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Air flow and spreading of pollution in an inhabited area

REPORT FROM THE STUDENT INTERNSHIP

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Summary

Abstract of the report will be there

Acknowledgements

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Contents

1 Introduction

The present work arose as the part of the authors student internship in Taiwan National Applied Research Laboratories (NARLabs). The report was written out in National Center for High-performance Computing.

2 Mathematical model

In the present work, the air-flow in the inhabited area is investigated together with the transport of the pollution emerging on the main road. The chosen simulation approach is a segregated one: (i) a steady state velocity field is pre-calculated using Navier-Stokes equations, and (ii) it is used in scalar transport equation to simulate advancement of the pollution.

The present section describing the used mathematical model is structured as follows: (i) a model geometry and a computational mesh generation are presented, (ii) used boundary conditions are summarized and (iii) the governing equations are briefly outlined.

2.1 Model geometry generation and boundary conditions

As stated, the air flow and the spread of the pollution in the inhabited area is of an interest. A studied part of the city is $L_{\mathrm{l}} = 500\,\mathrm{m}$ long, $L_{\mathrm{w}} = 500\,\mathrm{m}$ wide, and the highest building is $L_{\mathrm{h}} = 105\,\mathrm{m}$ tall. The available *stl* file together with its dimensions and the orientation in the chosen Cartesian coordinate system is depicted in Figure 1.

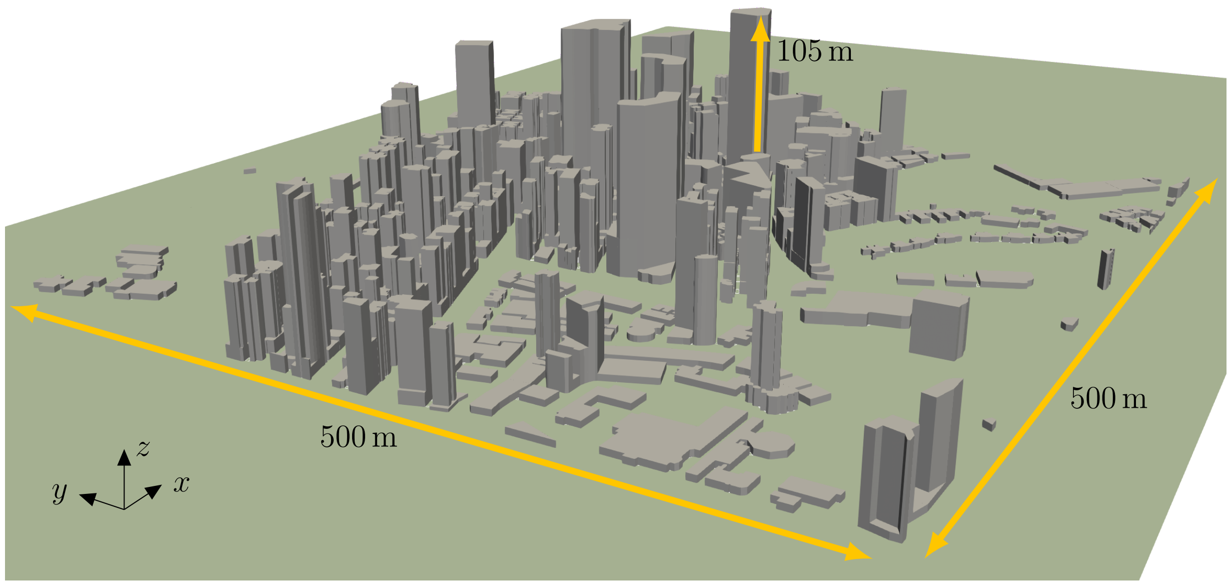
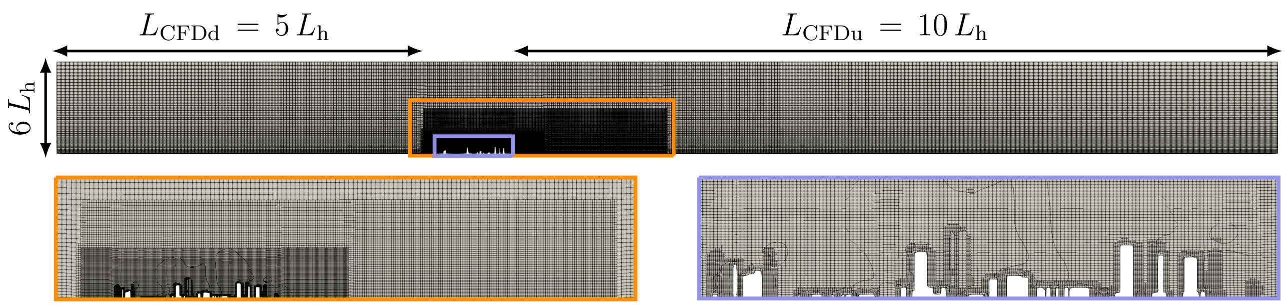


