

**SIMULATIONS OF STREET-CANYON AIR-QUALITY USING FLUID  
DYNAMICS AND AEROSOL MODELLING**

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**Abstract:** High concentrations of nitrogen dioxide and particulate matter are often observed locally in streets. Because of the spatial resolution limit, regional-scale chemical transport models cannot reproduce these high concentrations. Traditional local-scale methods such as computational fluid dynamics (CFD) often neglect chemical reactions and aerosol dynamics, which leads to inaccuracy in the simulation of local air quality. In this study, 2D CFD simulations performed by Code\_Saturne and OpenFOAM and coupled with the chemical aerosol module SSH-Aerosol are used to model pollutant dispersion, chemical reactions and aerosol dynamics during a period of 12 hours (from 4 a.m. to 4 p.m., local time, GMT+2h) in a street of Greater Paris. For both CFD codes, the setup is validated by comparing the simulated NO<sub>2</sub> and PM<sub>10</sub> concentrations with measurements. The impact of turbulence model and coupling strategy on reactive and non-reactive pollutant concentrations is assessed by comparing the concentrations simulated by two codes. This comparison of the CFD tools provides a qualitative estimation of the uncertainty associated with the modelling of the atmospheric flow and of the coupling between dispersion, chemistry and aerosol dynamics.

In order to understand the impact of chemical processes on aerosol formation, sensitivity tests concerning gas chemistry and aerosol dynamics are conducted. A non-neglectable under-estimation of some pollutant concentrations is observed when gas chemistry and aerosol dynamics are not taken into account. Gas chemistry significantly increases NO<sub>2</sub> concentrations in the street, which is underestimated by 41% on average when gas chemistry is not considered. Although the impact of gas chemistry on inorganic and organic condensables is limited, inorganic and organic aerosol concentrations in the street are largely impacted by aerosol dynamics. For inorganic aerosols the concentrations increase because of the formation of ammonium nitrate, partly due to the ammonia emission by traffic and partly due to the lack of thermodynamic equilibrium between gas and aerosols in the background regional concentration with high concentrations of nitric acid. For organic aerosols, the concentrations are strongly influenced by the increase of inorganic aerosols.

**Key words:** *CFD, Street canyon, secondary aerosols.*

## INTRODUCTION

High concentrations of nitrogen dioxide (NO<sub>2</sub>) and particulate matter (PM) are often observed in urban street canyons, becoming a global sanitary problem. In order to model these concentrations, it is necessary to model the dispersion and transportation of several species. Computational fluid dynamics (CFD) modeling is powerful in estimating the local-scale flow and air quality because of the high resolution. However, due to the high computational cost linked to the modelling of the flow, most CFD models treat pollutants as passive scalars and they do not take into account chemical reactions between different species (Zhang et al, 2020). Neglecting chemistry may lead an underestimation of some species, for example, nitrogen dioxide and organic condensables (Lugon et al, 2020), which are important to represent PM formation. Although chemical models are increasingly coupled with CFD models (Kikumoto et al, 2012; Zhong et al, 2014), most of these chemical models neglect the formation of condensables, because they were originally designed to simulate ozone formation (Kim and Ooka, 2011) and not PM. In this study, a chemical aerosol module taking into account the formation of condensables, SSH-Aerosol (Sartelet et al,

2020), is coupled to two CFD tools: Code\_Saturne (Archembeau et al, 2004) and OpenFoam (OpenFoam, 2020). Atmospheric dispersion, gas chemistry and aerosol dynamics are simulated and analysed in the following sections. To understand the role of chemistry and aerosol dynamics, passive simulations (passive case) as well as simulations with both chemistry and aerosol dynamics (chemistry case) are analysed.

## MODEL PRESENTATION

The CFD tools used are Code\_Saturne v6.2 and OpenFoam v2012. Different turbulence schemes are used in the two models. In Code\_Saturne, k- $\epsilon$  linear production is used to solve the turbulence while in OpenFoam, RNG k- $\epsilon$  model is employed. The 0-dimensional aerosol box model SSH-Aerosol is coupled to both CFD models. The modified version of the chemistry mechanism Carbon Bond Version 5 (CB05) (Yarwood et al, 2005) included in SSH-Aerosol is used for gas-phase chemistry. The coupling between SSH-Aerosol and the CFD models is realized through the application program interface (API).

## MODEL SETUP

The street “Boulevard Alsace-Lorraine” in Greater Paris is simulated by a 2-dimensional setup. Figure 1 shows the domain of the simulations. The building height (H) on both sides of the street is 8.5 m and the width (W) of the street is 27.5 m. This corresponds to an “intermediate” aspect ratio (0.31) (Lugon et al, 2020). Traffic is considered as a street emission source and is simulated as a surface source which is placed in the middle of the street. The inlet is set at the left and the top of the domain and the outlet is set at the right of the domain.

