MODELLING GAS FLOWS IN THE LOWER PULMONARY AIRWAYS

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The REO project

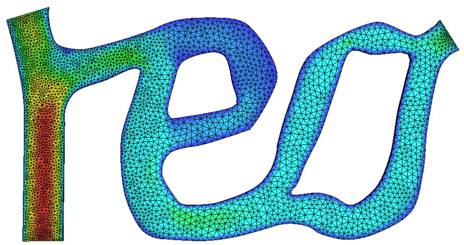
Joint project of the INRIA Paris-Rocquencourt and the Jacques-Louis Lions Laboratory (LJLL) of the Paris VI University.

Its research activities are aimed at

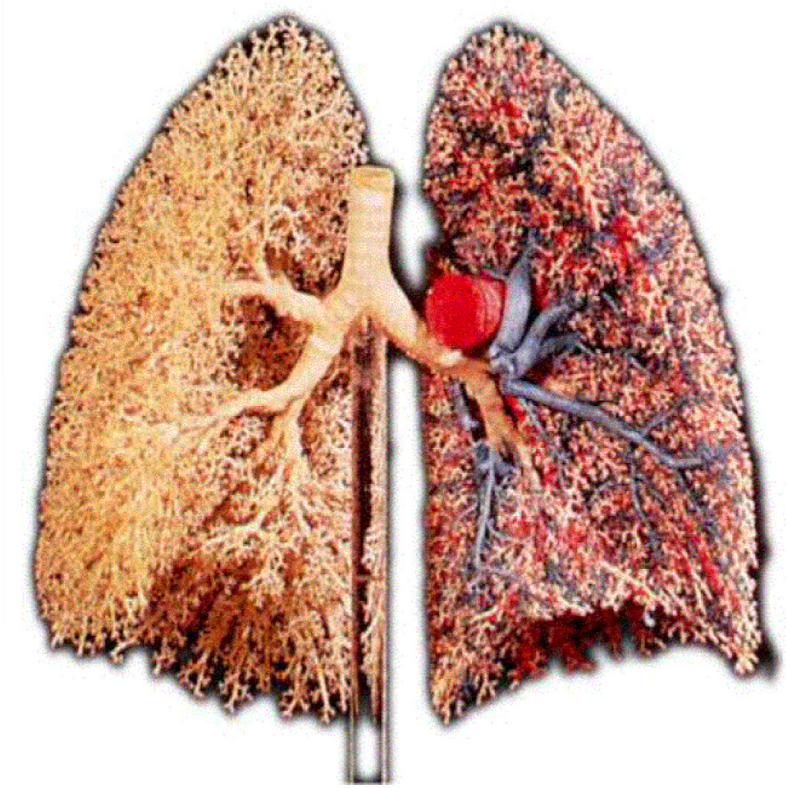
- ▷ modeling some aspects of the cardiovascular and respiratory systems, both in normal and pathological states;
- ▷ developing and analyzing efficient, robust and reliable numerical methods for the simulation of those models;
- ▷ developing simulation software to guide medical decision and to design more efficient medical devices.

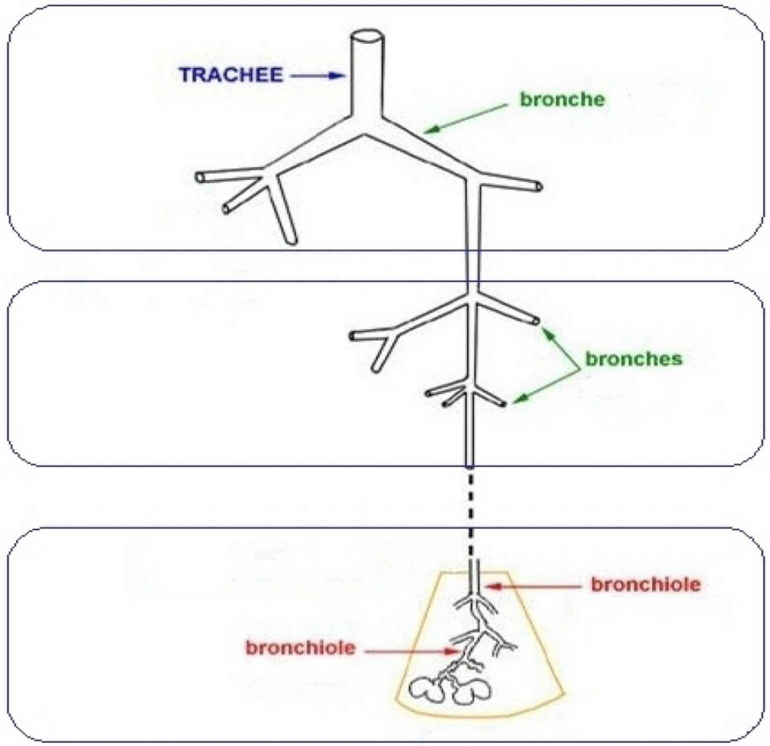
Head of the project: J.F. Gerbeau

Researchers involved in the modelling of flows in the lower respiratory airways (and whose results are presented here): L. Boudin, D. Götz, C. Grandmont, B. Grec, FS