Figure 1: Studied city geometry (used *stl* file) with its dimensions and chosen Cartesian coordinate system.

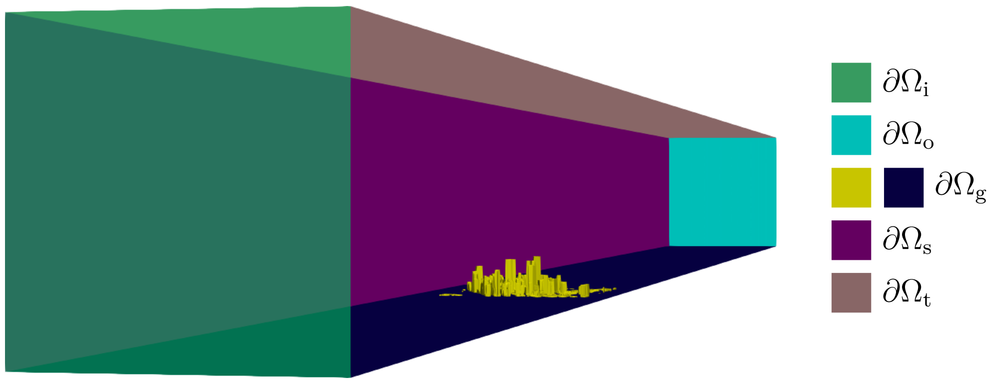
Computational mesh Computational mesh was prepared using the OpenFOAM `blockMesh` and `snappyHexMesh` utilities. The computational domain dimensions were determined based on the review by Pantusheva et al. [1]. In particular, we introduce both upstream, and downstream buffers in front of, and behind the city, which are in order $L_{\mathrm{CFDu}} = 5\,L_{\mathrm{h}}$, and $L_{\mathrm{CFDd}} = 10\,L_{\mathrm{h}}$ long. Furthermore, the computational domain is $L_{\mathrm{CFDh}} = 6\,L_{\mathrm{h}}$ high. The y-normal slices cut in the middle of the used computational mesh are shown in Figure 2. Note the grading of the computational mesh in the z-direction, and its refinement in the vicinity of the city.



$L_{\mathrm{CFDd}} = 5\,L_{\mathrm{h}}$
$L_{\mathrm{CFDu}} = 10\,L_{\mathrm{h}}$
$6\,L_{\mathrm{h}}$

Figure 2: y-normal slices through the half of the computational mesh.

Boundary conditions The model behavior in the computational domain (Ω) is described by partial differential equations outlined in the following subsection 2.2 (Governing equations). However, these need to be supplied with the consistent boundary conditions on the Ω boundary, $\partial\Omega$. As depicted in Figure 3, the computational domain boundary is split into (i) *inlet* ($\partial\Omega_{\mathrm{i}}$), (ii) *outlet* ($\partial\Omega_{\mathrm{o}}$), (iii) *ground* ($\partial\Omega_{\mathrm{g}}$), (iv) *sides* ($\partial\Omega_{\mathrm{s}}$), and (v) *top* ($\partial\Omega_{\mathrm{t}}$).



