CFD Optimization of a Vegetation Barrier

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Abstract. In this study we deal with a problem of particulate matter dispersion modelling in a presence of a vegetation. We present a method to evaluate the efficiency of the barrier and to optimize its parameters.

We use a CFD solver based on the RANS equations to model the air flow in a simplified 2D domain containing a vegetation block adjacent to a road, which serves as a source of the pollutant. Modelled physics captures the processes of a gravitational settling of the particles, dry deposition of the particles on the vegetation, turbulence generation by the road traffic and effect of the vegetation on the air flow.

To optimize the effectivity of the barrier we employ a gradient based optimization process. The results show that the optimized variant relies mainly on the effect of increased turbulent diffusion by a sparse vegetation and less on the dry deposition of the pollutant on the vegetation.

1 Introduction

Particulate matter (PM) in the atmosphere has a significant negative influence on the human health. It is a concern especially in the urban areas, where the road traffic constitutes a major source of the pollutants. Vegetation barriers were proposed as a means to the reduction of a harmful PM in the atmosphere. Due to the complexity of the problem, assessment of the effectivity of the barriers and its design is difficult without the computer simulations.

Many publications on the topic of mathematical modelling of the pollutant deposition on the vegetation are available. Among the most notable are the following: review [11] on the topic of dry deposition on the vegetation, reviews [9,5] on the vegetation in urban areas or modelling studies [13,17,15].

In this paper we present a method for the evaluation of the effectivity of the barriers and for the numerical optimization of the barrier properties. The model presented here is based on the work [20], where the influence of the atmospheric conditions on the barrier efficiency was investigated.

2 Numerical model

2.1 Physical model

Let us summarize the basic characteristics of the problem. We are interested in the air flow in the bottom layer of the atmosphere, approximately 200 meters thick. Such flow can be modelled as incompressible, but with variable density due to the acting of the gravity force. Three effects of the vegetation should be considered: effect on the air flow, i.e. slowdown or deflection of the flow, influence on the turbulence levels inside and near the vegetation, and the filtering of the particles present in the flow.

Fluid flow In our formulation of Reynolds-averaged Navier-Stokes (RANS) equations the pressure p and potential temperature θ are split into background component in hydrostatic balance and fluctuations, $p = p_0 + p'$ and $\theta = \theta_0 + \theta'$. Boussinesq approximation stating that changes in density are negligible everywhere except in the gravity term is utilized. Resulting set of equations is as follows:

$$\nabla \cdot \boldsymbol{u} = 0, \tag{1}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u} \cdot \nabla)\boldsymbol{u} + \nabla(p'/\rho_{\mathrm{ground}}) = \nu_E \nabla^2 \boldsymbol{u} + \boldsymbol{g} + \boldsymbol{S_u}, \tag{2}$$

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

Here vector $\boldsymbol{u}$ stands for velocity, ρ_{ground} is the value of the air density ρ at the ground level, $\nu_E = \nu_L + \nu_T$ is the effective kinematic viscosity, which is a sum of the laminar and turbulent viscosity, $\boldsymbol{g} = (0, g\frac{\theta'}{\theta_0}, 0)$ is the gravity term, $\boldsymbol{S_u}$ represent the momentum sink due to the vegetation and $\mathrm{Pr} = 0.75$ is the Prandtl number.

Turbulence Standard $k - \epsilon$ model is employed to model the turbulence. Equations for turbulence kinetic energy k and dissipation ϵ are as follows:

$$\frac{\partial \rho k}{\partial t} + \nabla \cdot (\rho k \boldsymbol{u}) = \nabla \cdot \left(\left(\mu_L + \frac{\mu_T}{\sigma_k} \right) \nabla k \right) + P_k - \rho \epsilon + \rho S_k, \tag{4}$$

$$\frac{\partial \rho \epsilon}{\partial t} + \nabla \cdot (\rho \epsilon \boldsymbol{u}) = \nabla \cdot \left(\left(\mu_L + \frac{\mu_T}{\sigma_\epsilon} \right) \nabla \epsilon \right) + C_{\epsilon 1} \frac{\epsilon}{k} P_k - C_{\epsilon 2} \rho \frac{\epsilon^2}{k} + \rho S_\epsilon. \tag{5}$$

