Macroscopic and kinetic diffusion models for gaseous mixtures in the context of respiration

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Collaborations with A. Bondesan[1], L. Boudin[2,3], M. Briant[1], C. Grandmont[3], S. Martin[1], V. Pavan[4], F. Salvarani[5]

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Context : impact of oxygen-helium mixture for respiration

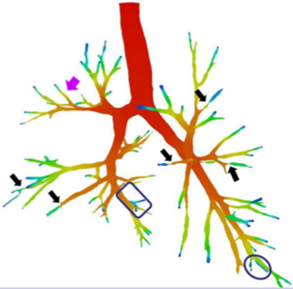
Oxhel: oxygen-helium mixture

Impact of inhaling Oxhel on the ventilation through the airways, blood oxygenation and aerosol deposition in the context of chronic obstructive lung diseases

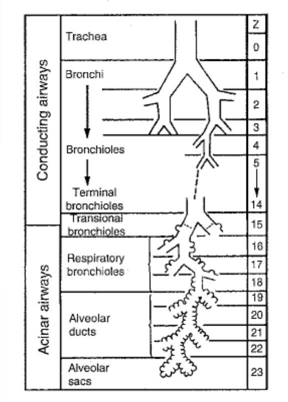
- Modeling the air as a mixture of several gases: N_2, O_2, (H_2O)
- In the context of respiration (gaseous exchanges): CO_2
- Oxhel for healing purposes: $N_2 \longrightarrow He$
- Expected improvements: respiration & oxygen transfer

First possible approach

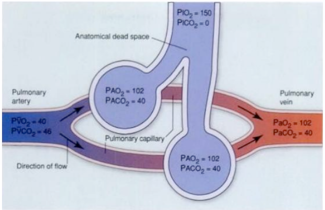
- Segmenting medical images
- Meshing the upper airways
- Simulating 3D flows
- No description of the lower airways
- Problematic for aerosol deposition



Airways modelling



- Decomposition of the respiratory tree in 2 parts
- Bronchi and bronchioles (1st - 16th gen.): convective regime
- Acini (17th - 23rd gen.): mainly diffusive regime and gaseous exchanges
- Integrated model of the ventilation process coupled with O_2 transfer into the blood [Martin, Maury (2013)]
- Taking into account the other gases: CO_2 and N_2/He



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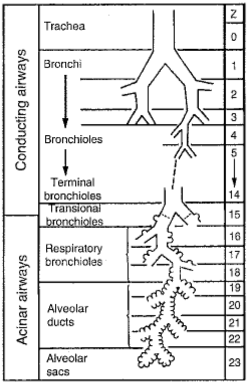

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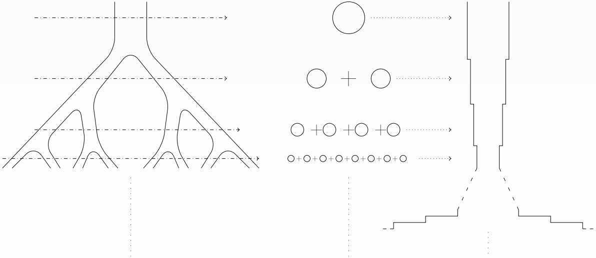
Diffusion models for gaseous mixtures

- Cross-diffusion model?
- Influence on oxygen transfer into the blood?

Collaboration with L. Boudin, C. Grandmont, S. Martin

Integrated model of the respiratory system for a mixture of three gases (O_2,CO_2,N_2/He)

- A lumped 0D mechanical model gives the entrance flux
- The geometry is reduced to a 1D domain
- Only longitudinal velocity u



- Discontinuous equivalent section S, computed from morphometric data
- Distinction between bronchial and alveolar part: $S = S_b + S_a$
- Alveoli starting from the 17th generation

Notation, for each species $1 \leq i \leq 3$

c_i concentration, M_i: molar mass, $\varrho_i = M_i c_i$: density

- Incompressibility: the total density $\varrho^0 = \sum_i \varrho_i$ is constant $\Longrightarrow$ relation between the c_i
- For two of the three species: mass conservation with simple diffusion

$$\partial_t(Sc_i) + \partial_x(S_b c_i u) + \partial_x(S_b N_i) = \mathcal{E}_i \quad \text{with} \quad N_i = -D_i \partial_x c_i, \qquad i = 1, 2$$

- Global mass conservation equation: coupling between u and the c_i

$$\varrho^0 \partial_t S + \varrho^0 \partial_x(S_b u) + \sum_j M_j \partial_x(S_b N_j) = \sum_j M_j \mathcal{E}_j$$