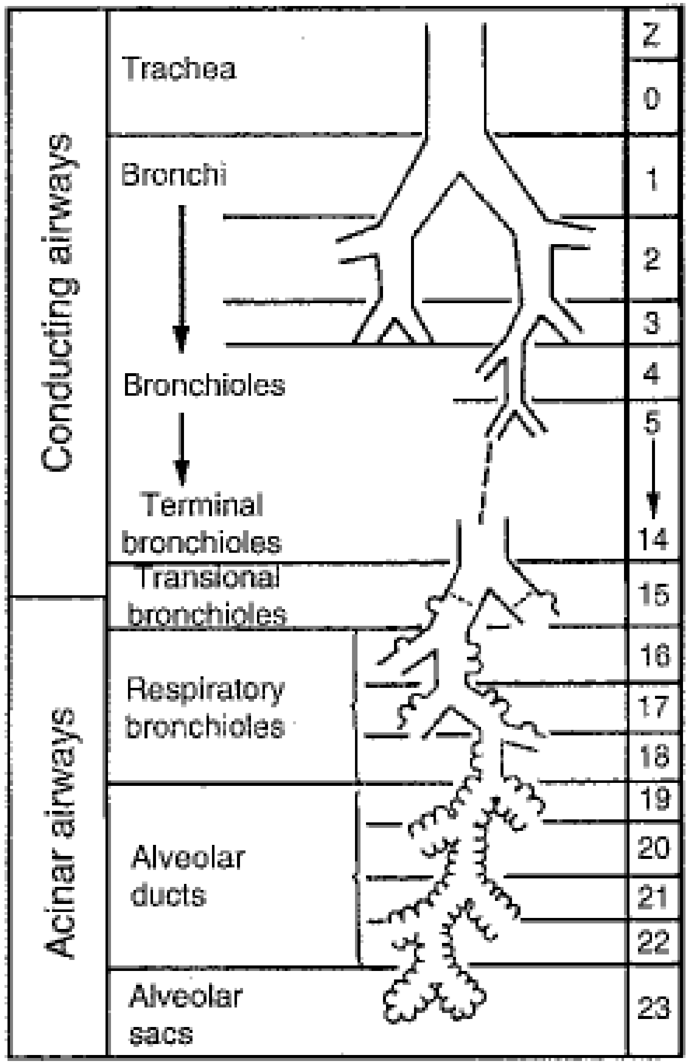
The human respiratory airways





23 generations tree (Weibel model)

Decomposition of the respiratory tree



Upper airways (1st - 8th generation): incompressible Navier-Stokes equations

Distal region (9th - 16th generation): Poiseuille flow in bronchioles

Acinar airways (17th - 23rd generation): oxygen diffusion in alveoli

Lower respiratory airways

In the acini: no convection, only diffusion

Air is a multi-component mixture:

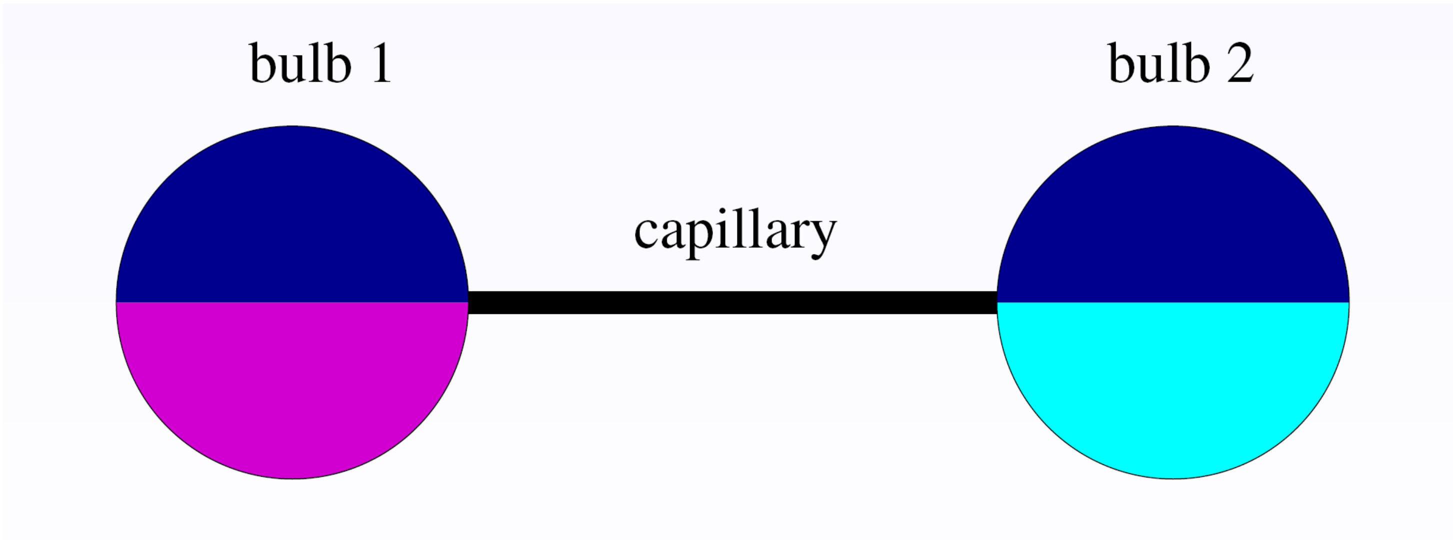
	nitrogen (N_2)	oxygen (O_2)	water (H_2O)	carbon dioxide (CO_2)
In atmosphere (dry)	78%	21%	0%	0%
In the lung (wet) before gas exchanges	74.3%	19.5%	6.2%	0%
In the lung (wet) after gas exchanges	74.3%	14.2%	6.2%	5.3%

Duncan and Toor experiment, 1962

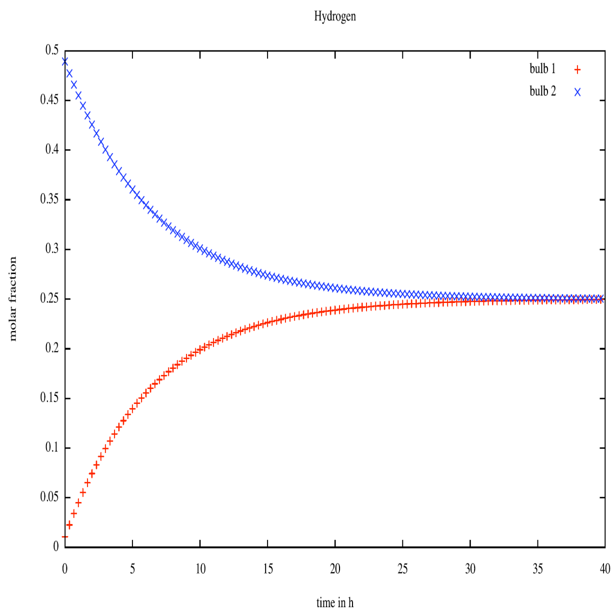
Mixture of three perfect gases:

In bulb 1:
49.9% of CO_2 and 50.1% of N_2

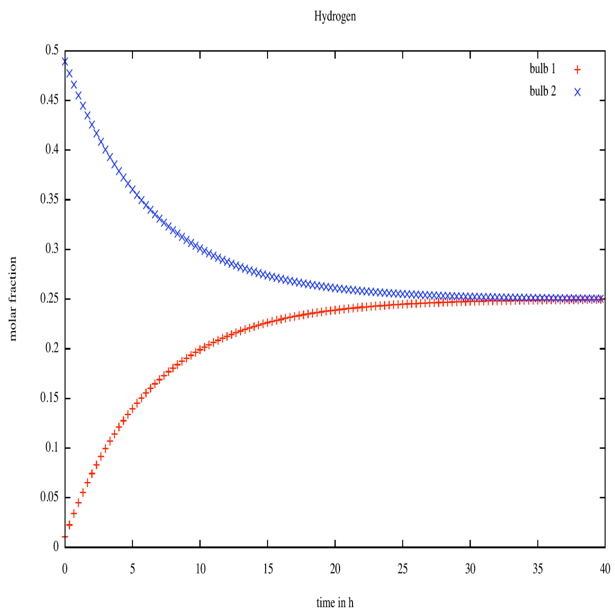
In bulb 2:
50.1% of H_2 and 49.9% of N_2

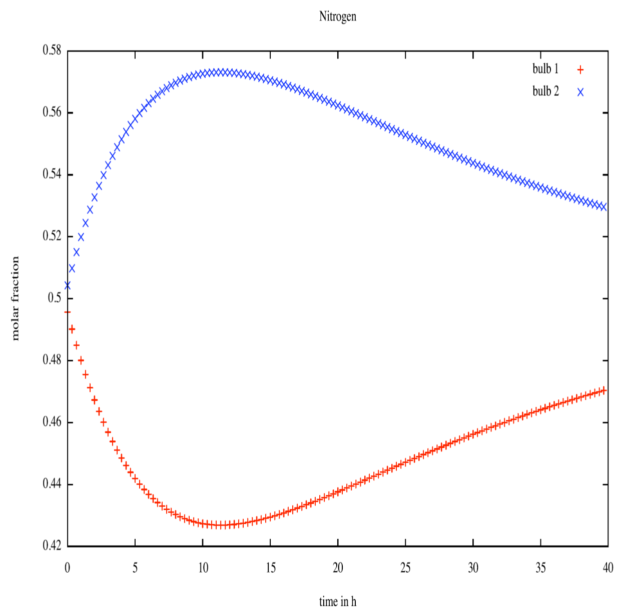


The uphill diffusion

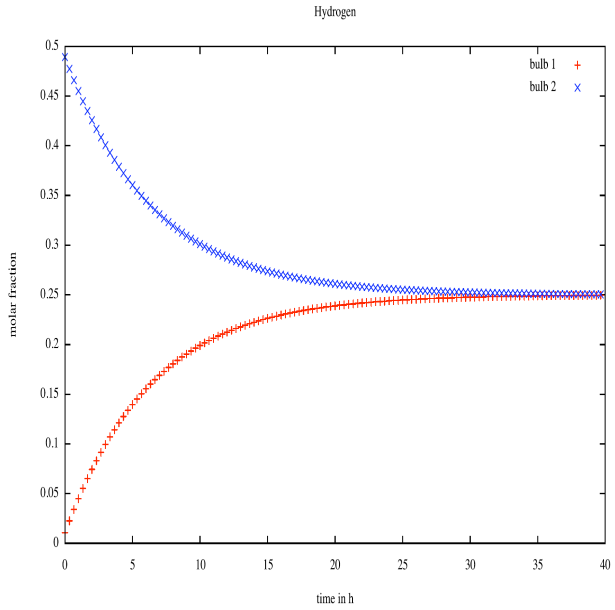


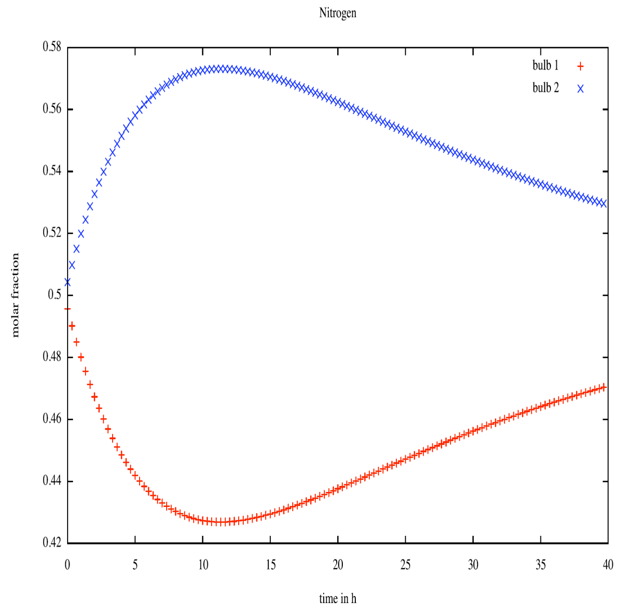
The uphill diffusion

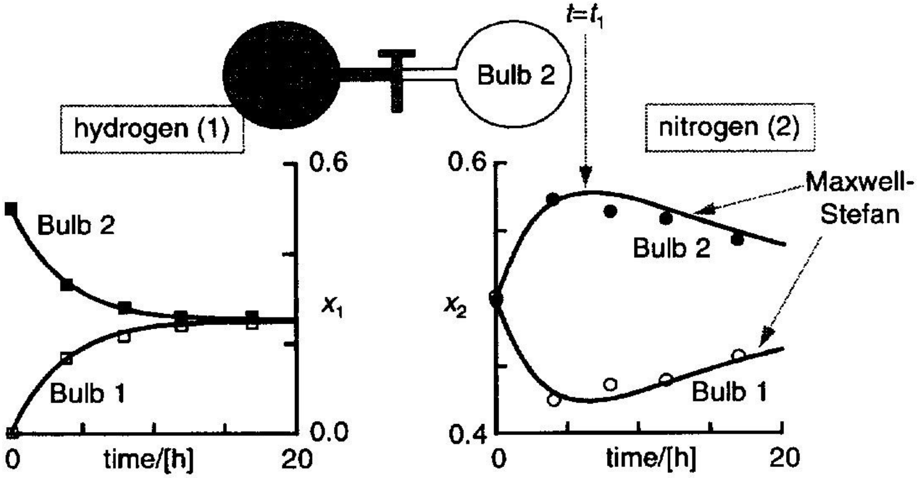




The uphill diffusion







Maxwell-Stefan model

Assumption: the total concentration $c_t = \sum c_i$ remains constant (no convection)

Conservation of mass (for each species):

$$\partial_t \xi_i + \nabla \cdot N_i = 0$$

c_i: concentration of species i,
$\xi_i = c_i / c_t$: molar fraction of species i