The model is completed by a relation between k, ϵ and the turbulent dynamic viscosity μ_T, $\mu_T = C_\mu \rho \frac{k^2}{\epsilon}$. In the equations above μ_L is the laminar dynamic viscosity, P_k is the production of the turbulence kinetic energy, and S_k and S_ϵ are sources of k and ϵ respectively. Both consist of a part due to the road traffic and a part due to the vegetation, $S_k = S_k^r + S_k^v$, $S_\epsilon = S_\epsilon^r + S_\epsilon^v$. Sources due to the road traffic are modelled by the model from [2], while sinks and sources due to the vegetation are described below.

Following constants of the model are used: $\sigma_k = 1.0$, $\sigma_\epsilon = 1.167$, $C_{\epsilon_1} = 1.44$, $C_{\epsilon_2} = 1.92$ and $C_\mu = 0.09$.

Particle transport Non dimensional mass fraction w of the pollutant in the air is calculated using the equation for the pollutant density,

$$\frac{\partial \rho w}{\partial t} + \nabla \cdot (\rho w \boldsymbol{u}) - (\rho w u_s)_y = \nabla \cdot \left(\frac{\nu_E}{\mathrm{Sc}} \nabla \rho w \right) + \rho f_c + S_w. \tag{6}$$

Here f_c is the source term and S_w is the vegetation deposition term. Based on the review and the discussion in [18], the Schmidt number $\mathrm{Sc} = 0.72$ was used. The settling velocity u_s of a spherical particle with the diameter d and density ρ_p is given by the Stokes' equation, $u_s = (d^2 \rho_p g C_c)/(18\mu)$, with the correction factor $C_c = 1 + \frac{\lambda}{d}(2.34 + 1.05 \exp(-0.39 d/\lambda))$, where $\lambda = 0.066$ µm is the mean free path of the particle in the air [4].

Vegetation We model the vegetation as horizontally homogenous, described by vertical *Leaf area density* (LAD) profile - foliage surface area per unit volume - and a leaf type (broadleaf or needle) and size of the leaf. Three effects of the vegetation are modelled: first, it is a momentum sink inside the vegetation block, $\boldsymbol{S}_u = -C_d \mathrm{LAD} |\boldsymbol{u}| \boldsymbol{u}$, present in the Eq. (2). Here $C_d = 0.3$ is the drag coefficient [7].

Secondly, it is the influence on the turbulence levels. Following [7], we model this term as

$$S_k^v = C_d \mathrm{LAD} (\beta_p |\boldsymbol{u}|^3 - \beta_d |\boldsymbol{u}| k), \quad S_\epsilon^v = C_{\epsilon_4} \frac{\epsilon}{k} S_k^v,$$

in Eqs. (4) and (5). Constants used are $\beta_p = 1.0$, $\beta_d = 5.1$ and $C_{\epsilon_4} = 0.9$.

And lastly, it is a particle sink term in Eq. (6), $S_w = -\mathrm{LAD} u_d \rho w$. The term is proportional to the deposition velocity u_d. Deposition velocity reflects four main processes by which particles depose on the leaves: Brownian diffusion, interception, impaction and gravitational settling. Its value generally depends on wind speed, particle size and vegetation properties. In this study we adopted the model from [12] derived for broadleaf trees.

2.2 Numerical methods

CFD solver Apart from the divergence constraint (1), all presented PDEs are in a form of a evolution equation, suitable for the discretization as described below. The divergence constraint is transformed into such form by employing method of artificial compressibility with parameter β so that we obtain

$$\frac{1}{\beta} \frac{\partial p'}{\partial t} + \nabla \cdot \boldsymbol{u} = 0. \tag{7}$$

The choice of the parameter β is discussed e.g. in [10], here we have used $\beta = 1000$.

The resulting set of equations is discretized using the finite volume method on unstructured grid. For the convective terms the AUSM+up scheme [8], designed for all speed flows, is used. Second order accuracy is achieved via the linear reconstruction, where gradients are calculated using least squares approach. To prevent artificial overshooting, Venkatakrishan limiter [19] is utilized.

