Modelling of air flows and transport of pollutants in an enclosed environment.

Final defense

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Table of Contents

Table of Contents

General Context

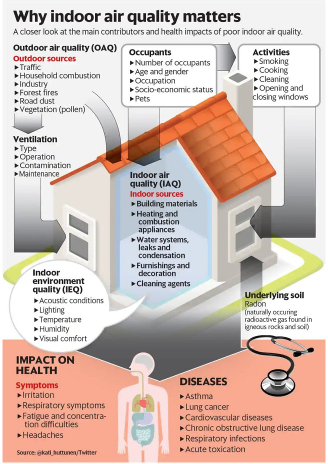


Figure: IAQ Infographic [1]

Indoor Environmental Quality (IEQ)

-> **Indoor Air Quality (IAQ) & Thermal Comfort**

-> IAQ indicators & Confinement indicators

-> we will use the **transport (ADR)** and **Navier-Stokes (CFD)** models

IAQ Indicators

ASHRAE [*ppm*]	**Building Bulletin** [*ppm*]	**Singapore** [*ppm*]
$1'000$	$1'500$	$1'000$

Table: CO_2 thresholds for IAQ [6][7]

Ethera sensors:

- $< 1'000$ (good IAQ)
- $1'000 - 1'700$ (advised to take action, i.e. ventilate etc)
- $> 1'700$ (poor IAQ resulting in fatigue, loss of concentration and others)

Road Map

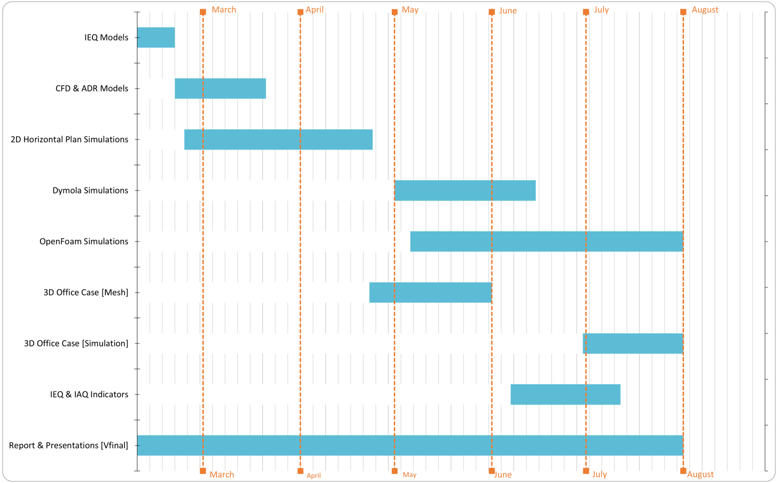


Figure: Gantt Chart [2]

Table of Contents

ADR Model

Transport Equation

$$\underbrace{\frac{\partial C}{\partial t}}_{\substack{\text{concentration}\\ \text{change over time}}} + \underbrace{\bar{u} \cdot \nabla C}_{\text{advection}} - \underbrace{k \Delta C}_{\text{diffusion}} + \underbrace{\mu C}_{\text{reaction}} = \bar{f} \qquad \text{in} \;\; \Omega \times [t_i, t_f]$$

where

- $C : \mathbb{R}^d \times [t_i, t_f] \to \mathbb{R}$: substance concentration
- $\bar{u} : \mathbb{R}^d \times [t_i, t_f] \to \mathbb{R}^d$: velocity field
- $k : \mathbb{R}^d \times [t_i, t_f] \to \mathbb{R}$: diffusion coefficient
- $\mu : \mathbb{R}^d \times [t_i, t_f] \to \mathbb{R}$: reaction coefficient
- $\bar{f} : \mathbb{R}^d \times [t_i, t_f] \to \mathbb{R}^d$: source term

and with the following notations:

- $\Omega \in \mathbb{R}^d$, $d = 2, 3$, is our considered domain
- t_i: initial time and t_f: final time
- $\bar{u}$: u is a vector field

CFD Model

Navier-Stokes Equations

$$\begin{cases} \rho_f \left.\dfrac{\partial \bar{u}_f}{\partial t}\right|_x + \rho_f(\bar{u}_f \cdot \nabla_x)\bar{u}_f - \nabla_x \cdot \bar{\bar{\sigma}}_f = \bar{f}_f^t & \text{in } \Omega_f^t \times [t_i, t_f] \\ \nabla_x \cdot \bar{u}_f = 0 & \text{in } \Omega_f^t \times [t_i, t_f] \end{cases}$$

where

- $\bar{u}_f$: fluid velocity $[m \cdot s^{-1}]$
- ρ_f: fluid density $[kg \cdot m^{-3}]$
- $\bar{f}_f^t$: external force $[kg \cdot m^{-3} \cdot s^{-1}]$

and with the following notations:

- $\left.\frac{\partial}{\partial t}\right|_x$: time derivative in the Eulerian reference frame
- ∇_x: gradient in the Eulerian reference frame
- $\bar{\bar{\sigma}}_f$: σ_f is a matrix field