N_i: molar flux of species i

Fick's law:

$$-\nabla \xi_i = \frac{N_i}{D_i}, \qquad D_i\text{: diffusion coefficient}$$

Maxwell-Stefan's model:

$$-\nabla \xi_i = \sum_{j \neq i} \frac{\xi_j N_i - \xi_i N_j}{D_{ij}}, \qquad D_{ij}\text{: binary diffusion coefficient}$$

Kinetic derivation of the Maxwell-Stefan diffusion equations

Mixture of $i \in \mathbb{N}$ species A_i

$f_i = f_i(t,x,v)$: number density function ($t \geq 0$, $x \in \mathbb{R}^d$, $v \in \mathbb{R}^d$)

$n_i(x,t)\,dx$: number of particles of the specie i at time t in an infinitesimal region of thickness dx centered in x

Link between f_i and n_i: $n_i(t,x) = \displaystyle\int_{\mathbb{R}^d} f_i(t,x,v)\,dv.$

Effect of a collision between two molecules of species i and j, with mass m_i and m_j, and velocity v', v'_* (with new velocities v and v_*):

The conservations of momentum and total energy lead to ($\omega \in S^{d-1}$):

$$v' = \frac{1}{m_i + m_j}(m_i v + m_j v_* + m_j |v - v_*|\,\omega)$$
$$v'_* = \frac{1}{m_i + m_j}(m_i v + m_j v_* - m_i |v - v_*|\,\omega).$$

The collision kernels

Mono-species collision kernels:

$$Q_i^{\mathrm{m}}(f,f)(v) = \int_{v_*\in\mathbb{R}^d}\int_{\omega\in S^{d-1}} B_i(v,v_*,\omega)\left[f(v')f(v'_*) - f(v)f(v_*)\right]\,dv_*d\omega$$

The cross sections B_i are supposed to satisfy the microreversibility assumptions:

$$B_i(v,v_*,\omega) = B_i(v_*,v,\omega), \qquad B_i(v,v_*,\omega) = B_i(v',v'_*,\omega).$$

Bi-species collision kernels ($i \neq j$):

$$Q_{ij}^{\mathrm{b}}(f,g)(v) = \int_{v_*\in\mathbb{R}^d}\int_{\omega\in S^{d-1}} B_{ij}(v,v_*,\omega)\left[f(v')g(v'_*) - f(v)g(v_*)\right]\,dv_*d\omega$$

The cross sections B_{ij} are supposed to satisfy the microreversibility assumptions:

$$B_{ij}(v,v_*,\omega) = B_{ji}(v_*,v,\omega) \qquad B_{ij}(v,v_*,\omega) = B_{ij}(v',v'_*,\omega).$$

The weak form of the collision kernels

Let $\psi : \mathbb{R}^d \to \mathbb{R}$ be functions such that the formulas $\int_{v\in\mathbb{R}^d} Q_i^{\mathrm{m}}(f,f)(v)\psi(v)\,dv$, $\int_{v\in\mathbb{R}^d} Q_{ij}^{\mathrm{b}}(f,g)(v)\,\psi_i(v)\,dv$ and $\int_{v\in\mathbb{R}^d} Q_{ji}^{\mathrm{b}}(g,f)(v)\,\psi_j(v)\,dv$ make sense. Then

$$\int_{v\in\mathbb{R}^d} Q_i^{\mathrm{m}}(f,f)(v)\,\psi(v)\,dv = -\frac{1}{4}\int_{v\in\mathbb{R}^d}\int_{v_*\in\mathbb{R}^d}\int_{\omega\in S^{d-1}} B_i(v,v_*,\omega)\left[f(v')f(v'_*) - f(v)f(v_*)\right]$$

$$\times\ \left[\psi(v') + \psi(v'_*) - \psi(v) - \psi(v_*)\right]\,dv\,dv_*\,d\omega$$

and

$$\int_{v\in\mathbb{R}^d} Q_{ij}^{\mathrm{b}}(f,g)(v)\,\psi_i(v)\,dv + \int_{v\in\mathbb{R}^d} Q_{ji}^{\mathrm{b}}(g,f)(v)\,\psi_j(v)\,dv =$$

$$-\frac{1}{2}\int_{v\in\mathbb{R}^d}\int_{v_*\in\mathbb{R}^d}\int_{\omega\in S^{d-1}} B_{ij}(v,v_*,\omega)\left[f(v')g(v'_*) - f(v)g(v_*)\right]\times$$

$$\left[\psi_i(v') + \psi_j(v'_*) - \psi_i(v) - \psi_j(v_*)\right]\,dv\,dv_*d\omega.$$

Conservation laws

Mono-species collision kernels:

$$\int_{v\in\mathbb{R}^d} Q_i^{\mathrm{m}}(f,f)(v) \begin{pmatrix} 1 \\ m_i\, v^{(k)} \\ m_i\, |v|^2/2 \end{pmatrix} dv = 0$$

Bi-species collision kernels ($i \neq j$):

$$\int_{v\in\mathbb{R}^d} Q_{ij}^{\mathrm{b}}(g,f)(v)\, dv = 0$$

$$\int_{v\in\mathbb{R}^d} Q_{ij}^{\mathrm{b}}(f,g)(v) \begin{pmatrix} m_i\, v^{(k)} \\ m_i\, |v|^2/2 \end{pmatrix} dv + \int_{v\in\mathbb{R}^d} Q_{ji}^{\mathrm{b}}(g,f)(v) \begin{pmatrix} m_j\, v^{(k)} \\ m_j\, |v|^2/2 \end{pmatrix} dv = 0$$

The H-theorem

Hypotheses: the quantities B_i, B_{ij} and φ_i are strictly positive a.e. ($i \in \mathbb{N}$, $j \neq i$)

First part of the H-theorem: For all $f_i \equiv f_i(v) \geq 0$ such that the following quantities are defined, one has

$$\sum_i \int_{v\in\mathbb{R}^d} Q_i^m(f_i, f_i)(v) \log\left(\frac{f_i(v)}{m_i^d}\right) dv + \sum_i \sum_{j\neq i} \int_{v\in\mathbb{R}^d} Q_{ij}^b(f_i, f_j)(v) \log\left(\frac{f_i(v)}{m_i^d}\right) dv \leq 0.$$

Second part of the H-theorem: the three following properties are equivalent:

- For all $v \in \mathbb{R}^d$: $\quad Q_i^m(f_i, f_i)(v) = 0 \quad \text{and} \quad Q_{ij}^b(f_i, f_j)(v) = 0,$

- $\displaystyle\sum_i \int_{v\in\mathbb{R}^d} Q_i^m(f_i, f_i)(v) \log\left(\frac{f_i(v)}{m_i^d}\right) dv + \sum_i \sum_{j\neq i} \int_{v\in\mathbb{R}^d} Q_{ij}^b(f_i, f_j)(v) \log\left(\frac{f_i(v)}{m_i^d}\right) dv = 0,$

- There exist $T_i = T_i(t,x) > 0$ and $u_i = u_i(t,x) \in \mathbb{R}^d$ such that

$$f_i(t,x,v) = n_i(t,x) \left(\frac{m_i}{2\,\pi\,T_i}\right)^{d/2} \exp\left(-\frac{m_i}{2T_i}|v-u_i|^2\right).$$

The Maxwell-Stefan diffusion limit of the kinetic model

Maxwellian case: $B_{ij}(v, v_*, \omega) = B_{ij}(\omega)$ and such that $B_{ij} \in L^1(S^{d-1})$ for all $i, j \in \mathbb{N}$.

For symmetry reasons: $B_{ij}(\omega) = B_{ij}(-\omega)$ for all $\omega \in S^{d-1}$.

The scaled Boltzmann equation (ε mean free path):

$$\varepsilon \frac{\partial f_i^\varepsilon}{\partial t} + v \cdot \nabla_x f_i^\varepsilon = \frac{1}{\varepsilon} \left[Q_i^{\mathrm{m}}(f_i^\varepsilon, f_i^\varepsilon) + \left(\sum_{j \neq i} Q_{ij}^{\mathrm{b}}(f_i^\varepsilon, f_j^\varepsilon) \right) \right].$$

Problem in a bounded spatial domain: $x \in \Omega \subset \mathbb{R}^d$, with regular boundary $\partial\Omega$,

Specular boundary conditions $f_i(t, x, v) = f_i(t, x, v - 2(v \cdot n_x) n_x)$,
$(t, x, v) \in \mathbb{R}^+ \times \mathbb{R}^n \times \partial\Omega$ for each and $i \in \mathbb{N}$

The initial conditions

The initial conditions are local Maxwellians, with the same temperature T and zero macroscopic velocity

$$f_i^{\text{in}}(v) = n_i^{\text{in}}(x) \left(\frac{m_i}{2\,\pi\,T}\right)^{d/2} e^{-m_i|v|^2/2T}.$$

We moreover impose that the initial conditions $f_i^{\text{in}}(x,v)$ ($i \in \mathbb{N}$) satisfy

$$\sum_i \int_{v\in\mathbb{R}^d} f_i^{\text{in}}(x,v)\,dv = 1$$

It is easy to prove that

$$\sum_i \frac{1}{\varepsilon} \int_{v\in\mathbb{R}^d} v\, f_i^{\text{in}}(x,v)\,dv = 0$$

Towards the diffusion limit

Macroscopic mass density: $\xi_i^\varepsilon(t,x) = m_i \int_{v\in\mathbb{R}^d} f_i^\varepsilon(t,x,v)\,dv$

Its limit: $\xi_i(t,x) = \lim_{\varepsilon\to 0} \xi_i^\varepsilon(t,x)$

Macroscopic flux: $N_i^\varepsilon(t,x) = \frac{m_i}{\varepsilon} \int_{v\in\mathbb{R}^d} v\, f_i^\varepsilon(t,x,v)\,dv$

Its limit: $N_i(t,x) = \lim_{\varepsilon\to 0} N_i^\varepsilon(t,x)$

Working hypothesis: N_i is finite (as usual, when dealing with diffusive limits).

Since the initial flux is zero, and the boundary conditions are of specular type: $N_i^\varepsilon(0,x) = 0$ for a.e. $x \in \Omega$ and $N_i^\varepsilon(t,x) = 0$ for all $t > 0$ and a.e. $x \in \partial\Omega$.

Formal passage to the limit

$f_i^\varepsilon \to f_i$; f_i is solution of $Q_i^{\mathrm{m}}(f_i, f_i) + \left(\sum_{j \neq i} Q_{ij}^{\mathrm{b}}(f_i, f_j) \right) = 0$

Thanks to the H-theorem: $f_i(t,x,v) = n_i(t,x) \left(\frac{m_i}{2\pi T_i} \right)^{d/2} \exp\left(-\frac{m_i}{2T_i} |v - u_i|^2 \right)$

Consequence: $\int_{\mathbb{R}^d} f_i(v) \begin{pmatrix} 1 \\ m_i v^{(k)} \\ m_i |v|^2/2 \end{pmatrix} dv = \begin{pmatrix} n_i \\ m_i n_i u_i^{(k)} \\ m_i n_i (|u_i|^2 + dT_i)/2 \end{pmatrix}$

- The hypothesis $N_i^\varepsilon = O(1)$ implies $u_i(t,x) = 0$ in the limit

- When $i \neq j$: $f_i(v') f_j(v'_*) = f_i(v) f_j(v_*)$, that is

$$\frac{m_i}{2T_i} |v'|^2 + \frac{m_j}{2T_j} |v'_*|^2 = \frac{m_i}{2T_i} |v|^2 + \frac{m_j}{2T_j} |v_*|^2 .$$

The conservation of energy implies $T_i = T_j$ for all $i \neq j$.

The mass conservation

We integrate the Boltzmann equation with respect to v in $\mathbb{R}^d$

$$\frac{\partial}{\partial t}\int_{\mathbb{R}^d} f_i^\varepsilon(v)\,dv + \frac{1}{\varepsilon}\sum_{k=1}^{d}\frac{\partial}{\partial x_k}\int_{\mathbb{R}^d} v^{(k)}\,f_i^\varepsilon(v)\,dv = 0$$

Notation: $v^{(k)}$ means the k-th component of the vector v.

Letting $\varepsilon \longrightarrow 0$ and multiplying by m_i, we get

$$\frac{\partial \xi_i}{\partial t} + \nabla_x \cdot N_i = 0,$$

which is the continuity equation.