🟩 $\partial\Omega_{\mathrm{i}}$
🟦 $\partial\Omega_{\mathrm{o}}$
🟨 ■ $\partial\Omega_{\mathrm{g}}$
🟪 $\partial\Omega_{\mathrm{s}}$
🟫 $\partial\Omega_{\mathrm{t}}$

Figure 3: Boundaries of the computational domain.

Used boundary conditions are utilized from [1, 2] and summarized in Table 1. Starting with flow variables, uniform Dirichlet (*fixedValue*), and OpenFOAM inletOutlet boundary conditions are prescribed for velocity ($\boldsymbol{u}$) at Ω_{i}, and Ω_{o}, respectively. At Ω_{g}, we standardly assume *noSlip* boundary condition, and finally the sides of the geometry (Ω_{s} and Ω_{t}) are treated as the symmetry (*slip*). This setting is supplemented with OpenFOAM *totalPressure* boundary condition for pressure (p) at Ω_{o}, and zeroGradient (*zeroGrad*) elsewhere.

As described in the later subsection, $k-\varepsilon$ turbulence model is used to estimate unresolved eddy dissipation. The turbulence model requires specification of the boundary conditions for turbulent kinetic energy (k), rate of dissipation of the turbulent kinetic energy (ε), and the turbulent viscosity (ν_{t}). At Ω_{i}, we use OpenFOAM turbulentIntensityKineticEnergyInlet (*turbIntKinEngInlet*), and turbulentMixingLengthDissipationRateInlet (*turbMixDissRateInlet*) boundary conditions, which calculate the inlet k and ε, respectively, based on specified value of the inlet turbulence intensity I_{i}. At the Ω_{g}, standard wall functions are utilized *kqRWallFunction*, *epsWallFunction*, and *nutkWallFunction*, in order for k, ε, and ν_{t}. And finally, *zeroGrad* boundary condition is prescribed elsewhere.

Scalar transport equation describing the spreading of the pollution y_{P} is supplied with the *fixedValue* boundary condition at Ω_{g}, defining the source of the pollution on the main road, and *zeroGrad* boundary condition elsewhere.

Table 1: Used boundary conditions.

variable	Ω_{i}	Ω_{o}	Ω_{g}	Ω_{s}	Ω_{t}
$\boldsymbol{u}$	fixedValue	inletOutlet	noSlip	slip	slip
p	zeroGrad	totalPressure	zeroGrad	zeroGrad	zeroGrad
k	turbIntKinEngInlet	zeroGrad	kqRWallFunction	zeroGrad	zeroGrad
ε	turbMixDissRateInlet	zeroGrad	epsWallFunction	zeroGrad	zeroGrad
ν_{t}	fixedValue	zeroGrad	nutkWallFunction	zeroGrad	zeroGrad
y_{P}	zeroGrad	zeroGrad	fixedValue	zeroGrad	zeroGrad

2.2 Governing equations

The description of the chosen governing equations is split into two parts, (i) air-flow governing equations, and (ii) the pollution scalar transport.

Flow governing equations Steady state isothermal incompressible flow of the Newtonian gas is assumed. Adopting Boussinesq hypothesis, and noting the mean time velocity, $\boldsymbol{u} = (u_x, u_y, u_z)^{\intercal}$, and the mean time turbulent pressure, $\tilde{p}$, the flow can be described by Reynolds-averaged Navier-Stokes (RANS) equations in a form,

$$\nabla \cdot (\boldsymbol{u}\boldsymbol{u}^{\intercal}) - \nabla \cdot [(\nu + \nu_{\mathrm{t}})\,(\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^{\intercal})] = -\nabla \tilde{p}\,, \tag{1}$$

$$\nabla \cdot (\boldsymbol{u}) = 0 \tag{2}$$

where ν is the gas kinematic viscosity, and ν_{t} is the turbulent eddy viscosity.