CFD Model - Notations

Fluid stress tensor $\bar{\bar{\sigma}}_f$ $[N \cdot m^{-2}]$:

$$\bar{\bar{\sigma}}_f = -p_f \bar{I} + 2\mu_f \bar{D}(\bar{u}_f)$$

where

- p_f: pressure field $[kg \cdot m^{-1} \cdot s^{-2}]$
- $\bar{I}$: identity tensor
- μ_f: dynamic viscosity $[kg \cdot m^{-1} \cdot s^{-1}]$

Deformation tensor $\bar{D}(\bar{u}_f)$ $[m \cdot s^{-1}]$:

$$\bar{D}(\bar{u}_f) = \frac{1}{2}\left(\nabla_x \bar{u}_f + (\nabla_x \bar{u}_f)^\top\right)$$

Zero-equation turbulence model [1]

Turbulent viscosity:

$$\mu_{f,t} = 0.03874 \rho_f \bar{u}_f l$$

where

- $\bar{u}_f$: local mean velocity
- l: distance to the nearest closure

Effective viscosity:

$$\mu_{f,eff} = \mu_{f,t} + \mu_f$$

where

- μ_f: laminar viscosity

[1] *A zero-equation turbulence model for indoor airflow simulation*

Pulse Respiration Profiles

Created with the **Pulse Physiology** software:

Figure: Pulse Physiology logo [8]

	Female	**Male**
Year $[yr]$	27	27
Height $[cm]$	160	190
Weight $[kg]$	55	77
Exercise Intensity $[-]$	9.29×10^{-5}	1.32×10^{-4}

Table: Profiles of 2 people in office

Note: The exercise intensity is low as it consists of office work that does not represent a huge effort.

Source terms

Transport Equation

$$\underbrace{\frac{\partial C}{\partial t}}_{\substack{\text{concentration}\\ \text{change over time}}} + \underbrace{\bar{u} \cdot \nabla C}_{\text{advection}} - \underbrace{k \Delta C}_{\text{diffusion}} + \underbrace{\mu C}_{\text{reaction}} = \bar{f} \qquad \text{in } \Omega \times [t_i, t_f]$$

Source term modelled with Pulse: Carbon Dioxide Production Rate $[mL/min]$

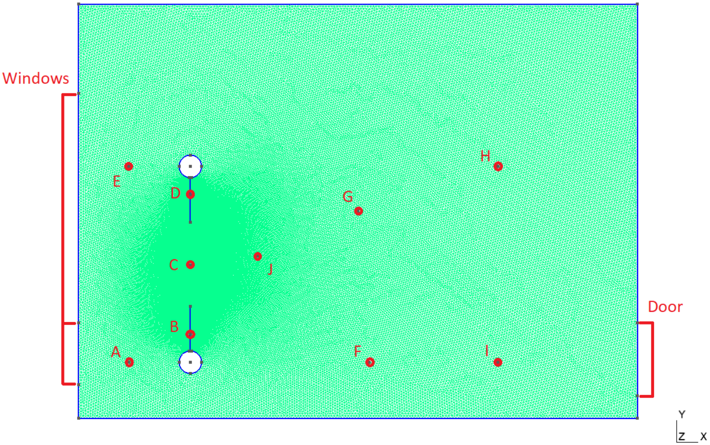
Navier-Stokes Equations

$$\begin{cases} \rho_f \left.\dfrac{\partial \bar{u}_f}{\partial t}\right|_x + \rho_f (\bar{u}_f \cdot \nabla_x) \bar{u}_f - \nabla_x \cdot \bar{\bar{\sigma}}_f = \bar{f}_f^t & \text{in } \Omega_f^t \times [t_i, t_f] \\ \nabla_x \cdot \bar{u}_f = 0 & \text{in } \Omega_f^t \times [t_i, t_f] \end{cases}$$

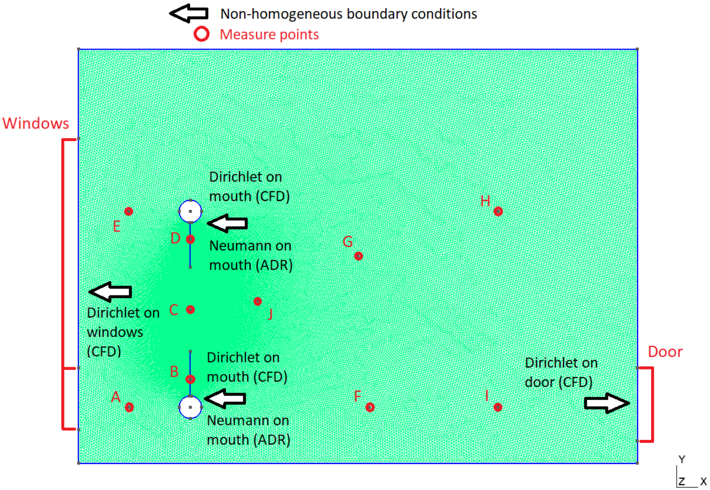
Source term modelled with Pulse: Expiratory Flow $[mL/s]$

Table of Contents

Geometry (horizontal plan) - Office room at UFR



Geometry (horizontal plan) - Office room at UFR



Model Setup & Respiration Movement

Simulation setup:

Parameter	Quantity	Value	Unit
k	diffusion coefficient	1.6×10^{-5}	$m^2 \cdot s^{-1}$
ρ	fluid density	1.23	$kg \cdot m^{-3}$
μ	dynamic viscosity	1×10^{-4}	$Pa \cdot s$