Gradients on the cell faces needed for the calculation of the diffusive terms are evaluated using the Gauss-Green theorem on a dual cell associated with the face.

The discretized system forms a set of ordinary differential equations, which are solved using an implicit BDF2 method. In every time step (outer iteration), first the system of the Navier-Stokes equations (2, 3, 7) is solved, followed by the system of the $k - \epsilon$ equations (4, 5) and then by the system of the passive scalar equations (6). Values of turbulent viscosity, coupling together turbulence equations with the Navier-Stokes equations, are taken from the previous time step.

Each of these nonlinear systems is solved by the Newton method. Inner linear systems are solved using matrix-free GMRES solver. The linear systems are preconditioned by ILU(3) preconditioner. Necessary evaluations of the Jacobians are done via finite differences. Significant cost of these operations is reduced by two complementing approaches: via matrix coloring, which exploit the sparseness of the Jacobian, and by calculating the preconditioner matrices (as well as the Jacobians) only every 20th time step.

Since we are solving only for a steady-state solution, we continuously adapt the time step in order to accelerate the convergence. The adapting criterion is based on the number of the iterations of the linear solvers in one outer iteration. Time stepping proceeds until a steady-state solution is reached.

The solver is written in C++. PETSc library [1] is used for the nonlinear system solution.

Optimization PDE-constrained optimization problem could be written in the following form:

$$\text{Find } \min_{p \in P} J(\boldsymbol{W}, p) \quad \text{subject to} \quad F(\boldsymbol{W}, p) = 0 \tag{8}$$

and constrained by

$$p_i^{min} \leq p_i \leq p_i^{max} \quad i = 1...n, \tag{9}$$

$$g_j(p) \leq 0 \quad j = 1...m. \tag{10}$$

Here $J(\boldsymbol{W}, p)$ is a cost function and $F(\boldsymbol{W}, p)$ is the system of steady-state PDEs, $\boldsymbol{W}$ is the state vector and p is the vector of parameters. Allowed values of parameters are limited by p_i^{min} and p_i^{max}, while functions g_j represents nonlinear constraints.

To solve the optimization problem, method of moving asymptotes (MMA) [16] implemented in NLopt optimization package [6] was employed.

Since the MMA is a gradient-based method, the CFD solver has to facilitate the evaluation of not only the cost function at a given point in the parameter space, but also its derivatives with respect to the parameters. This was done via a direct sensitivity approach [3].

3 Application to the model problem

3.1 Case settings

Figure 1 shows the sketch of the computational domain. Four sources of pollutant, representing the road, are placed between 23 m and 42 m from the inlet at height 0.8 m. Vegetation block of height 15 m is placed downstream from the road.

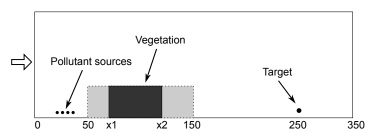

Fig. 1. Sketch of the domain (not to scale)

We model the particles of diameter 10 µm and density 1000 kg/m^3. Each source of the pollutant has the intensity 1 µg/s. No resuspension of the particles fallen on the ground is allowed. Density of the traffic is set to 4 passenger cars and 1 heavy duty vehicle per minute in each of the four lanes.

As in [20], logarithmic wind profile is prescribed at the inlet with $u_{\mathrm{ref}} = 5$ m/s at height $y_{\mathrm{ref}} = 10$ m. Roughness parameter z_0 is set to 0.1 m. The atmosphere is under weakly stable stratification ($\partial T/\partial y = 0$ K/m). For further details on the boundary conditions for the fluid flow and the pollutant equations see [20]. For the turbulence equations, boundary conditions and wall functions according to [14] are used.

The optimization cost function J is the value of the pollutant concentration at $x = 250$ m from the inlet at height 2 m. Vector of parameters $p = (x_1, x_2, \mathrm{LAI})$ consists of starting and end point of the vegetation block and its *Leaf Area Index*, which is a ratio of a total leaf area relative to the ground area. Following constraints are placed on the parameters:

- Position of the vegetation: $x_{min} \leq x_1 \leq x_2 \leq x_{max}$ with $x_{min} = 50$ m and $x_{max} = 150.0$ m.
- Maximal leaf area index: $0.0 \leq \mathrm{LAI} \leq \mathrm{LAI}_{max}$ with $\mathrm{LAI}_{max} = 9.0$.