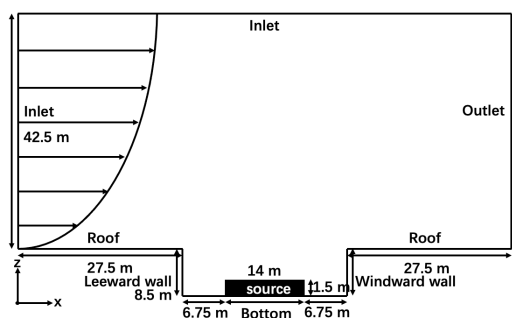


Figure 1. Street canyon domain of the model.

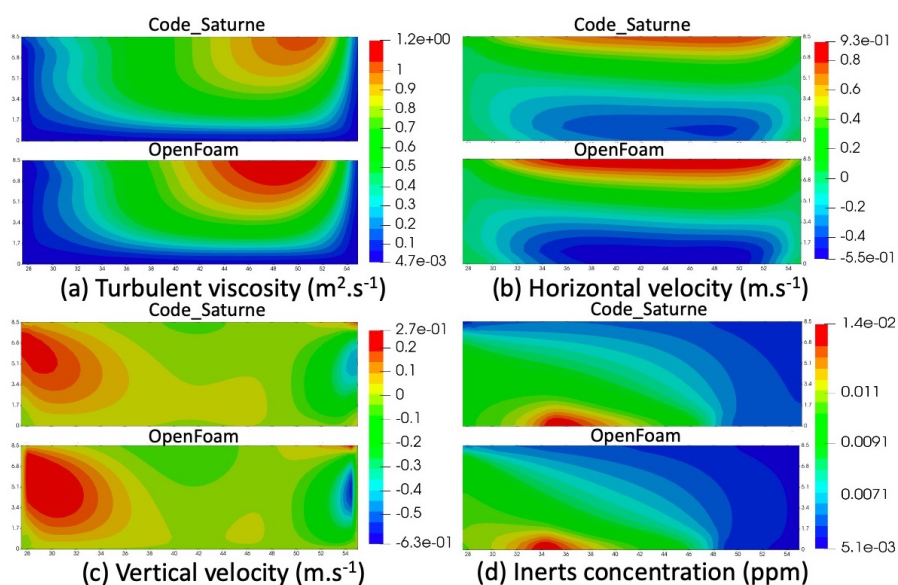
The simulation lasts 12.5h from 4h30 to 17h on the 30<sup>th</sup> April, 2014 in local time of Paris (GMT+2), with a constant time step  $\Delta t$  of 0.5 s . The first 30 minutes is the model spin-up time. Meteorological boundary conditions including hourly-varying temperature (T), humidity (H) and friction velocity ( $u$ ) are obtained from Weather Research and Forecasting (WRF) simulations (Sartelet et al, 2018). Wind direction is set perpendicular to the length of the street. Hourly-varying background concentration of simulation species is acquired from regional-scale simulations (Sartelet et al, 2018) and the hourly-varying traffic emission is calculated from the COPERT (Computer Program to calculate Emissions from Road Transport, version 2019, EMEP/EEA, 2019) methodology (Kim et al, 2022). These boundary conditions are interpolated linearly in time. As detailed in Lin et al. (2022), the simulated concentrations of NO<sub>2</sub> and PM<sub>10</sub> compare well with observations.