Table: Model Parameters

Video of respiratory movement:

[Video]

Resolution with Feelpp (2D horizontal plan) - 4h simulation

BuildingSystems Model

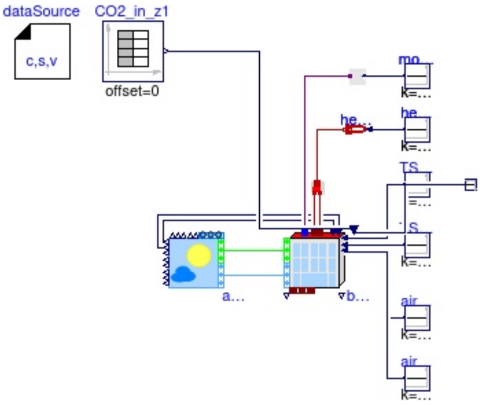
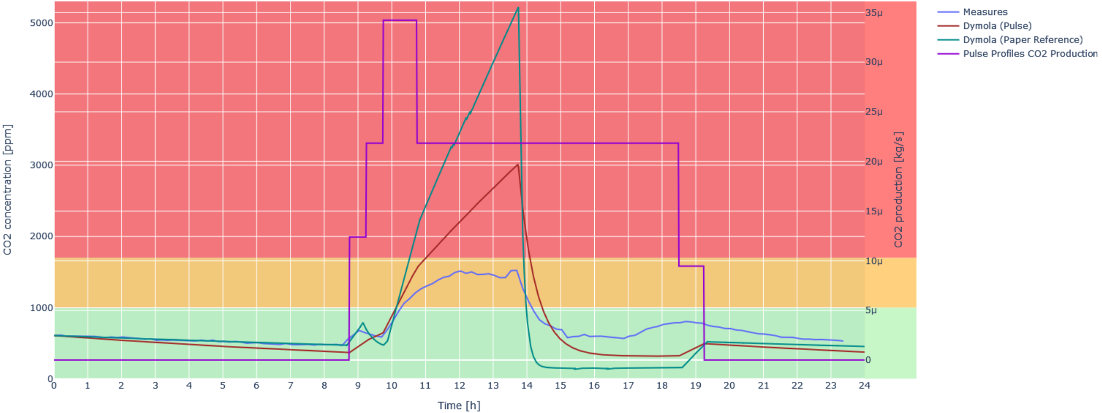


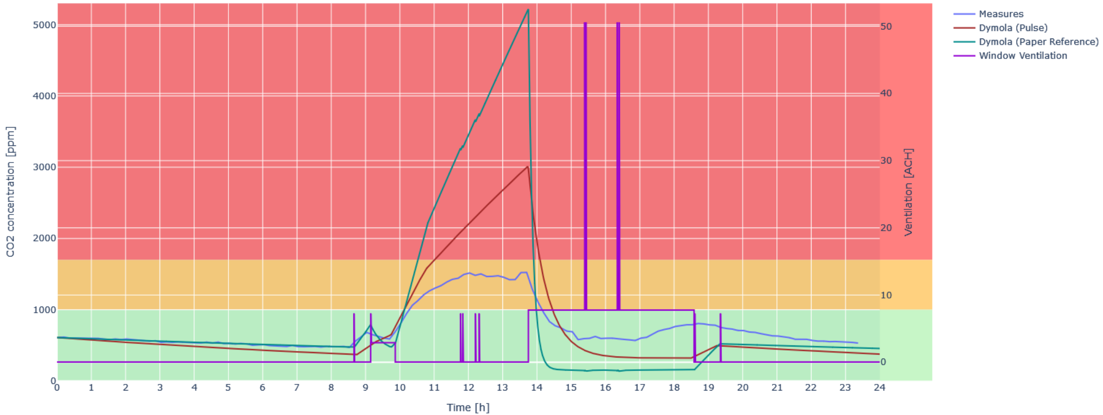
Figure: Modelisation of office 228

- Open-source library from Modelica used for building energy simulation at room, building and district levels
- Library is used in the Ktirio project for thermal simulation
- **2 zones:** one zone modelling the office room and a second zone modelling the corridor

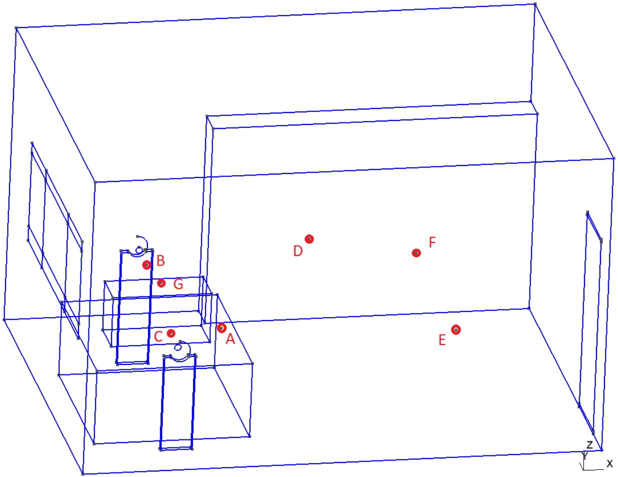
Resolution with BuildingSystems



Resolution with BuildingSystems



Geometry (3D) - Office room at UFR



3D Model Setup

Simulation setup:

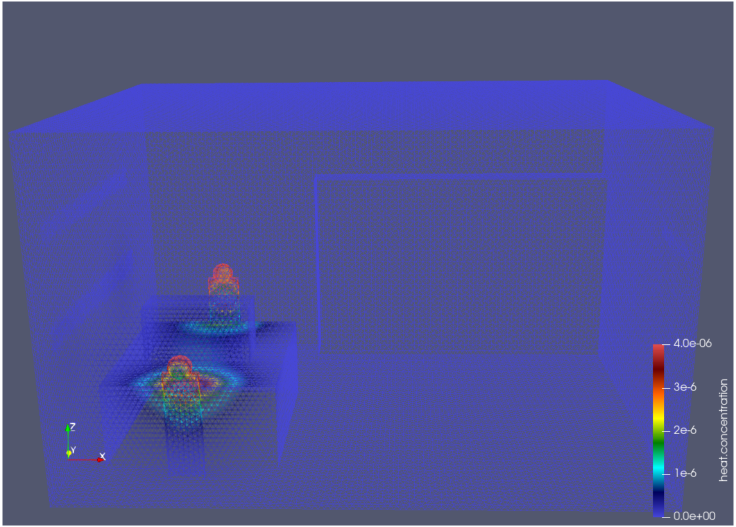
Condition	Marker	Value
inlet for flow velocity	Mouth_m	2.960×10^{-9}
inlet for flow velocity	Mouth_f	8.783×10^{-9}
flux on concentration	Mouth_m	2.418×10^{-7}
flux on concentration	Mouth_f	1.748×10^{-7}

Table: Boundary Conditions

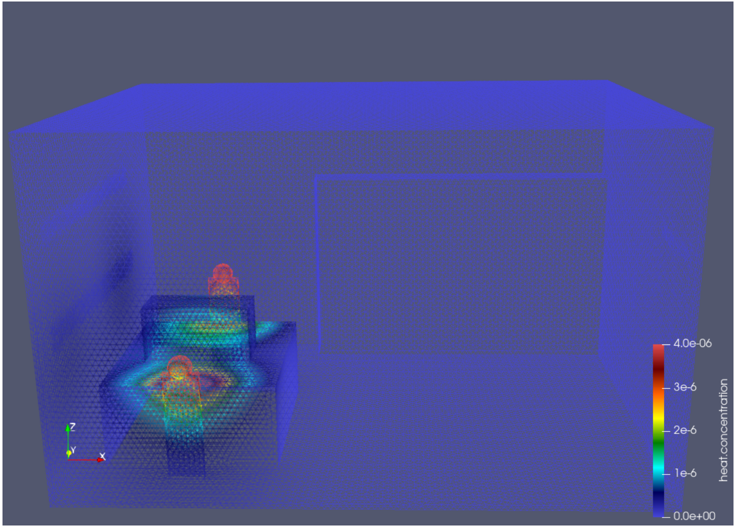
-> **no ventilation**

-> 2-step simulation: **stationnary** and **transient** step

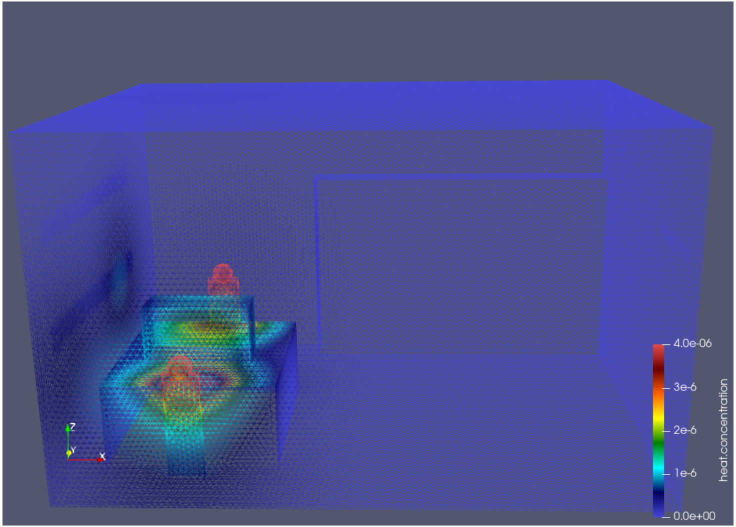
Resolution with Feelpp (3D) - Concentration after 1h



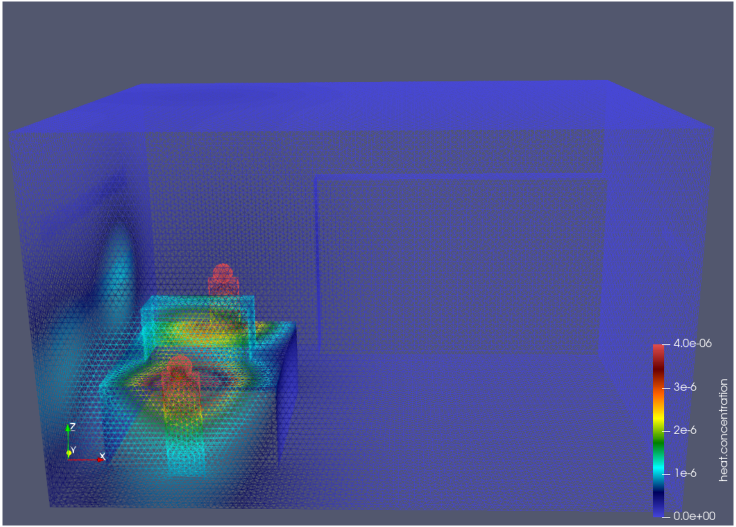
Resolution with Feelpp (3D) - Concentration after 2h



