Size-varying respiratory aerosols modeling

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CEMRACS 2018

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Introduction

Purpose

- Modeling of particles (aerosol) motion in the lung.
- Understanding aerosol deposition maps on bronchi walls.
- Influence of the radius growth (water vapor exchange) on the aerosol deposition.

Previous model

Fluid particle model : L. Boudin, C. Grandmont, A. Lorz and A. Moussa, Modelling and Numerics for Respiratory Aerosols (2015).
Model assumptions :

- The aerosol volume fraction in the mixture remains negligible.
- No interaction between particles.
- Aerosol can have an effect on the fluid (Retroaction effect).

Model description

We denote by Ω the fluid domain, which is a cylinder or a branch and is assumed to be fix in time.

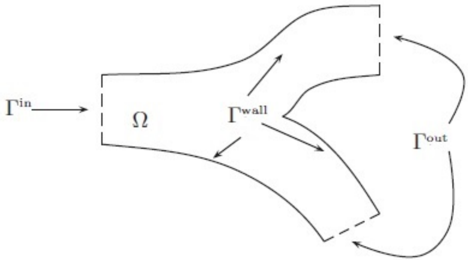


FIGURE – Domain

Fluid equations

(u, p) represents the fluid velocity and its pressure satisfying a Navier-Stokes equation :

$$\left\{ \begin{array}{rcl} \rho_{\text{air}}[\partial_t u + (u \cdot \nabla)u] - \eta\Delta u + \nabla p & = & F, \\ \text{div}(u) = 0, & & \end{array} \right. \quad \text{on } \mathbb{R}^+ \times \Omega,$$

completed with the following boundary and initial conditions :

$$\left\{ \begin{array}{rcl} u & = & u^{\text{in}}, \text{ on } \Gamma^{\text{in}}, \\ u & = & 0, \text{ on } \Gamma^{\text{wall}}, \\ \sigma(u,p) \cdot n & = & 0, \text{ on } \Gamma^{\text{out}}, \\ u(0,\cdot) & = & u_0, \text{ on } \Omega, \end{array} \right.$$

where $\sigma(u, p)$ is the stress tensor and F is the particles retroaction term defined as follows :

$$\begin{array}{rcl} \alpha & = & \dfrac{6\pi\eta r}{m}, \\ F & = & -\displaystyle\int m\alpha(u - v) f dv. \end{array}$$

Density equation

For all $t \in \mathbb{R}^+$, $x \in \Omega$ and $v \in \mathbb{R}^3$, $f(t, x, v)$ represents the number of droplets located in the elementary volume of the domain, at time t, position x and velocity v. The density f satisfies the following equation :

$$\partial_t f + v \cdot \nabla_x f + \mathrm{div}_v(\alpha(u - v)f) = 0, \text{ on } \mathbb{R}^+ \times \Omega \times \mathbb{R}^3,$$

completed with the following initial and boundary conditions :

$$\begin{cases} f &= 0, \text{ on } \Gamma^{\text{wall}} \times \mathbb{R}^3, \text{ if } v \cdot n \leq 0, \\ f_{|t=0} &= f_{\text{init}}, \text{ on } \Omega \times \mathbb{R}^3 . \end{cases}$$

Radius growth and temperature variation

ODE System : We denote by T_d the droplet temperature, r_d the droplet radius, T_{air} the air temperature and $Y_{\text{v,air}}$ the water vapor mass fraction in the air.

$$\begin{aligned}
\dot{r}_d &= a(r_d, T_d, Y_{\text{v,air}}),\\
\dot{T}_d &= b(r_d, T_d, T_{\text{air}}, Y_{\text{v,air}}),\\
\dot{T}_{\text{air}} &= c(r_d, T_d, T_{\text{air}}),\\
\dot{Y}_{\text{v,air}} &= d(r_d, T_d, Y_{\text{v,air}}).
\end{aligned}$$

P. W Longest and M. Hindle, Numerical model to characterize the size increase of combination drug and hygroscopic excipient nanoparticle aerosols (2011).