## COMPARISON OF CODE\_SATURNE AND OPENFOAM SIMULATIONS

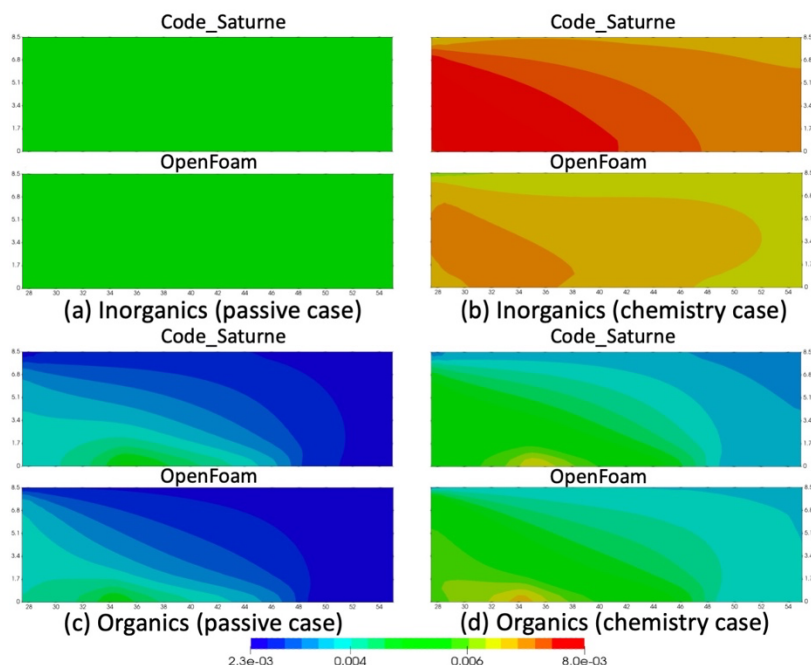
As discussed in Lin et al (2022), the simulations conducted with Code\_Saturne and OpenFoam lead to slight differences in NO<sub>2</sub> ( $67.6 \mu\text{g} \cdot \text{m}^{-3}$  in OpenFoam and  $70.0 \mu\text{g} \cdot \text{m}^{-3}$  in Code\_Saturne) and PM<sub>10</sub> ( $22.3 \mu\text{g} \cdot \text{m}^{-3}$  in OpenFoam and  $23.4 \mu\text{g} \cdot \text{m}^{-3}$  in Code\_Saturne) concentrations. In this section, simulations conducted by the two CFD tools are presented and a detailed comparison between the different compounds of particles is computed and analyzed.

Figure 2 compares the time-averaged air flow field and the time-averaged concentration field of inert particle components in the street canyon. As shown in Figure 2 (a), the differences in turbulent scheme result in a larger turbulent viscosity at the top of the street in OpenFoam than in Code\_Saturne. The horizontal and vertical wind velocity fields are also higher at the top of the street and lower at the bottom, as shown in Figure 2 (b) and Figure 2 (c). In OpenFoam, the vortex simulated in the street is also slightly

larger, with larger wind speed in the vortex. These differences in the flow field results in differences in the concentration field. Figure 2 (d) shows the comparison of time-averaged inert particle (dust, black carbon) concentrations in the street. Inert particles are not chemically reactive. Although their spatial distribution is similar in two models, the inert concentration averaged over the canyon is slightly lower in OpenFoam ( $9.0 \mu\text{g} \cdot \text{m}^{-3}$ ) than in Code\_Saturne ( $10.0 \mu\text{g} \cdot \text{m}^{-3}$ ); as the turbulent viscosity is higher in OpenFoam, emitted pollutants are more dispersed out of the canyon. In addition, because of the longer vortex in the x direction in OpenFoam, the concentrations are higher in the leeward side compared to Code\_Saturne.



**Figure 2.** Time-average flow field and inert concentration field in Code\_Saturne and OpenFoam.



**Figure 3.** Time-averaged inorganic and organic concentrations in Code\_Saturne and OpenFoam, the unit is ppm. Considering the reactive compounds of particles, Figure 3 compares the time-average inorganic and organic aerosol concentrations in the passive and chemistry cases. For inorganic aerosols in Figure 3 (a) and (b), the average concentration in Code\_Saturne is slightly larger than in OpenFoam both in the passive and the chemistry cases: in the passive case, the street-average inorganic concentration is  $5.8 \mu\text{g} \cdot \text{m}^{-3}$  in

OpenFoam and  $6.1 \mu\text{g}\cdot\text{m}^{-3}$  in Code\_Saturne; In the chemistry case, the street-average inorganic concentration is  $7.9 \mu\text{g}\cdot\text{m}^{-3}$  in OpenFoam and  $8.2 \mu\text{g}\cdot\text{m}^{-3}$  in Code\_Saturne. This can be explained by the different turbulent models, which result in slightly different exchanges between the street and the background concentrations above the street. A large fraction of inorganics comes from the background concentrations (boundary conditions) as shown by the uniformity of concentrations in Figure 3(a). For organic aerosols, in the passive case, the spatial distribution difference is similar to inert matter in Figure 2 (c), as there are strong emissions in the street. The average organics concentration in OpenFoam ( $3.5 \mu\text{g}\cdot\text{m}^{-3}$ ) is lower than in Code\_Saturne ( $3.9 \mu\text{g}\cdot\text{m}^{-3}$ ), which is caused by the different turbulence scheme. In the chemistry case, organic aerosol concentrations near the ground at the leeward side in OpenFoam ( $5.4 \mu\text{g}\cdot\text{m}^{-3}$  on average) is however slightly larger than in Code\_Saturne ( $5.3 \mu\text{g}\cdot\text{m}^{-3}$  on average). This may be caused by the different velocities in the two models.