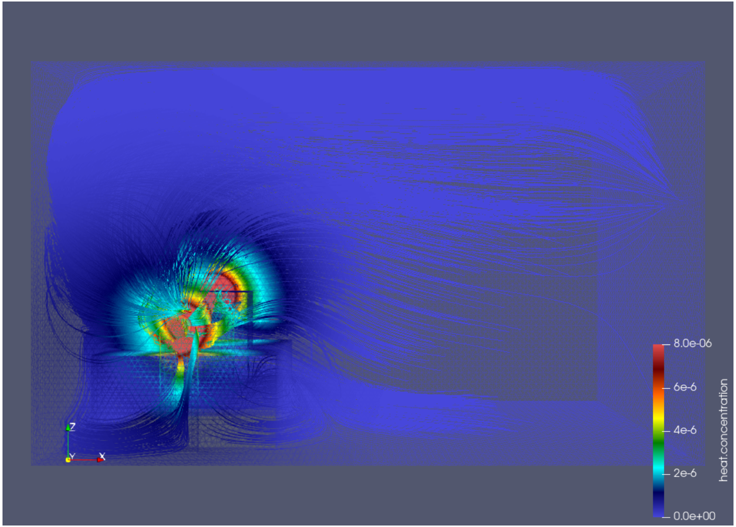
Resolution with Feelpp (3D) - Concentration after 3h



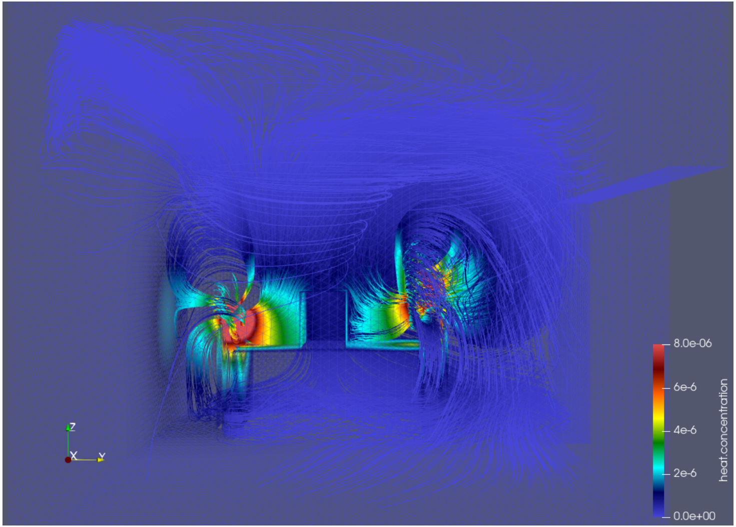
Resolution with Feelpp (3D) - Concentration after 4h



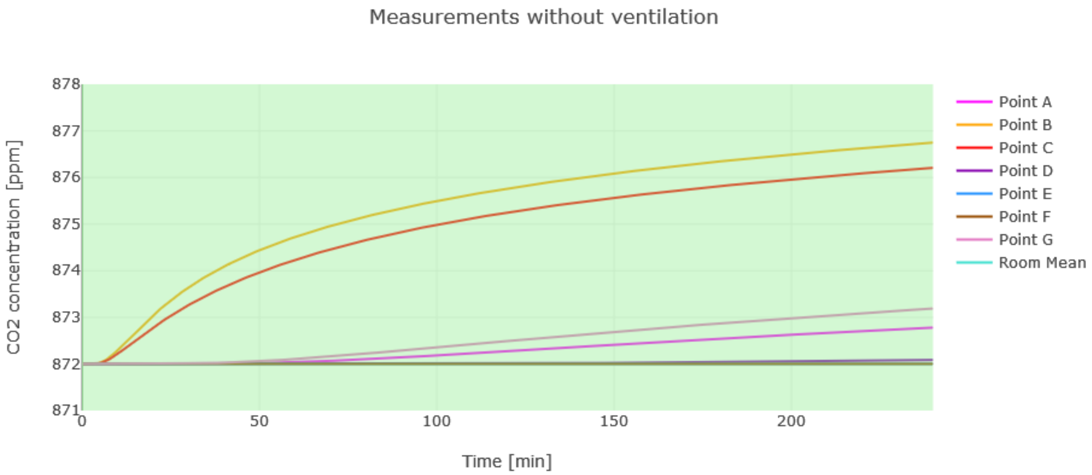
Resolution with Feelpp (3D) - Concentration stream after 4h