An Aerosol-fluid model with radius growth

We keep the same Navier-Stokes equation for the velocity field and add to the density function f the radius variable $r \in \mathbb{R}^+$. The new Vlasov-type equation writes :

$$\partial_t f + v \cdot \nabla_x f + \mathrm{div}_v(\alpha(u - v)f) + \nabla_r(a(r, Y_{\mathrm{v,air}})f) = 0.$$

We complete by considering an advection diffusion equation for the evolution of water vapor mass fraction $Y_{\mathrm{v,air}}$:

$$\partial_t Y_{\mathrm{v,air}} + (u \cdot \nabla) Y_{\mathrm{v,air}} - D\Delta Y_{\mathrm{v,air}} = S_y,$$

completed with the following boundary and initial conditions :

$$\left\{ \begin{array}{rcl} Y_{\mathrm{v,air}} & = & Y_{\mathrm{v,air,in}},\ \text{on } \Gamma^{\mathrm{in}}, \\ Y_{\mathrm{v,air}} & = & Y_{\mathrm{v,wall}},\ \text{on } \Gamma^{\mathrm{wall}}, \\ \frac{\partial}{\partial n} Y_{\mathrm{v,air}} & = & 0,\ \text{on } \Gamma^{\mathrm{out}}, \\ Y_{\mathrm{v,air}}(0, \cdot) & = & Y_{\mathrm{v,air,0}},\ \text{on } \Omega. \end{array} \right.$$

Definition of the source term S_y

Proposition

Under the assumption that $u = 0$, $\nabla Y_{v,air} = 0$ on $\partial\Omega$ and

$$S_y(t,x) = -\frac{\rho_w}{\rho_{air}} \int_{\mathbb{R}^3 \times \mathbb{R}^+} 4\pi r^2 a(r, Y_{v,air}) f(t,x,v,r) dvdr,$$

the mass conservation is satisfied :

$$\frac{d}{dt}\left(\int \frac{4}{3}\pi \rho_w r^3 f dxdvdr + \int \rho_{air} Y_{v,air} dx \right) = 0, \ \forall t \geq 0.$$

Remark

The mass conservation is in accordance with the one satisfied by the ODE system.

Numerical scheme

For the fluid and water vapor mass fraction computation, we apply a finite element method on freefem. For the Vlasov equation we discretise the density f as a weighted sum of dirac masses :

$$f(t,x,v,r) \sim f^N(t,x,v,r) := \sum_{i=1}^{N_{\text{num}}} \omega_i \, \delta_{x_i(t),v_i(t),r_i(t)}(x,v,r),$$

where $t \to (x_i(t), v_i(t))$ is the trajectory of the i^{th} particle in the phase space and $r_i(t)$ its radius. The number of initial particles N_{Num} is related to the physical aerosol particles N_{Aero} as follows :

$$N_{\text{Aero}} = \sum_{i=1}^{N_{\text{num}}} \omega_i.$$

Scheme algorithm

Iteration loop on $n \geq 0$

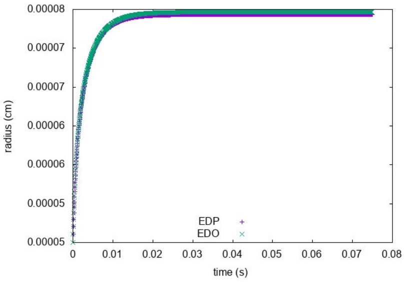
1. Computation of u^n with retroaction source term coming from the previous time step.
2. Computation of $Y^n_{\mathrm{v,air}}$ using u^n and the source term coming from the previous time step.

Local time loop for particles on $\tilde{n} \geq 0$

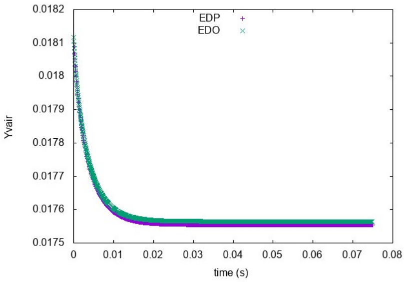
- Incrementation of the radius $r_i^{\tilde{n}}$ for the i^{th} particle (RK4).
- Computation of the velocity $v_i^{\tilde{n}}$ (implicit scheme).
- Computation of the position $x_i^{\tilde{n}}$ (explicit scheme).

$2D$ Numerical tests

Implementing the ODE model on Scilab and the aerosol-fluid model on Freefem we get :



(a) Radii comparison



(b) $Y_{\mathrm{v,air}}$ comparison

here Ω is a tube, the diffusion and the fluid velocity u are equal to 0.