## IMPACT OF CHEMISTRY ON THE FORMATION OF GAS AND AEROSOLS

### Impact of chemistry on NO<sub>2</sub>

The gas chemistry has a large impact on reactive gaseous species, which influences the formation of some secondary pollutants. Figure 4 presents the time-average NO<sub>2</sub> concentration in the street. Gas chemistry promotes its formation in the street, leading to an average increase of 40.5% in Code\_Saturne and 46.7% in OpenFoam. The impact of gas chemistry is more significant in OpenFoam than in Code\_Saturne, especially the flow differences between the two models lead to slightly more accumulation of emitted pollutants, such as NO, on the leeward side of the street. NO forms NO<sub>2</sub>, as it accumulates to the leeward side.

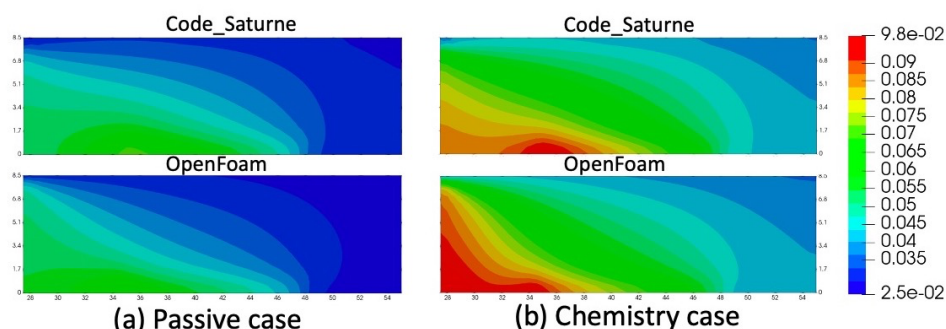


Figure 4. Time-average NO<sub>2</sub> concentration field in Code\_Saturne and OpenFoam, the unit is ppm.

### Impact of chemistry on inorganic and organic aerosols

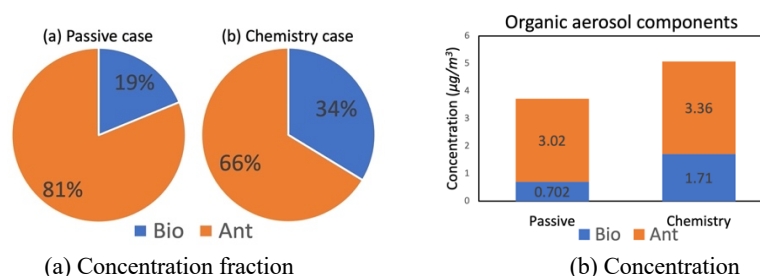
Gas chemistry and aerosol dynamics lead to a significant increase of the average concentration of PM<sub>10</sub> in the street. For the inorganic components of PM<sub>10</sub>, the increase mainly comes from the increase of ammonium nitrate. In Code\_Saturne and in OpenFoam, the increase of ammonium nitrate concentration is comparable ( $+1.9 \mu\text{g}\cdot\text{m}^{-3}$  on average in both OpenFoam and Code\_Saturne). Ammonium nitrate is not directly emitted from the traffic, but is formed from the condensation of ammonia (NH<sub>3</sub>) and nitric acid (HNO<sub>3</sub>). NH<sub>3</sub> is emitted from the traffic, and HNO<sub>3</sub> is formed from the oxidation of NO<sub>2</sub>. As the formation of HNO<sub>3</sub> from NO<sub>2</sub> is too slow to be formed efficiently in the street, the increase of ammonium nitrate is mostly due to aerosol dynamics, and not gas chemistry.

For organic aerosols, as is shown in Figure 5 (a), the fraction of biogenic organic compounds in the chemistry case is significantly larger than in the passive case. Figure 5 (b) shows the concentration of biogenic and anthropogenic compounds on average in the passive and chemistry cases, when chemistry is activated, more than 70% of the organic aerosols increase comes from the increase of biogenic compounds. As biogenic organic aerosols are assumed to be hydrophilic in the model while most anthropogenic organic aerosols are hydrophobic, the increase of ammonium nitrate enhances the condensation of hydrophilic species, and hence biogenic organic aerosols.

## CONCLUSIONS

The formation of gaseous and particle concentrations in a street of Greater Paris was simulated with two different CFD tools coupled with the same chemical model. Different turbulent schemes and pollutant

dispersion only slightly impact the airflow and the concentrations. The gas and aerosol chemistry significantly impacts the formation of secondary gaseous concentrations, such as  $\text{NO}_2$ , and to a lesser extent the formation of inorganic and organic aerosols. Inorganics increase because of ammonia emission. The increase of organics is partly due to the increase of hydrophilic compounds (biogenics) enhanced by the increase of inorganic concentrations.



**Figure 5.** Time-average anthropogenic and biogenic concentration fraction in passive case and chemistry cases. Bio represents biogenic compounds; Ant represents anthropogenic compounds.

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