Resolution with Feelpp (3D) - Concentration stream after 4h



Resolution with Feelpp (3D) - 4h simulation



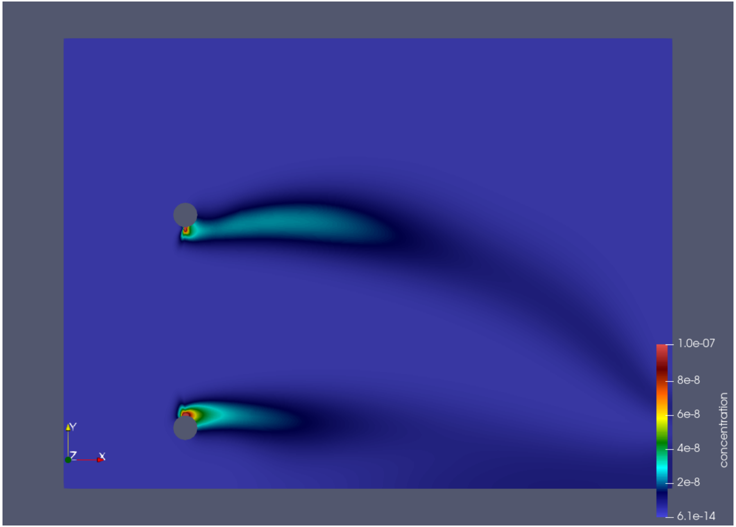
OpenFOAM

- One of the leading open source software for **C**omputational **F**luid **D**ynamics
- Carry out 2D simulations in horizontal plan
- Implementation of the `scalartransportsimpleFoam` solver

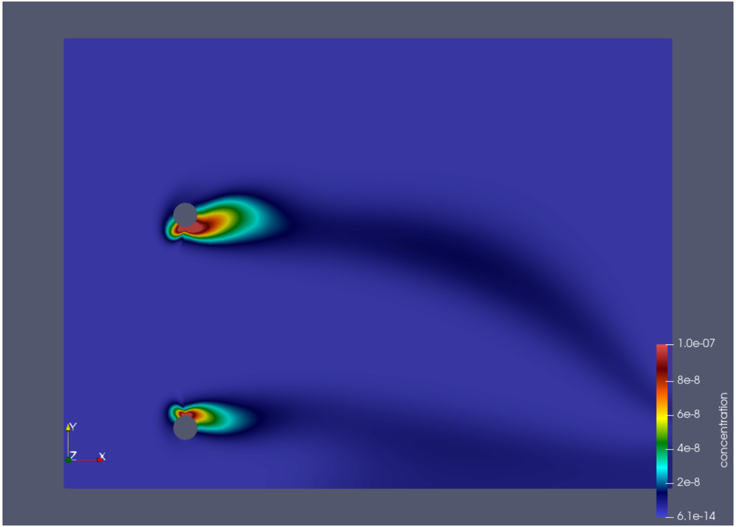
Open∇FOAM®

Figure: OpenFOAM logo [9]

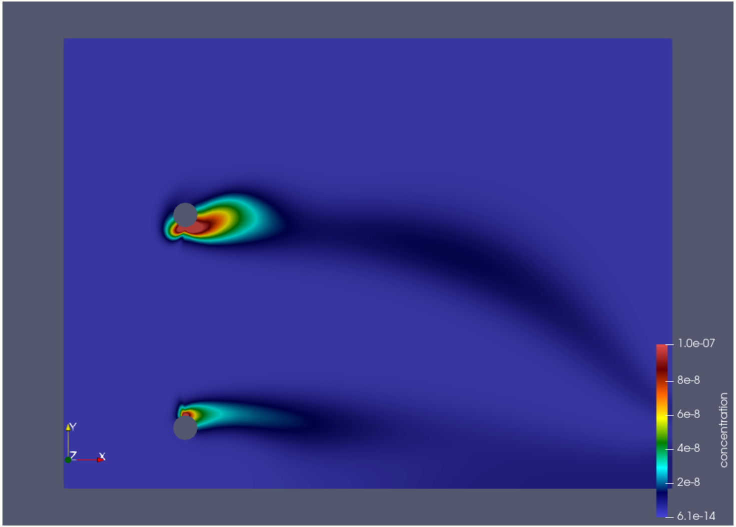
Resolution with OpenFOAM - Concentration after 10min



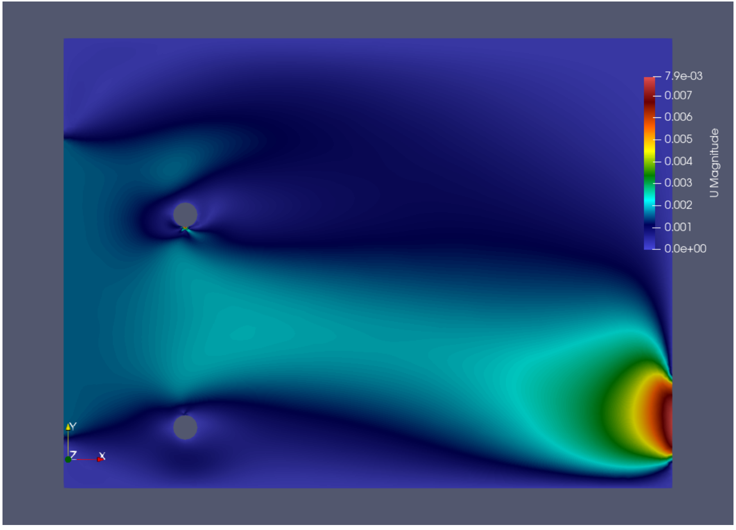
Resolution with OpenFOAM - Concentration after 30min



