Road Dust Emission Modelling

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Abstract *Atmospheric particulate matter (PM) is a well known risk to human health. Vehicular traffic is one of the major sources of particulates in an urban setting. Here we study a problem of road dust dispersion. Using CFD solver based on RANS equations, we investigate the effect of a vegetation barrier on the concentration of airborne PM induced by road traffic. Simplified 2D model of a porous obstacle adjacent to a road source of PM10 serves as an idealization of a real-world situation. Importance of several model parameters is estimated using direct sensitivity approach.*

Keywords *Vegetation barrier, Particulate matter, RANS modelling, Air quality*

1 Introduction

Near road vegetation barriers have been suggested as a way to mitigate the particulate matter pollution in neighbouring areas. Its effectivity is influenced by a number of parameters: atmospheric conditions, properties of the particulates, vegetation type or its position (see eg. [5], [3] and references therein).

Here we set out to explore the effect of various parameters on the particle concentration behind the barrier using simplified 2D model.

2 Numerical Model

Flow in the domain is modelled using equations of incompressible turbulent flow,

$$\frac{1}{\beta}\frac{\partial p'}{\partial t} + \nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} + \nabla(p'/\rho_0) = \nu_E \nabla^2 \boldsymbol{u} + \boldsymbol{g} + \boldsymbol{S}_{\boldsymbol{u}}, \tag{2}$$

$$\frac{\partial \theta}{\partial t} + \nabla \cdot (\theta \boldsymbol{u}) = \frac{\nu_E}{\mathrm{Pr}}\left(\nabla \cdot (1/\rho \nabla \theta)\right). \tag{3}$$

Here pressure and density are split into background component in hydrostatic balance and fluctuations, $p = p_0 + p'$ and $\rho = \rho_0 + \rho'$. Vector $\boldsymbol{u}$ stands for velocity, ν_E is the effective viscosity, $\nu_E = \nu + \nu_T$, $\boldsymbol{g}$ is the gravity term, $\boldsymbol{g} = (0, -g, 0)$. Term $\boldsymbol{F}$ represents momentum sink due to the vegetation, which we describe later, θ is a potential temperature and $\mathrm{Pr} = 0.75$ is Prandtl Number.

Artificial compressibility with parameter β is utilized to transform the divergence constraint of incompressible flow $\nabla \cdot \boldsymbol{u} = 0$ to evolution equation of pressure fluctuation (1).

Algebraic mixing-length model according to [1] is used to account for effects of turbulence.

2.1 Particle transport

Concentration of particulate matter C is modelled as passive scalar,

$$\frac{\partial \rho C}{\partial t} + \nabla \cdot (\rho C \boldsymbol{u}) - (\rho C u_s)_y = \nabla \cdot \left(\frac{\nu_E}{\mathrm{Sc}} \nabla C \right) + \rho f_c + S_C. \tag{4}$$

Here u_s is settling velocity of the particle, $\mathrm{Sc} = 0.72$ is Schmidt Number, f_c is the source term and S_c is the vegetation deposition term, described below.

For spherical particle with diameter d and density ρ_p, settling velocity is given by Stokes' law,

$$u_s = \frac{d^2 \rho_p g C_c}{18\mu} \tag{5}$$

with correction factor $C_c = 1 + \frac{\lambda}{d}\left(2.34 + 1.05 \exp(-0.39 d/\lambda)\right)$, where $\lambda = 0.066\,\mu\mathrm{m}$ is mean free path of the particle in the air.

2.2 Effects of the vegetation

Near-road vegetation has two effects: First is the aerodynamic effect of the block, obstructing the air flowing through it. It also serves as a sink for the pollutant, as the particles in the flow deposit on the leaves and branches.

In our model, vegetation block is described by its Leaf Area Density (LAD) profile, characterizing its vertical structure, and porosity coefficient c representing the spatial density of the plants.

The aerodynamic effect is modeled through the term

$$\boldsymbol{S}_u = -\rho c \mathrm{LAD} |\boldsymbol{u}| \boldsymbol{u}, \tag{6}$$

while the deposition term, present in the equation for particle concentration C has the form

$$S_C = -\rho c \mathrm{LAD} u_d C. \tag{7}$$

Here u_d is the deposition velocity, which is a fraction of particle flow rate towards the leaf surface over the particle concentration. Based on a literature survey ([3], [4]), we have chosen constant value of $u_d = \ 0.01 \mathrm{ms}^{-1}$.

2.3 Discretization

Discretization of the equations is done using finite volume method. Numerical flux AUSM$^+$-up [2], designed for flows at all speed regimes, is employed for convective fluxes evaluation. Second order accuracy in space is achieved via linear reconstruction, where gradients are evaluated by means of least squares approach. Venkatakrishnan limiter [6] is used to prevent unphysical oscillations. Resulting system of ODEs is discretized in time using BDF2 method.