The balance of momentum

We multiply the Boltzmann equation by $v^{(l)}$ and integrate with respect to v

$$\varepsilon \frac{\partial}{\partial t} \int_{\mathbb{R}^d} v^{(l)}\, f_i^\varepsilon \, dv + \sum_{k=1}^{d} \frac{\partial}{\partial x_k} \int_{\mathbb{R}^d} v^{(l)}\, v^{(k)}\, f_i^\varepsilon \, dv = \frac{1}{\varepsilon} \sum_{j \neq i} \int_{\mathbb{R}^d} v^{(l)} Q_{ij}^{\mathrm{b}}(f_i^\varepsilon, f_j^\varepsilon)(v)\, dv.$$

Letting $\varepsilon \to 0$ and multiplying by m_i, we get

$$\nabla \xi_i(t,x) = \sum_{j \neq i} \frac{1}{D_{ij}} [N_j(t,x)\xi_i(t,x) - N_i(t,x)\xi_j(t,x)], \qquad D_{ij}^{-1} = \frac{\|B_{ij}\|_{L^1(S^{d-1})}}{(m_i + m_j)T}$$

Summing over all i and using initial data and specular boundary conditions:

$$\sum_i \xi_i(t,x) = \sum_i n_i^{\mathrm{in}}(x) = 1 \qquad \nabla \cdot \left(\sum_i N_i(t,x) \right) = 0$$

Simulations of a three-component mixture, in the 1D spatial case

$$
\begin{aligned}
\partial_t \xi_i + \partial_x N_i &= 0,\\
N_1 + N_2 + N_3 &= 0,\\
\frac{\xi_2 N_1 - \xi_1 N_2}{D_{12}} + \frac{\xi_3 N_1 - \xi_1 N_3}{D_{13}} &= -\partial_x \xi_1,\\
\frac{\xi_1 N_2 - \xi_2 N_1}{D_{12}} + \frac{\xi_3 N_2 - \xi_2 N_3}{D_{23}} &= -\partial_x \xi_2,
\end{aligned}
$$

Bounded domain $\Omega = (0,1)$.

Initial conditions $\xi_i(0,\cdot) = \xi_i^{\text{in}} \in L^\infty(\Omega)$

Boundary conditions: $N_i(t,0) = N_i(t,1) = 0, \qquad 1 \le i \le 3$.

$\partial_x \sum_i N_i = 0$ and $N_i(t,0) = N_i(t,1) = 0$ imply $\sum_i N_i = 0$

Reduced form of the system

We use only the two sets of unknowns (ξ_1, N_1) and (ξ_2, N_2), $(1 \le i \le 2)$

$$\begin{aligned} \partial_t \xi_i + \partial_x N_i &= 0, \\ \frac{1}{D_{13}} N_1 + \alpha N_1 \xi_2 - \alpha N_2 \xi_1 &= -\partial_x \xi_1, \\ \frac{1}{D_{23}} N_2 - \beta N_1 \xi_2 + \beta N_2 \xi_1 &= -\partial_x \xi_2, \end{aligned}$$

where

$$\alpha = \left(\frac{1}{D_{12}} - \frac{1}{D_{13}} \right), \qquad \beta = \left(\frac{1}{D_{12}} - \frac{1}{D_{23}} \right).$$

NB: $(\xi_3, N_3) = (1 - \xi_1 - \xi_2, -N_1 - N_2)$

Discretization of the problem

We assume that $D_{23} \geq D_{13} \geq D_{12}$, i. e. $\alpha,\ \beta \geq 0$

Regular subdivision $(x_j)_{0\leq j\leq J}$ of $\Omega = (0,1)$, with $J \geq 1$. $\Delta x = 1/J > 0$, so that $x_j = j\Delta x$

The mole fractions ξ_i are computed at the centers $x_{j+1/2} := (j+1/2)\Delta x$ of each interval $[x_j, x_{j+1}]$, $0 \leq j \leq J-1$

The molar fluxes N_i are computed at the nodes of the subdivision x_j, $0 \leq j \leq J$.

For each species $i \in \{1,2\}$, we consider the approximations ($\Delta t > 0$)

$$\begin{aligned} \xi_i^{(k,j)} &\simeq \xi_i(k\Delta t, x_{j+1/2}), \qquad k \in \mathbb{N}, \quad 0 \leq j \leq J-1, \\ N_i^{(k,j)} &\simeq N_i(k\Delta t, x_j), \qquad k \in \mathbb{N}, \quad 0 \leq j \leq J, \end{aligned}$$

$$\xi_i^{(k,j-1/2)} = \frac{1}{2}\left(\xi_i^{(k,j)} + \xi_i^{(k,j-1)}\right), \qquad k \in \mathbb{N}, \quad 1 \leq j \leq J-1.$$

Further discretizations . . .

The initial and boundary conditions ($0 \le j \le J-1,\ k \in \mathbb{N}$):

$$\xi_i^{(0,j)} = \xi_i^{\text{in}}(x_{j+1/2}), \qquad N_i^{(k,0)} = N_i^{(k,J)} = 0$$

The continuity equations ($k \in \mathbb{N}$ and $1 \le j \le J-1$):

$$\xi_i^{(k+1,j)} = \xi_i^{(k,j)} - \frac{\Delta t}{\Delta x^2}\left[N_i^{(k,j+1)}\Delta x - N_i^{(k,j)}\Delta x\right]$$

The momentum equations: linear system of unknowns $N_1^{(k,j)}\Delta x$ and $N_2^{(k,j)}\Delta x$:

$$\begin{aligned}
\left[\frac{1}{D_{13}} + \alpha\xi_2^{(k,j-1/2)}\right] N_1^{(k,j)} - \alpha\xi_1^{(k,j-1/2)} N_2^{(k,j)} &= \frac{\xi_1^{(k,j-1)} - \xi_1^{(k,j)}}{\Delta x} \\
-\beta\xi_2^{(k,j-1/2)} N_1^{(k,j)} + \left[\frac{1}{D_{23}} + \beta\xi_1^{(k,j-1/2)}\right] N_2^{(k,j)} &= \frac{\xi_2^{(k,j-1)} - \xi_2^{(k,j)}}{\Delta x}
\end{aligned}$$

Properties of the numerical scheme

Conservation of the total masses $\|\xi_i(t)\|_{L^1_x}$, $i \in \{1,2\}$:

$$\sum_{j=0}^{J-1} \xi_i^{(k+1,j)} = \sum_{j=0}^{J-1} \xi_i^{(k,j)} + \frac{\Delta t}{\Delta x^2} \sum_{j=0}^{J-1} \Delta x \left[N_i^{(k,j)} - N_i^{(k,j+1)} \right] = \sum_{j=0}^{J} \xi_i^{(k,j)}.$$

for any $k \in \mathbb{N}$

The numerical scheme, where we choose $D_{12} = D_{13}$, is of first order in time and second order in space. Moreover, it is L^∞-stable if

$$D_{23} \frac{\Delta t}{\Delta x^2} \leq \frac{1}{2}.$$

The stability proof

Since ξ_1 satisfies a heat equation, the standard stability condition is obvious (beacuse $D_{12} \leq D_{23}$).