Resolution with OpenFOAM - Concentration after 4h



Resolution with OpenFOAM - Ventilation velocity



Calculation of IAQ Indicator

$$\Sigma IAQ_{\text{index}} = 100 - \left(W_{P_1} \cdot PD_{P_1} + W_{P_2} \cdot PD_{P_2} + \cdots + W_{P_j} \cdot PD_{P_j}\right)$$

where $W_{P_1,...,P_j}$ are the weights associated to the different pollutants $P_1, \ldots, P_j$ considered. These weights are given by the following relations:

$$W_i = \frac{\Delta c_i}{\sum_{i=1}^{j} \Delta c_i} \,, \qquad \sum_{i=1}^{j} W_i = 1 \,,$$

with Δc_i the excess concentration defined by

$$\Delta c_i = c_i - c_{\text{ref}} \,,$$

where c_i is the concentration of pollutant P_i and c_{ref} the associated reference concentration. [10][11]

IAQ Indicators - Scenario of a working day

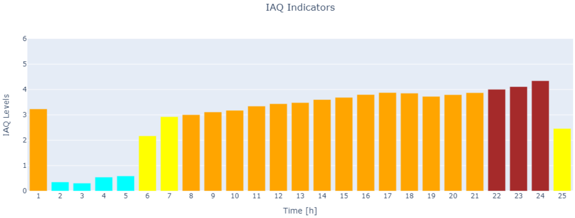


Figure: Self-made indicators

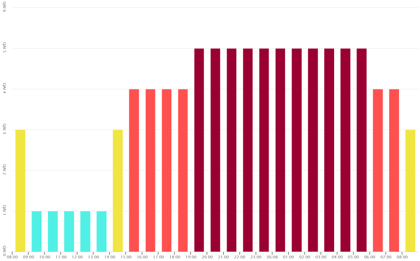


Figure: Ethera indicators

ICO Indicators - Scenario of a working day

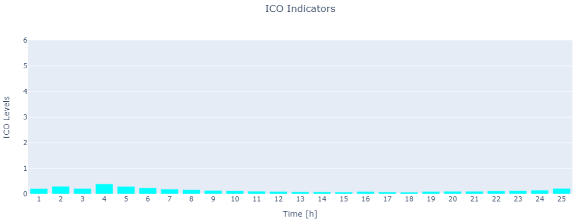


Figure: Self-made indicators

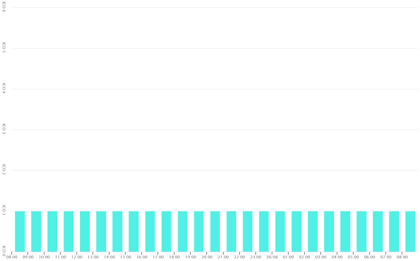


Figure: Ethera indicators

Table of Contents

-> We manage to make simulations with more or less coherent visualisation results

-> We are generally not coinciding with the measures

-> There are several possible reasons for these differences e.g.

- the complicated modelling of natural ventilation
- physical effects that are not taken into account
- possible slight variations in measurements
- the respiration profiles

-> Further exploration of OpenFOAM and its parameterisation

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ADR Model

Convective Heat Equation

$$\rho C_p \left(\frac{\partial T}{\partial t} + \bar{\beta} \cdot \nabla T \right) - \nabla \cdot (k \nabla T) = \bar{f} \qquad \text{in } \Omega \times [t_i, t_f] \,, \tag{2}$$

with

- T $[K]$: temperature
- C_p $[J \cdot kg^{-1} \cdot K^{-1}]$: specific heat
- ρ $[kg \cdot m^{-3}]$: fluid density
- $\bar{\beta}$ $[m \cdot s^{-1}]$: fluid velocity
- k $[m^2 \cdot s^{-1}]$: diffusion coefficient
- $\bar{f}$ $[J \cdot m^{-3} \cdot s^{-1}]$: source term

ADR Model

$$\rho\left(\frac{\partial C}{\partial t} + \bar{\beta}\cdot\nabla C\right) - \nabla\cdot(k\nabla C) = \bar{f} \qquad \text{in } \Omega\times[t_i, t_f]\ , \tag{3}$$

with

- C: substance concentration
- ρ $[kg \cdot m^{-3}]$: fluid density
- $\bar{\beta}$ $[m \cdot s^{-1}]$: fluid velocity
- k $[m^2 \cdot s^{-1}]$: diffusion coefficient
- $\bar{f}$ $[kg \cdot m^{-3} \cdot s^{-1}]$: source term

CFD Model - Variational formulation

The boundary of the domain $\Omega_f^t \in \mathbb{R}^d$, $d = 2, 3$:

$$\partial\Omega_f^t = \Gamma^t = \Gamma_D^t \cup \Gamma_N^t$$

has the following boundary conditions:

$$\begin{aligned} \bar{u}_f &= \bar{g}_D^t \quad \text{on } \Gamma_D^t \times [t_i, t_f] \\ \bar{\bar{\sigma}}_f \bar{n}_f &= \bar{g}_N^t \quad \text{on } \Gamma_N^t \times [t_i, t_f] \end{aligned}$$

where the functions $\bar{g}_D^t \in L^2(\Gamma_D^t)$ and $\bar{g}_N^t \in L^2(\Gamma_N^t)$ are supposed to be known.