– Maximal total amount of trees planted: $(x_2 - x_1)\mathrm{LAI} \leq \mathrm{VEG}_{max}$ with $\mathrm{VEG}_{max} = 270.0$. That could represent eg. forest of length 30 m and LAI 9 or length 100 m and LAI 2.7.

3.2 Results

Since our method searches only for a local minimum, three different initial points were used to rule out a possibility that only a local minimum in the vicinity of a initial position was found. The optimization procedure ended in the same point for all of the initial points. The initial configurations and corresponding solutions are listed in Tab. 1. The optimized variant represents

Variant	Initial point	Solution	J (Initial)	J (Final)	#Evaluations
A	$(90.0, 110.0, 4.5)$	$(50.0, 150.0, 0.810)$	0.0407	0.0338	39
B	$(80.0, 110.0, 6.75)$	$(50.0, 150.0, 0.810)$	0.0419	0.0338	45
C	$(60.0, 90.0, 8.1)$	$(50.0, 150.0, 0.810)$	0.0402	0.0338	67

Table 1. Three initial variants and corresponding solutions. The initial and final points are listed in the form of the parameter vector $p = (x_1, x_2, \mathrm{LAI})$.

a sparse vegetation block spanning the whole allowed interval. The obtained LAI = 0.81 lies well below the value given by the constraint on the maximal amount of trees planted, which allowed for a LAI = 2.7 for a block spanning the whole interval.

As evident from the Tab. 1, the cost function (i.e. the concentration behind the barrier) was reduced by 15% - 20% in all three cases. This reduction is further visible on the left panel of Fig. 2, where the vertical profiles of the particle concentration at $x = 250$ m is shown. Three initial variants and the final variant are complemented by a variant with no vegetation present.

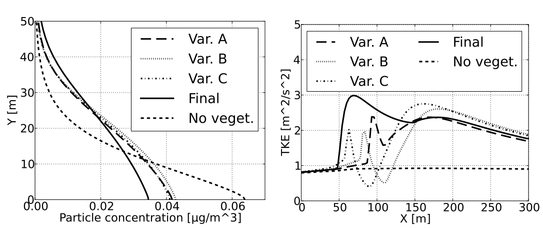

Fig. 2. Vertical profile of particle concentration at x = 250 m (left) and horizontal profile of turbulence kinetic energy at height 10 m (right).

Table 2 shows that less than 10% of the injected pollutant was deposed either on the ground or on the vegetation in all cases, and less than 5% in the optimized variant. The rest was redistributed to the higher layers

	Variant A	Variant B	Variant C	Final variant
Deposition on the vegetation	2.88%	4.30%	5.51%	2.43%
Deposition on the ground	2.88%	2.95%	2.75%	2.32%

Table 2. Percentage of the injected pollutant deposed on the vegetation and on the ground.

of the atmosphere, where the higher velocity of the flow allowed for faster dilution. Therefore, the most important effect of the sparse vegetation here is the disturbance of the flow, leading to the increased levels of turbulence and increased turbulent diffusion, which results in faster redistribution to the higher layers. This is demonstrated on the right panel of Fig. 2, where the horizontal profiles of the turbulence kinetic energy are shown for all variants.

4 Discussion

A method for evaluation the effects of vegetation barriers on pollution dispersion was developed and its usability was demonstrated on a simple test case. There are several shortcomings of the method. First, it is suitable only for a limited number of parameters. In the current implementation when 100 parameters are optimized the amount of time for the CFD solution in every step of the optimization loop is roughly equal to the time needed for the gradient evaluation. For higher number of parameters it would be therefore more suitable to use the adjoint method for the gradient calculation.

Secondly, there is a significant uncertainty in vegetation properties, as these are difficult to estimate. Quantification of this uncertainty should therefore be in order.

