XXXVI Jornada de Matemática de la Zona Sur
Universidad Católica de Temuco
24, 25 y 26 de abril de 2024, Temuco, Chile

Nonlinear convection-diffusion model of lung capillary perfusion and gas exchange

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Abstract

Pulmonary capillary perfusion and gas exchange are the fundamental physical processes that allow for respiration to occur at the microscale. Present-day computational simulations of these phenomena are often based on low-dimensional mathematical models on idealized alveolar geometries, where the chemical reactions between O_2-CO_2 and haemoglobin are simplified [1, 2]. However, these models fail to capture the complex chemical reactions that take place in pulmonary capillary blood, and overlook the effect of porous alveolar structure. In our study, we develop a coupled perfusion and gas exchange model that reflects physiological gas and Hb dynamics in pulmonary capillaries. To this end, we formulate a system of two coupled nonlinear convection-diffusion boundary value problems. We derive the equations from continuum balance laws, incorporating an experimentally-validated relationship between gas partial pressures and Hb saturations through a fully coupled Hill equation-like model [3]. We numerically solve these problems using a finite element scheme in a simple slab capillary domain, on a range of blood flow velocity fields and blood pH values. Moreover, we perform numerical simulations in a 3D alveolar domain reconstructed from μ-CT rat lung images, which were morphologically manipulated in order to simulate various degrees of emphysema. Numerical perfusion experiments agree with expected blood pressure drops and velocity fields in the lung capillary domain [4]. Additionally, numerical gas exchange simulations reconstruct physiological O_2 and CO_2 partial pressure and Hb saturation dynamics in the capillary domain, and reproduce the $\sim$ 100 ms equilibrium time of O_2 [5]. Further, these simulations replicate Bohr and Haldane effects in blood, and provide a fast and effective framework for estimating whole-lung diffusing capacities for O_2 and CO_2, whose values show a marked decrease during emphysema. We envision that this model broadens the applicability of computational lung simulations in clinical settings, specially during exercise and pathological conditions that alter perfusion dynamics and the overall lung gas exchanging function.

References

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