We thus have: $\bar{u}_f : \Omega_f^t \times [t_i, t_f] \to \mathbb{R}^d$ and $\bar{f}_f^t : \Omega_f^t \times [t_i, t_f] \to \mathbb{R}^d$.

CFD Model - Variational formulation

Find $(\bar{u}_f, p_f) \in V \times Q$ such that $\forall(\bar{v}, q) \in W \times Q$:

$$\begin{cases} \rho_f \int_{\Omega_f^t} \left.\frac{\partial \bar{u}_f}{\partial t}\right|_x \cdot \bar{v} + \rho_f \int_{\Omega_f^t} (\bar{u}_f \cdot \nabla_x)\bar{u}_f \cdot \bar{v} + \int_{\Omega_f^t} \bar{\bar{\sigma}}_f : \nabla_x \bar{v} - \int_{\Gamma_N^t} \bar{g}_N^t \cdot \bar{v} = \int_{\Omega_f^t} \bar{f}_f^t \cdot \bar{v} \\ \int_{\Omega_f^t} q \nabla_x \cdot \bar{u}_f = 0 \end{cases}$$

where

$$V = \left\{ H^1_{(\bar{g}_D^t, \Gamma_D^t)}(\Omega_f^t) \right\}^d , \quad Q = L^2(\Omega_f^t) , \quad W = \left\{ H^1_{(0, \Gamma_D^t)}(\Omega_f^t) \right\}^d$$

CFD Model - Spatial discretization

Find $(\bar{u}_{f,\delta}, p_{f,\delta}) \in V_\delta \times Q_\delta$ such that $\forall(\bar{v}, q) \in W_\delta \times Q_\delta$:

$$\begin{cases} \rho_f \displaystyle\int_{\Omega^t_{f,\delta}} \left.\frac{\partial \bar{u}_{f,\delta}}{\partial t}\right|_x \cdot \bar{v} + \rho_f \int_{\Omega^t_{f,\delta}} (\bar{u}_{f,\delta} \cdot \nabla_x)\bar{u}_{f,\delta} \cdot \bar{v} \\ \qquad + \displaystyle\int_{\Omega^t_{f,\delta}} \bar{\bar{\sigma}}_{f,\delta} : \nabla_x \bar{v} - \int_{\Gamma^t_{N,\delta}} \bar{g}^t_N \cdot \bar{v} = \int_{\Omega^t_{f,\delta}} \bar{f}^t_{f,\delta} \cdot \bar{v} \\ \displaystyle\int_{\Omega^t_{f,\delta}} q \nabla_x \cdot \bar{u}_{f,\delta} = 0 \end{cases}$$

where

$$V_\delta = \left\{ H^1_{(\bar{g}^t_D, \Gamma^t_{D,\delta})}(\Omega^t_{f,\delta}) \right\}^d \cap \left\{ P^M_c(\Omega^t_{f,\delta}) \right\}^d \quad \text{and} \quad W_\delta = \left\{ H^1_{(0, \Gamma^t_{D,\delta})}(\Omega^t_{f,\delta}) \right\}^d \cap \left\{ P^N_c(\Omega^t_{f,\delta}) \right\}^d$$

CFD Model - Time discretization using *BDF* scheme

Find $(\bar{u}_{f,\delta}, p_{f,\delta}) \in V_\delta \times Q_\delta$ such that $\forall(\bar{v}, q) \in W_\delta \times Q_\delta$:

$$
\begin{cases}
\rho_f \dfrac{\beta_{-1}}{\Delta t} \displaystyle\int_{\Omega_{f,\delta}^{t_{n+1}}} \bar{u}_{f,\delta}^{n+1} \cdot \bar{v} + \rho_f \int_{\Omega_{f,\delta}^{t_{n+1}}} (\bar{u}_{f,\delta}^{n+1} \cdot \nabla_x) \bar{u}_{f,\delta}^{n+1} \cdot \bar{v} \\
\qquad + \displaystyle\int_{\Omega_{f,\delta}^{t_{n+1}}} \bar{\bar{\sigma}}_{f,\delta}^{n+1} : \nabla_x \bar{v} - \int_{\Gamma_{N,\delta}^{t_{n+1}}} \bar{g}_N^{t_{n+1}} \cdot \bar{v} = \int_{\Omega_{f,\delta}^{t_{n+1}}} \bar{\tilde{f}}_f^{t_{n+1}} \cdot \bar{v} \\
\qquad \displaystyle\int_{\Omega_{f,\delta}^{t_{n+1}}} q \nabla_x \cdot \bar{u}_{f,\delta}^{n+1} = 0
\end{cases}
$$

where

$$
\left.\frac{\partial \bar{u}_{f,\delta}^{n+1}}{\partial t}\right|_x \approx \frac{\beta_{-1}}{\Delta t} \bar{u}_{f,\delta}^{n+1} - \sum_{j=0}^{q-1} \frac{\beta_j}{\Delta t} \bar{u}_{f,\delta}^{n-j} \quad \text{and} \quad \bar{\tilde{f}}_f^{t_{n+1}} = \bar{f}_f^{t_{n+1}} + \sum_{j=0}^{q-1} \frac{\beta_j}{\Delta t} \bar{u}_{f,\delta}^{n-j}
$$