Thirdly, our method optimizes only for a single target, while in reality we may be interested in several targets at once. To take that into account, multi-objective optimization should be employed.

Lastly, optimization procedure sought only for the local minimum. Here we have used multiple initial points to assess whether we have found the global minimum, however, such approach is not sufficiently rigorous and could be difficult to apply when higher number of parameters is used.

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References

1. S. Balay, S. Abhyankar, M. Adams, J. Brown, P. Brune, K. Buschelman, L. Dalcin, V. Eijkhout, W. Gropp, D. Kaushik, M. Knepley,

L. McInnes, K. Rupp, B. Smith, S. Zampini, and H. Zhang, *PETSc Web page*, `http://www.mcs.anl.gov/petsc`, 2015.
2. D. Bäumer, B. Vogel, and F. Fiedler, *A new parameterisation of motorway-induced turbulence and its application in a numerical model*, Atmos. Environ. **39**:31 (2005), 5750–5759.
3. M. Gunzburger, *Perspectives in flow control and optimization*, Society for Industrial and Applied Mathematics, 2002.
4. W. Hinds, *Aerosol technology: Properties, behavior, and measurement of airborne particles*, Wiley, 1999.
5. S. Janhäll, *Review on urban vegetation and particle air pollution - deposition and dispersion*, Atmos. Environ. **105** (2015), 130–137.
6. S. Johnson, *The NLopt nonlinear-optimization package*, `http://ab-initio.mit.edu/wiki/index.php/NLopt`, 2015.
7. G. Katul, L. Mahrt, D. Poggi, and C. Sanz, *One- and two-equation models for canopy turbulence*, Bound. Layer Meteor. **113** (2004), 81–109.
8. M.-S. Liou, *A sequel to AUSM, part II: AUSM+-up for all speeds*, J. Comput. Phys. **214** (2006), 137–170.
9. T. Litschke and W. Kuttler, *On the reduction of urban particle concentration by vegetation - a review*, Meteorol. Z. **17** (2008), 229–240.
10. F. Muldoon and S. Acharya, *A modification of the artificial compressibility algorithm with improved convergence characteristics*, Int. J. Numer. Meth. Fl. **55**:4 (2007), 307–345.
11. A. Petroff, A. Mailliat, M. Amielh, and F. Anselmet, *Aerosol dry deposition on vegetative canopies. Part I: Review of present knowledge*, Atmos. Environ. **42** (2008), 3625–3653.
12. A. Petroff, L. Zhang, S. Pryor, and Y. Belot, *An extended dry deposition model for aerosols onto broadleaf canopies*, J. Aerosol Sci. **40**:3 (2009), 218–240.
13. M. Raupach, N. Woods, G. Dorr, J. Leys, and H. Cleugh, *The entrapment of particles by windbreaks*, Atmos. Environ. **35** (2001), 3373–3383.
14. P. Richards and R. Hoxey, *Appropriate boundary conditions for computational wind engineering models using the k-ϵ turbulence model*, J. Wind Eng. Ind. Aerodyn. **46 & 47** (1993), 145–153.
15. J. Steffens, Y. Wang, and K. Zhang, *Exploration of effects of a vegetation barrier on particle size distributions in a near-road environment*, Atmos. Environ. **50** (2012), 120–128.
16. K. Svanberg, *A class of globally convergent optimization methods based on conservative convex separable approximations*, SIAM J. Optim. **12**:2 (2002), 555–573.
17. A. Tiwary, H. Morvanb, and J. Colls, *Modelling the size-dependent collection efficiency of hedgerows for ambient aerosols*, Aerosol Science **37** (2005), 990–1015.
18. Y. Tominaga and T. Stathopoulos, *Turbulent Schmidt numbers for CFD analysis with various types of flowfield*, Atmos. Environ. **41** (2007), 8091–8099.
19. V. Venkatakrishnan, *Convergence to steady state solutions of the euler equations on unstructured grids with limiters*, J. Comput. Phys. **118** (1995), 120–130.
20. V. Šíp and L. Beneš, *Modelling the effects of a vegetation barrier on road dust dispersion*, Appl. Mech. Mater. **821** (2016), 105–112.