- Source term $\mathcal{E}_i$ modelling the gaseous exchanges
  - Activated from the 17th generation
  - For oxygen and carbon dioxide
  - Basic principles of O_2/CO_2 uptake/release along the pulmonary capillary
- If cross-diffusion effects, Maxwell-Stefan's model for the fluxes N_i:

$$-\partial_x c_i \propto \sum_j \frac{c_j N_i - c_i N_j}{D_{ij}} - \sum_j \partial_x c_j$$

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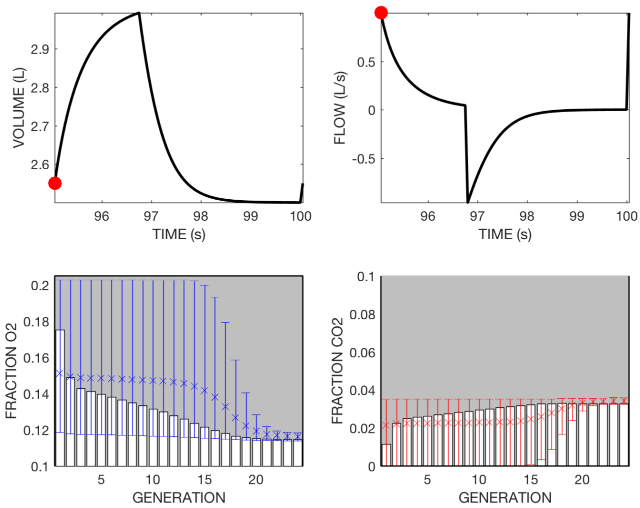
Preliminary results: ventilation for simple diffusion



Kinetic description and hydrodynamic limit

For mixtures

Obtain a macroscopic cross-diffusion model of Maxwell-Stefan's type as an hydrodynamic limit of kinetic models

- Kinetic description: $f_i(t, x, v)$ distribution fonction of species i
- Boltzmann equation for mixtures

$$\varepsilon \partial_t f_i + v \cdot \nabla_x f_i = \frac{1}{\varepsilon} \sum_j Q_{ij}(f_i, f_j), \qquad \forall i$$

- Q_{ij}: collision operators
- Elastic collisions: conservation of mass and momentum
- Fluid regime: Kn $\sim \varepsilon$
  Equilibria of the collision operators: local Maxwellians

$$f_i(t, x, v) = c_i(t, x) \left(\frac{m_i}{2\pi kT} \right)^{3/2} \exp\left(-\frac{m_i}{2kT} |v - \varepsilon u_i(t, x)|^2 \right).$$

- Diffusion predominant over convection : Ma $\sim \varepsilon$

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Diffusive asymptotics for multi-species Boltzmann eq.

Two possible approaches

- Perturbative method (leads the Fick's equations)
  Based on Chapman-Enskog expansion
  [Bardos, Golse, Levermore], [Bisi, Desvillettes]
- Moment method (leads the Maxwell-Stefan's equations)
  Based on the assumption of a local equilibrium
  [Levermore], [Müller, Ruggieri]

Ansatz

The distribution fonctions f_i^ε are local Maxwellians with velocities $\varepsilon u_i^\varepsilon$

- The macroscopic concentration c_i^ε is the moment of order 0 of f_i^ε
- The macroscopic flux $\varepsilon c_i^\varepsilon u_i^\varepsilon$ is the moment of order 1 in v of f_i^ε

$$\int_{\mathbb{R}^3} f_i^\varepsilon(v)dv = c_i^\varepsilon \qquad \text{and} \qquad \int_{\mathbb{R}^3} v\, f_i^\varepsilon(v)dv = \varepsilon c_i^\varepsilon u_i^\varepsilon = \varepsilon N_i^\varepsilon.$$

$$\boxed{\varepsilon \partial_t f_i^\varepsilon + v \cdot \nabla_x f_i^\varepsilon = \frac{1}{\varepsilon} \sum_j Q_{ij}(f_i^\varepsilon, f_j^\varepsilon), \quad \forall i}$$