In general, there exist numerous various approaches of ν_{t} estimation. In the present work, the OpenFOAM variant of $k - \varepsilon$ turbulence model is used to calculate the turbulent eddy viscosity as,

$$\nu_{\mathrm{t}} = \frac{k}{\varepsilon}\,, \tag{3}$$

where k, and ε are the turbulence kinetic energy, and its rate of the dissipation, respectively. For more information on the calculation of the k and ε, see e.g. [3, 4].

Pollution transport governing equation Assuming constant mass density, the transient dispersion of the polluting gas in the carrier gas can be estimated employing standard scalar variable transport equation in a form,

$$\frac{\partial(y_{\mathrm{P}})}{\partial t} + \nabla \cdot (\boldsymbol{u}\, y_{\mathrm{P}}) - \nabla \cdot ((D\, +\, D_{\mathrm{t}})\nabla y_{\mathrm{P}}) = 0\,, \tag{4}$$

where $\boldsymbol{u}$ is the mean-time velocity obtain from solution of (1,2), y_{P} is the molar fraction of the polluting gas, t is time, and D and D_{t} are in order molar and turbulent diffusivities of the polluting gas. Remark that no source of the pollution is assumed on the right hand side of the equation (4), as the source of the pollution is ensured by proper application of the boundary conditions.

Furthermore, the turbulent diffusivity, D_{t}, is calculated using Schmidt number (Sc) defined as,

$$\mathrm{Sc} = \frac{\nu + \nu_{\mathrm{t}}}{D + D_t}\,, \tag{5}$$

where $\nu + \nu_{\mathrm{t}}$ are the gas kinematic and the turbulent viscosities, respectively. Note that a standard assumption of the constant Schmidt number is adopted [5], and ν_{t} is estimated from from (3).

2.3 Model parameters

The above described mathematical model has several tunable parameters that can be split into two groups, (i) thermophysical parameters of the flowing gas, and (ii) boundary conditions

The flow of the air at the common temperature of the $T = 25\,°\mathrm{C}$ has been assumed. The value of the gas kinematic viscosity has been calculated from Sutherland equation [6] as $\nu = 1.53 \cdot 10^{-5}\,\mathrm{m}^2\,\mathrm{s}^{-1}$, and the value of the pollution molar diffusivity from Fuller equation [7] as $D = 1.72 \cdot 10^{-5}\,\mathrm{m}^2\,\mathrm{s}^{-1}$. As in [5], the Schmidt number has been assumed constant and equal $\mathrm{Sc} =\ 0.9$.

To complete the description of the prepared model, it remains to specify the inlet values of the velocity, and the turbulence intensity, and the value of the pollution molar fraction on the ground of the main road.finish

3 Computational environment

NCHC servers use Singularity container platform [8] and Slurm workload manager [9] to run user-defined tasks. Thus,

(i) custom singularity container, which includes necessary packages installed and compiled inside, is prepared, and

(ii) Slurm task (which runs within the container) is prepared and run at the computational server.

3.1 Preparation of the singularity container

Assuming you have super-user permission and singularity installed on local (see step-by-step guide in [10]), a preparation of the singularity container image from docker ubuntu:latest release can be done as follows:

1. Navigate outside the home directory and work here, e.g.:

   ```
   mkdir /tmp/
   mkdir /tmp/test
   cd /tmp/test/
   ```

2. New container (`./ubuntu`) can be built from ubuntu docker repository using:

   ```
   sudo singularity build --sandbox ./ubuntu docker://ubuntu:latest
   ```

   Note: `--sandbox` flag allows to write into container later

Shell inside container can be opened using:

```
sudo singularity shell ./ubuntu --writable
```

where `--writable` flag again allows to write into container and install packages here.