3 Case settings

Computational domain is 300 m long and 150 m high. Four-lane road is modelled as four line sources of PM10 particulates, placed at 23.125, 29.375, 35.625 and 41.875 m from the inlet at height 0.8 m. Intensity of each source is 1 mg/m/s. The vegetation barrier of length 30 m and height 15 m is located at 50 m from the inlet. Its porosity coefficient is $c = 0.3$.

Size of the computational grid is 300 x 120 cells, height of a first cell above ground is 14 cm.

Following boundary conditions are prescribed:

- Inlet: Prescribed log wind velocity profile with $u_{\text{ref}} = 5\,\text{ms}^{-1}$ at 50 m height, coupled with constant temperature of 20°C. Neumann BC for pressure.
- Bottom: No-slip condition for velocity, Neumann BC for pressure and potential temperature.
- Outlet and top: Pressure prescribed according to barometric formula, Neumann BC for velocity and potential temperature.

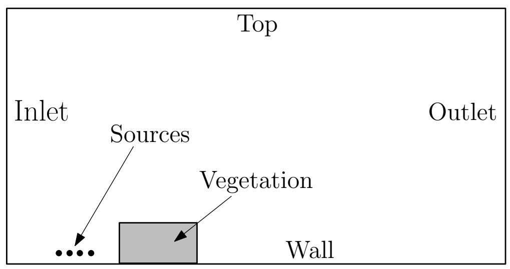

Figure 1: Sketch of a computational domain.

4 Sensitivity analysis

Constructed model involves large number of parameters we can estimate only approximately - eg. atmospheric conditions, or vegetation properties. To assess their relative importance, we employed direct sensitivity approach as outlined below. This will help us to identify most influential parameters, on which we can focus in our future studies.

4.1 Method description

Consider calculated steady-state solution $\boldsymbol{W}$ of PDE expressed as

$$\boldsymbol{F}(\boldsymbol{W}) = 0. \tag{8}$$

We are interested in value of a objective function $J(\boldsymbol{W}, \boldsymbol{p}) = \hat{J}(\boldsymbol{p})$ and its derivatives with respect to the set of parameters $\boldsymbol{p}$, $\frac{d\hat{J}}{d\boldsymbol{p}}$. Denoting m and m length of vectors $\boldsymbol{W}$ and $\boldsymbol{p}$ respectively, we use chain rule to obtain

$$\underbrace{\frac{d\hat{J}}{d\boldsymbol{p}}}_{\text{1 x m}} = \underbrace{\frac{\partial J}{\partial \boldsymbol{W}}}_{\text{1 x n}} \underbrace{\frac{\partial \boldsymbol{W}}{\partial \boldsymbol{p}}}_{\text{n x m}} + \underbrace{\frac{\partial J}{\partial \boldsymbol{p}}}_{\text{1 x m}} . \tag{9}$$

Partial derivatives $\frac{\partial \boldsymbol{W}}{\partial \boldsymbol{p}}$ and $\frac{\partial J}{\partial \boldsymbol{p}}$ are easily calculated by hand. The term $\frac{\partial \boldsymbol{W}}{\partial \boldsymbol{p}}$ is computed from system of linear equations, which is obtained by taking a derivative of Eq. (8) and using chain rule again,

$$\frac{d\boldsymbol{F}}{d\boldsymbol{p}} = 0 \tag{10}$$

$$\underbrace{\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{W}}}_{\mathrm{n\,x\,n}} \cdot \underbrace{\frac{\partial \boldsymbol{W}}{\partial \boldsymbol{p}}}_{\mathrm{n\,x\,m}} = - \underbrace{\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{p}}}_{\mathrm{n\,x\,m}} . \tag{11}$$

Terms $\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{W}}$ and $\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{p}}$ are calculated using finite differencing.

5 Results

5.1 Simulation results

Figure 2 shows isolines of velocity and particle mass concentration for calculated case. Effect of vegetation block (located between 50 and 80 m from the inlet) on flow field is substantial. Reduction of the particle concentration behind the barrier is partly caused by diffusion in the atmosphere, partly by the deposition in the vegetation block and partly by settling of the particles on the ground.

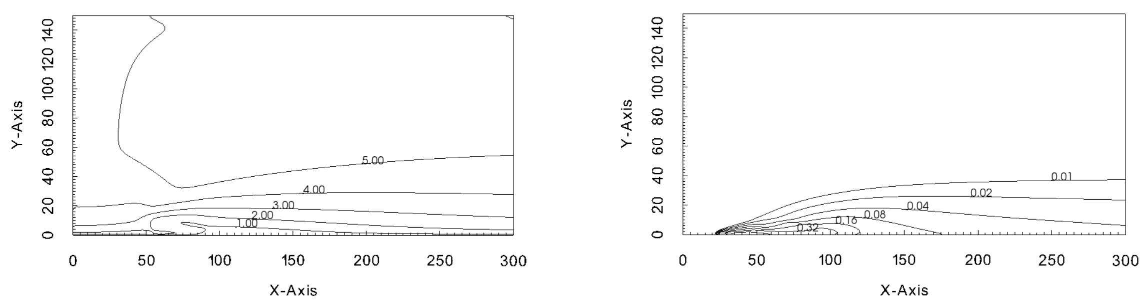

Figure 2: Isolines of velocity magnitude [m/s] (left) and particle mass concentration [µgm^{-3}] (right).