- Conservation property:

$$\int_{\mathbb{R}^3} Q_{ij}(f,g)(v)\, dv = 0, \qquad \forall i,j$$

- Mass conservation equation

$$\varepsilon \frac{\partial}{\partial t} \left(\int_{\mathbb{R}^3} f_i^\varepsilon(v)\, dv \right) + \nabla_x \cdot \left(\int_{\mathbb{R}^3} v\, f_i^\varepsilon(v)\, dv \right) = 0.$$

$$\partial_t c_i^\varepsilon + \nabla_x \cdot N_i^\varepsilon = 0.$$

- Conservation property:

$$\int_{\mathbb{R}^3} Q_{ij}(f,g)(v)\, m_i\, v\, dv + \int_{\mathbb{R}^3} Q_{ji}(g,f)(v)\, m_j\, v\, dv = 0, \qquad \forall i,j$$

- Momentum equation

$$\varepsilon \frac{\partial}{\partial t} \int_{\mathbb{R}^3} v\, f_i^\varepsilon(v)\, dv + \int_{\mathbb{R}^3} v\, \nabla_x \cdot (v\, f_i^\varepsilon(v))\, dv = \frac{1}{\varepsilon} \sum_{j \neq i} \int_{\mathbb{R}^3} v\, Q_{ij}(f_i^\varepsilon, f_j^\varepsilon)(v)\, dv.$$

Divergence term

- Use of the Ansatz, explicit computations of moments of Maxwellian terms

$$\int_{\mathbb{R}^3} v\, \nabla_x \cdot (v\, f_i^\varepsilon(v))\, dv = \frac{kT}{m_i} \nabla_x c_i^\varepsilon + \varepsilon^2 \nabla_x \cdot \left(c_i^\varepsilon u_i^\varepsilon \otimes u_i^\varepsilon \right).$$

Collision term

- If restrictive assumptions on the cross section $\Longrightarrow$ explicit computations
- In any case, Galilean invariance of the collision rules and use of Schur's lemma

$$\lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \sum_{j \neq i} \int_{\mathbb{R}^3} v\, Q_{ij}(f_i^\varepsilon, f_j^\varepsilon)(v)\, dv = \frac{c_i c_j (u_i - u_j)}{D_{ij}}.$$

- Explicit form of the binary diffusion coefficients D_{ij}

At the limit $\varepsilon \to 0$

$$\partial_t c_i + \nabla \cdot N_i = 0, \qquad \& \qquad \nabla_x c_i = -\sum_{j \neq i} \frac{c_j N_i - c_i N_j}{D_{ij}}.$$

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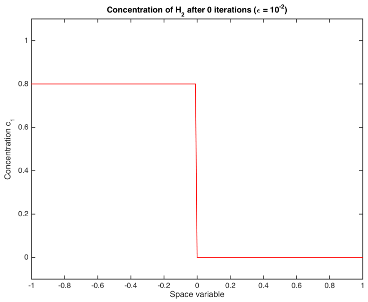
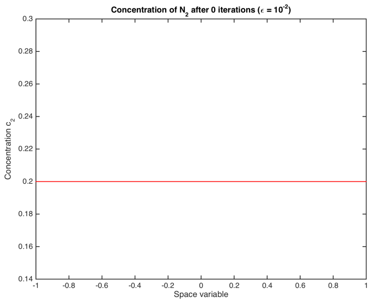
Beyond the formal convergence

- Rigorous convergence
- Asymptotic-preserving numerical scheme
  - Based on the moment method as for the formal convergence
  - Asymptotic-preserving behavior
  - Existence & positivity of the solutions (concentrations)

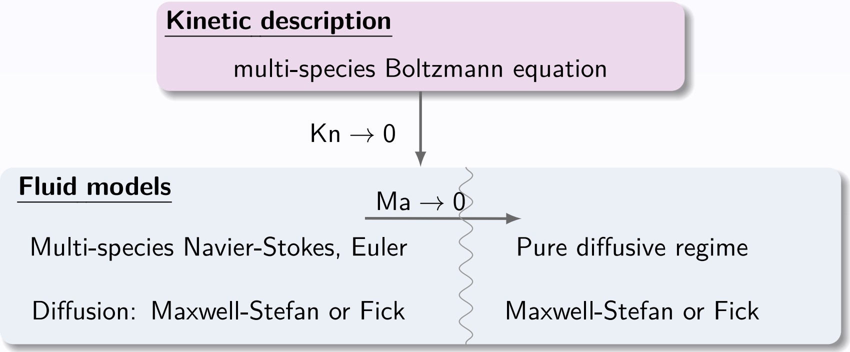




Collaboration with A. Bondesan, L. Boudin, M. Briant

Conclusion and prospects

- Hydrodynamic limit for mixtures



- Respiration
  - Influence of Oxhel?
  - Influence of the diffusion model?
  - Aerosol description and deposition?
  - Cemracs project: Size-varying respiratory aerosols modeling