Let us denote $\sigma = \Delta t / \Delta x^2$ and set, for $u, v \in [0,1]$,

$$A(u,v) = \sigma D_{23} \frac{2 + \beta D_{12}(u-v)}{2 + \beta D_{23}(u+v)}.$$

One can check that

$$\begin{aligned} \frac{\partial A}{\partial u} &= -2\beta D_{23}\sigma \frac{(D_{23} - D_{12})(1-v)}{[2 + \beta D_{23}(u+v)]^2} \leq 0, \\ \frac{\partial A}{\partial v} &= -2\beta D_{23}\sigma \frac{(D_{23} + D_{12}) + (D_{23} - D_{12})u}{[2 + \beta D_{23}(u+v)]^2} \leq 0. \end{aligned}$$

It is easy to prove that $\sigma D_{12} \leq A(u,v) \leq \sigma D_{23}, \qquad \forall\, u,v \in [0,1]$

The stability proof - II

Let $X = \xi_1^{(k,j-1)}$, $Y = \xi_1^{(k,j)}$ and $Z = \xi_1^{(k,j+1)}$ (all lie in $[0,1]$).

The discretized conservation of mass becomes

$$\xi_2^{(k+1,j)} = (1 - A(Y,Z) - A(Y,X))\xi_2^{(k,j)} + A(Z,Y)\xi_2^{(k,j+1)} + A(X,Y)\xi_2^{(k,j-1)}.$$

$\xi_2^{(k+1,j)}$ is still positive if the stability condition holds

The stability proof - III

$\xi_1^{(k,j)} + \xi_2^{(k,j)} \leq 1$ for any j: by induction on $k \in \mathbb{N}$.

a) The case $k = 0$: $\xi_1^{\text{in}} + \xi_2^{\text{in}} \leq 1$.

b) By assuming $\xi_1^{(k,j)} + \xi_2^{(k,j)} \leq 1$ for any j, then the same property holds at iteration $k+1$: we have $\xi_1^{(k+1,j)} + \xi_2^{k+1,j} \leq F(X,Y,Z)$, where

$$F(X,Y,Z) = (1-2\sigma D_{12})Y + \sigma D_{12}(X+Z) + (1 - A(Y,Z) - A(Y,X))(1-Y) \\ + A(Z,Y)(1-Z) + A(X,Y)(1-X) = 1.$$

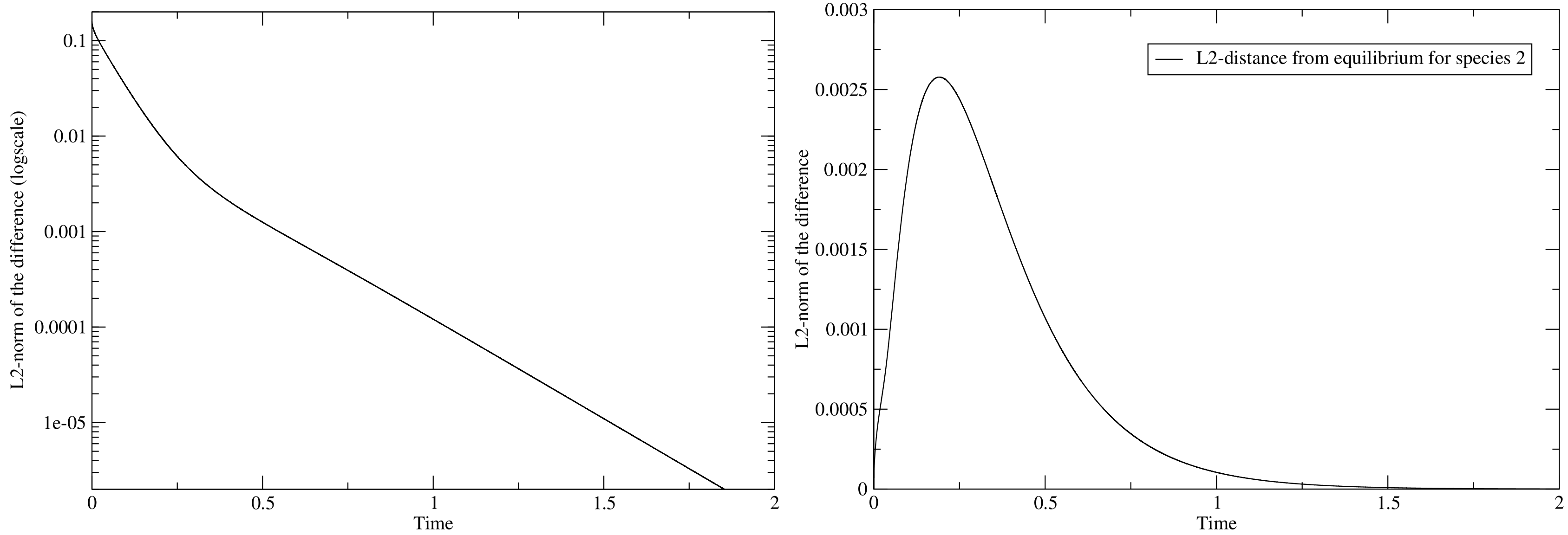
When $\alpha \neq 0$, the scheme seems to remain stable under the same condition

Numerical tests: the asymptotic behaviour (w.r.t time)

The *Duncan and Toor experiment*: $D_{12} = 0.833$, $D_{13} = 0.680$ and $D_{23} = 0.168$.