Addition of temperature variation

Keeping the same Navier-Stokes equation we add to the density function f the droplet temperature $T \in \mathbb{R}$. The new Vlasov-type equation writes :

$$\partial_t f + v \cdot \nabla_x f + \mathrm{div}_v(\alpha(u-v)f) + \nabla_r(a(r, T, Y_{v,air})f) + \nabla_T(b(r, T, T_{\mathrm{air}}, Y_{v,air})f) = 0,$$

We complete by considering an advection diffusion equation for the air temperature T_{air} :

$$\rho_{\mathrm{air}} Cp_{\mathrm{air}}[\partial_t T_{\mathrm{air}} + (u \cdot \nabla) T_{\mathrm{air}}] - K_{\mathrm{air}} \Delta T_{\mathrm{air}} = S_T, \ \text{ on } \mathbb{R}^+ \times \Omega,$$

completed with the following boundary and initial conditions :

$$\begin{cases} T_{\mathrm{air}} &= T_{\mathrm{air,in}}, \ \text{ on } \Gamma^{\mathrm{in}}, \\ T_{\mathrm{air}} &= T_{\mathrm{wall}}, \ \text{ on } \Gamma^{\mathrm{wall}}, \\ \frac{\partial}{\partial n} T_{\mathrm{air}} &= 0, \ \text{ on } \Gamma^{\mathrm{out}}, \\ T_{\mathrm{air}}(0, \cdot) &= T_{\mathrm{air},0}, \ \text{ on } \Omega. \end{cases}$$

Definition of the source term S_T

Proposition

Under the assumption that $\nabla T_{air} = 0$, $u = 0$ on $\partial\Omega$ and

$$S_T(t,x) = \int [4\pi \rho_w r^2 L_v a(r,T,Y_{v,air}) - mCp_d b(r,T,T_{air},Y_{v,air})] f dv dr dT,$$

the thermal energy balance writes :

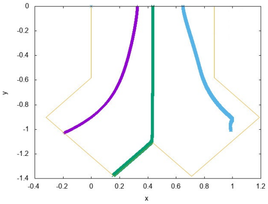
$$\rho_{air} Cp_{air} \int \partial_t T_{air} dx + Cp_d \int mb(r,T,T_{air},Y_{v,air}) f dx dv dr dT = \int 4\pi L_v r^2 \rho_w a(r,T,Y_{V,air}) f dx dv dr dT.$$

Remark

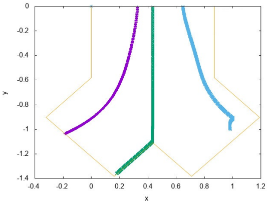
The thermal energy balance is in accordance with the one satisfied by the ODE system.

2*D* Numerical tests

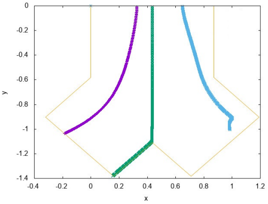
Particle position comparison with/without temperature variation



(a) With temperature



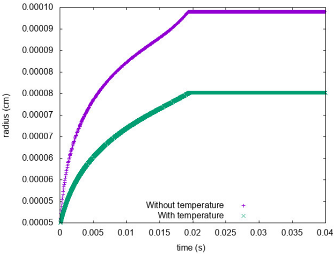
(b) Without temperature

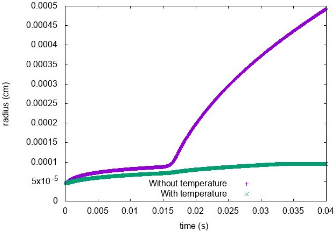


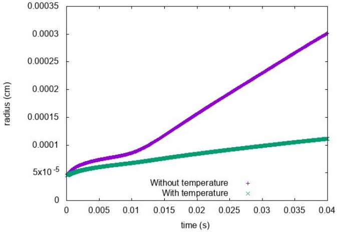
(c) Without radius growth

2*D* Numerical tests

Radii comparison with/without temperature variation

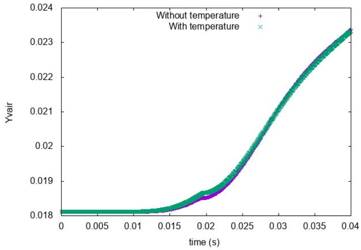


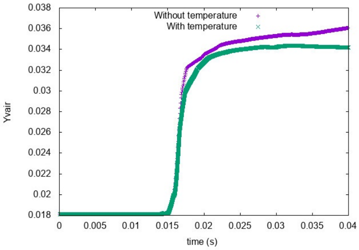


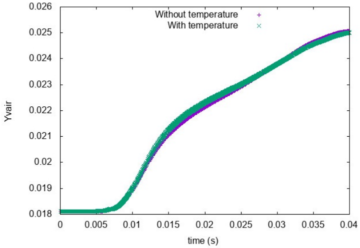


2D Numerical tests

$Y_{\mathbf{v,air}}$ comparison with/without temperature variation







Conclusion and prospects

Conclusion

- The radius growth rate is between 2 and 10.
- Including temperature variation in the model decreases the radius growth rate.

Prospects

- $3D$ implementation.
- Considering a multiple bifurcation tree.
- Existence and uniqueness of the coupled problem.
- Numerical tests on the aerosol deposition maps.

Thank you for your attention