5.2 Sensitivity analysis

In our case, we have chosen the objective function to be the value of particle concentration density at point 250 m from the inlet (170 m behind the barrier) at height 2 m. Sensitivity analysis was carried out for following parameters: atmospheric temperature lapse rate $\gamma = \frac{\partial T}{\partial y}$, inlet velocity (at the top of the domain) u_{ref}, terrain roughness z_0, particle diameter d and density ρ_p, and particle deposition velocity on the vegetation u_d and vegetation block porosity c.

Using second order of approximation in space, the linear system (11) did not converge for some of the parameters. Therefore the analysis was carried out using also first order approximation. Results are compared in Table 5.2. Missing values due to the failure of solving system (11) are replaced with “NA”.

To take into account variability of the parameters, product of the derivative with estimated possible difference from the base value Δ is also included. Since the value of Δ is estimated, only order of magnitude of the resulting product should be considered for further conclusions.

			1ST ORDER		2ND ORDER	
PARAMETER	VALUE	Δ	$\frac{d\hat{J}}{dp}$	$\Delta \cdot \frac{d\hat{J}}{dp}$	$\frac{d\hat{J}}{dp}$	$\Delta \cdot \frac{d\hat{J}}{dp}$
u_{ref}	5.0×10^{1}	5.0	-1.41×10^{-2}	-7.07×10^{-2}	NA	NA
d	1.0×10^{-5}	1.0×10^{-5}	-1.41×10^{3}	-1.41×10^{-2}	-1.10×10^{3}	-1.10×10^{-2}
c	3.0×10^{-1}	1.0×10^{-1}	-5.53×10^{-2}	-5.53×10^{-3}	NA	NA
u_d	1.0×10^{-2}	1.0×10^{-2}	-2.36×10^{-1}	-2.36×10^{-3}	-2.24×10^{-1}	-2.24×10^{-3}
z_0	2.0×10^{-1}	1.0×10^{-1}	1.00×10^{-2}	1.00×10^{-3}	NA	NA
ρ_p	1.0×10^{3}	5.0×10^{2}	-8.18×10^{-7}	-4.09×10^{-4}	-1.25×10^{-6}	-6.24×10^{-4}
γ	0.0	1.0×10^{-2}	5.02×10^{-3}	5.02×10^{-5}	NA	NA

Table 1: Sensitivity analysis results

5.3 Discussion

Firstly, let us note that the difference between the calculated derivatives using first and second order approximation (where available) is at most 35%. Even though this difference is substantial, the trends and orders of magnitudes agree, which allows us to reason about the parameter importance from the first order calculation.

From the analysis, inlet wind velocity u_{ref} appears to be the most influential parameter. This is not surprising, as inlet wind velocity has direct effect on the entire flow field, and it asserts the need for separate simulations for different wind condition. The other atmospheric condition, atmospheric stratification described by temperature lapse rate γ, is orders of magnitude less important.

Particle properties (namely diameter d and to a lesser extent density ρ_p) play crucial role as well. Larger and denser particles fall and get deposited on the ground faster than smaller ones, and therefore do not travel as far. From this result it is apparent that different classes of particles should be simulated separately.

The influence of deposition velocity u_d is far from negligible, therefore the approximation with constant value, as used here, is not satisfactory for further studies. As mentioned in [3], deposition velocity depends, among others, on particle properties (diameter and density), wind speed, air humidity, air turbulence or plant species. Deposition model taking this complexity into account should be adopted.

Nomenclature

$\boldsymbol{u}$	Velocity	$[\mathrm{m\,s^{-1}}]$
γ	Temperature lapse rate	$[\mathrm{K\,m^{-1}}]$
ν, ν_T, ν_E	Kinematic, turbulent kinematic and effective kinematic viscosity	$[\mathrm{m\,s^{-2}}]$

ρ	Air density	$[\mathrm{kg\,m^{-3}}]$
ρ_p	Particle density	$[\mathrm{kg\,m^{-3}}]$
θ	Potential temperature	[K]
C	Particulate matter concentration	[1]
c	Vegetation porosity coefficient	[1]
d	Particle diameter	[m]
g	Gravitational acceleration	$[\mathrm{m\,s^{-1}}]$
p	Air pressure	[Pa]
T	Temperature	[K]
t	Time	[s]
u_d	Deposition velocity	$[\mathrm{m\,s^{-1}}]$
u_s	Particle settling velocity	$[\mathrm{m\,s^{-1}}]$
u_{ref}	Reference velocity	$[\mathrm{m\,s^{-1}}]$
z_0	Terrain roughness	[m]
LAD	Leaf Area Density	$[\mathrm{m^{-1}}]$

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