Openfoam.org/v10 and other used packages can be installed inside the container as:

```
apt update
apt install python3 python3-pip wget vim software-properties-common
    python3-tk     pip3 install matplotlib
sh -c "wget -O - https://dl.openfoam.org/gpg.key >
    /etc/apt/trusted.gpg.d/openfoam.asc"
add-apt-repository http://dl.openfoam.org/ubuntu
apt update
apt install openfoam10
```

Compilation of the custom solver inside container is done as follows:

1. Source OpenFOAM in the container shell:
   ```
   . /opt/openfoam10/etc/bashrc
   ```
2. Navigate to solver folder, e.g.:
   ```
   cd /tmp/pollutionFoam
   ```
3. Compile solver executing:
   `wmake`.

When everything is installed, the `.sif` container file can be built from prepared `/tmp/test/ubuntu` directory using:

```
sudo singularity build /tmp/test/ubuntu.sif /tmp/test/ubuntu/
```

Following the above listed guideline, singularity container image `ubuntu.sif` is created. This can be uploaded to NCHC servers and used as described in following subsection.

3.2 Developed OpenFOAMCase python class documentation

3.3 Preparation of Slurm control script and running the task

4 Numerical experiments

Some nice results her.

5 Conclusions

And conclusion here

6 Nomenclature

c_i	....	Molar concentration of i-th molar specie
c_T	....	Total molar concentration
Co	....	Courant number
d	....	Diameter
D_i	....	Molar diffusivity of i-th molar specie
D_i^eff	....	Effective molar diffusivity of i-th molar specie
$\boldsymbol{d}_\mathrm{PN}$	....	Vector connecting centroids of P and N
f	....	Face of the cell
$\boldsymbol{f}_b$	....	Body forces acting on cell
$\boldsymbol{g}$	....	Gravitational acceleration
h	....	Specific enthalpy
I	....	Time interval
I^h	....	Discretized time interval
m	....	Number of discretized FV cells
M	....	Molar mass
n	....	Number of species
$\boldsymbol{n}$	....	Outer normal vector
$\boldsymbol{n}_f$	....	Outer normal vector of the face f
p	....	Pressure
p_ref	....	Reference pressure
$\tilde{p}$	....	Kinematic pressure
Q	....	Computational domain
r_i	....	Reaction source of the i-th molar specie
R^g	....	Universal gas constant
Re	....	Reynolds number
s_ϕ	....	Source of the ϕ
$\boldsymbol{S}_f$	....	Face area vector
t	....	Time
T	....	Temperature
T_ref	....	Reference temperature
$\boldsymbol{u} = (u, v, w)$	....	Velocity
y_i	....	Molar fraction of the i-molar specie
α	....	Heat transfer coefficient
ε	....	Porosity
Γ_ϕ	....	Diffusivity of ϕ
κ	....	Permeability
λ	....	Heat conductivity
μ	....	Dynamic viscosity
ν	....	Kinematic viscosity
Ω	....	Domain
Ω^h	....	Discretized domain
Ω_P^h	....	Cell P
$\delta\Omega_i^h$	....	Volume of the cell
$\partial\Omega$	....	Domain boundary
ϕ	....	Intensive tensorial quantity
ϕ_P	....	Value of ϕ in the cell centroid of cell P

ϕ_f	....	Value of ϕ in the face centroid of face f
$\mathbf{\Phi}_\phi$	....	Flux intensity of ϕ
$\mathbf{\Phi}_{\phi,\mathrm{conv}}$	....	Convective flux intensity of ϕ
$\mathbf{\Phi}_{\phi,\mathrm{diff}}$	....	Diffusive flux intensity of ϕ
ρ	....	Fluid mass density
Σ	....	Total stress tensor
τ	....	Tortuosity
$\boldsymbol{\tau}$	....	Viscous stress tensor
∇	....	Nabla differential operator

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Potencial appendix here.