alveolar sac.

The figure (5.5) show the gas transportation from the blood to the alveolar sac, in the right side we can see the

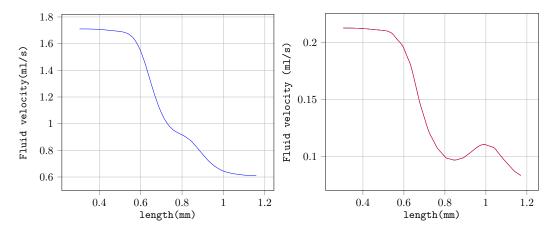


FIGURA 5.4. Inflow in the alveolar sac

dilution of carbon dioxide as a consequence of the gas inhaled.

Making the curve in line straight down the middle in the alveolar sac for the CO2 concentration, we can see the carbon dioxide stratification. That curve changes depending of the maneuver like in the figure on right side (see figure (5.6)). Those values increase as a consequence of the gas exchange with blood  $CO_2$  concentration from 0.065;

The oscillation for the stress in the wall  $\partial\Omega$  of the alveolar sac is showed in figure ( ??fig:6)). When the

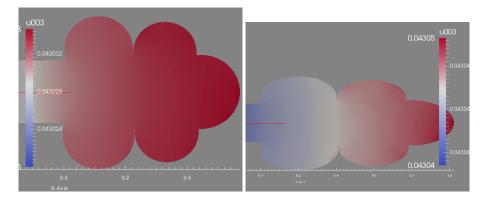


FIGURA 5.5.  $CO_2$  concentration in the alveolar sac

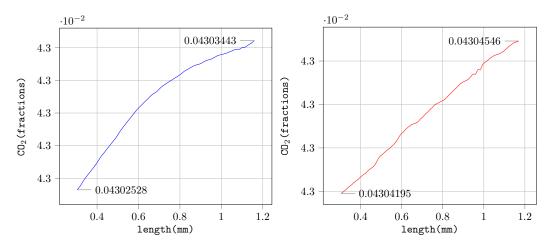


FIGURA 5.6. Stratification of the  $CO_2$ 

alveolar sac is submitted to fast and strong maneuver, we could see the differences from a normal maneuver very smooth.

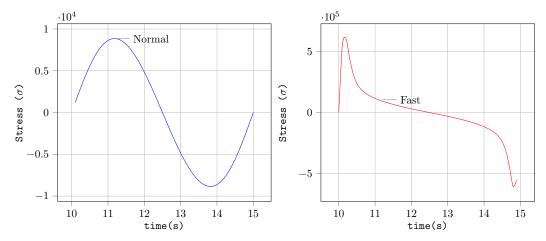


FIGURA 5.7. Stress for normal breath

Those figures for the  $CO_2$  showed that the gas is diluted or concentrated according the maneuver that the subject done (normal or fast respiratory maneuver) and the carbon dioxide was not affected with the stress in the wall of the alveolar sac for a normal maneuver. The stress changed following the pattern of respiration like a sinusoidal curve, but in a forced maneuver the stress did not follow the same pattern.

**6. Conclusion.** The model of the dynamics of gases in Arbitrary Lagrangian-Eulerian coordinates help to control a moving domain; this analysis showed that the dissipation of energy for the fluid and gas transport depend of fluid properties and the velocity of domain deformation of the alveolar sac. Furthermore, the dissipation for the concentration of carbon dioxide, it does not depend on fluid velocity as a consequence of incompressible fluid and the amount of CO<sub>2</sub> in the alveolar sacs, depends upon the number of capillaries in the wall and it is not affected by the expired force maneuver, but the stratification of gas concentration is affected by the gas flow is coming to the alveolar sac.

The analysis shows the relation between the value of domain deformation and viscosity of fluid.

$$2\lambda\nu\|\hat{F}^{-1}\|_{\hat{\mathcal{L}}^{\infty}} + \|\hat{F}^{-1}\|_{\hat{\mathcal{L}}^{\infty}} \|\operatorname{div}(\partial_t \hat{T})\|_{\hat{\mathcal{L}}^{\infty}} > 0$$

The analysis showed that the functional spaces for the existence of weak solution for the fluid and CO<sub>2</sub> concentration are

$$\hat{u} \in \hat{\mathcal{L}}^{\infty}(0,T;\hat{\mathcal{L}}^2(\hat{\Omega})) \cap \hat{\mathcal{L}}^2(0,T;\mathcal{H}^1_0(\hat{\Omega})) \cap \hat{\mathcal{L}}^2(0,T;\hat{\mathcal{L}}^2(\hat{\Omega})).$$

$$\hat{C} \in \hat{\mathcal{L}}^{\infty}(0,T;\hat{\mathcal{L}}^2(\hat{\Omega})) \cap \hat{\mathcal{L}}^2(0,T;\mathcal{H}^1(\hat{\Omega})) \cap \hat{\mathcal{L}}^2(0,T;\hat{\mathcal{L}}^2(\hat{\Omega}))$$

Future work: Analysis of dynamics of gases considering fluid-structure interaction, and analysis of dynamics in the lung pathology.

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