The initial condition:

$$\xi_1^{\text{in}}(x) = \begin{cases} 0.8 & \text{if } 0 \le x < 0.5 \\ 0 & \text{if } 0.5 \le x \le 1 \end{cases} \quad \text{and} \quad \xi_2^{\text{in}}(x) = 0.2, \quad \text{for all } x \in \Omega.$$



Time evolution of $H(t)$ and $\|\xi_2 - \bar{\xi}_2\|^2_{L^2(\Omega)}$

Comparison with the theoretical result

Theorem: Let $\xi_1^{\text{in}}, \xi_2^{\text{in}}$ two non-negative functions in $L^\infty(\Omega)$ such that $\xi_1^{\text{in}} + \xi_2^{\text{in}} \le 1$.

The initial-boundary value problem whith $D_{12} = D_{13}$, admits unique smooth solutions (ξ_1, N_1) and (ξ_2, N_2) for all time.

ξ_1 and ξ_2 remain positive, and

$$\|\xi_1(t,\cdot)\|_{L^1(\Omega)} = \|\xi_1^{\text{in}}\|_{L^1(\Omega)}, \qquad \|\xi_2(t,\cdot)\|_{L^1(\Omega)} = \|\xi_2^{\text{in}}\|_{L^1(\Omega)}, \qquad \forall\, t \in \mathbb{R}_+.$$

The mole fractions (ξ_i) asymptotically converge to $\bar{\xi}_i := \|\xi_i^{\text{in}}\|_{L^1(\Omega)} / \operatorname{meas}(\Omega)$.

Moreover, let $K \ge 0$ a suitable constant and

$$H(t) = \frac{K}{2}\int_\Omega (\xi_1 - \bar{\xi}_1)^2\, dx + \frac{1}{2}\int_\Omega (\xi_2 - \bar{\xi}_2)^2\, dx.$$

Then:

$$H(t) \le H(0)\exp\left(-2\theta \min(D_{12}, D_{23})\, C_{d,\Omega} t\right),$$

for any $\theta \in]0,1[$, where $C_{d,\Omega}$ is the best constant of the Poincaré inequality on $\Omega \in \mathbb{R}^d$.

Numerical tests: the uphill diffusion

The *semi-degenerate Duncan and Toor experiment*:
$D_{12} = D_{13} = 0.833$ ($\alpha = 0$) and $D_{23} = 0.168$.

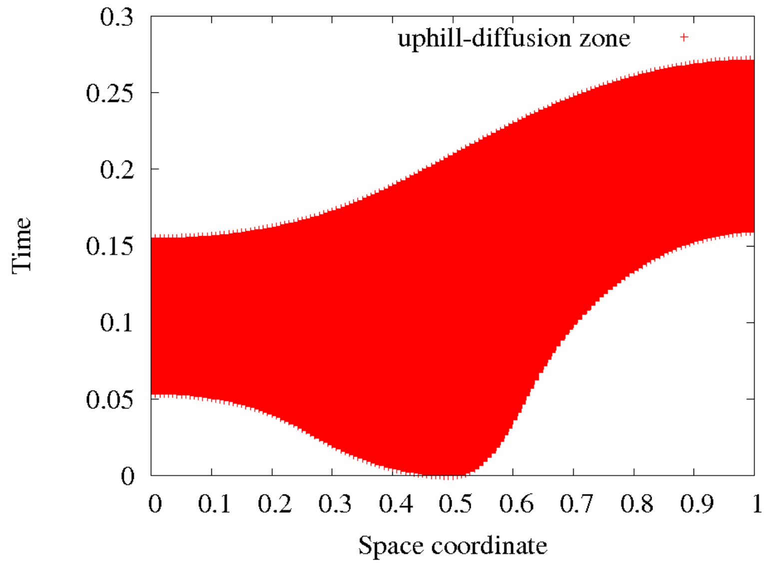
Two sets of initial data:

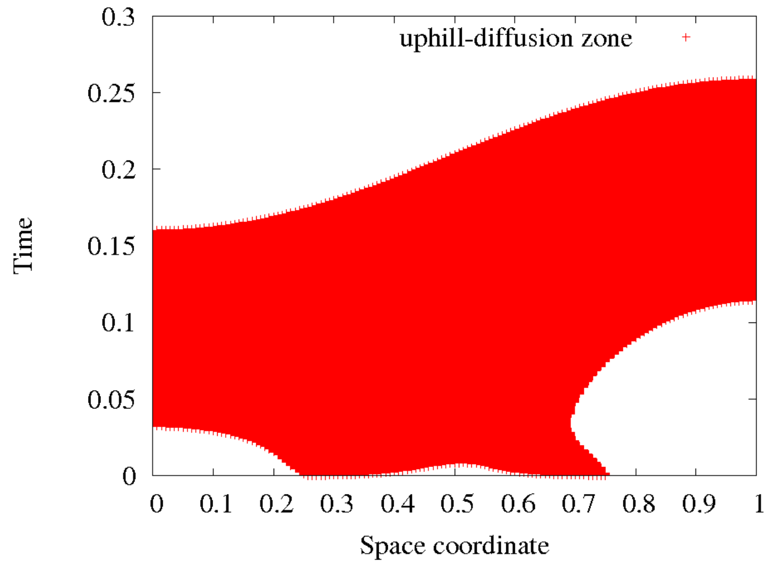
$$\xi_1^{\text{in}}(x) = \begin{cases} 0.8 & \text{if } 0 \le x < 0.5 \\ 0 & \text{if } 0.5 \le x \le 1 \end{cases} \qquad \text{and} \qquad \xi_2^{\text{in}}(x) = 0.2, \qquad \text{for all } x \in \Omega.$$

and

$$\xi_1^{\text{in}}(x) = \begin{cases} 0.8 & \text{if } 0 \le x < 0.25 \\ 1.6(0.75 - x) & \text{if } 0.25 \le x < 0.75, \\ 0 & \text{if } 0.75 \le x \le 1 \end{cases} \qquad \xi_2^{\text{in}}(x) = 0.2 \text{ for all } x \in \Omega.$$

Space-time localization of uphill diffusion





Regions where $N_2 \partial_x \xi_2 \geq 0$ for the two choices of initial data

The next step: taking gas exchange into account

Boundary conditions

$c_{O_2} = 0.20,$	$c_{CO_2} = 0,$	incoming fresh air on entrance
$c_{O_2} = 0.14,$	$c_{CO_2} = 0.06,$	alveolar air on exits

For the other species, zero outflux condition on $\partial\Omega$.

Gas exchange in the alveoli

Loss of O_2 and gain of CO_2
Total flux equal to zero on the boundary

$c_{O_2} = 0.14,$	on alveoli
$c_{CO_2} = 0.06,$	on alveoli