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Application of Detached Eddy Simulation to neighbourhood scale gases atmospheric dispersion modelling

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HIGHLIGHTS

- A model for the simulation of gases dispersion in urban terrain based on DES-SA.
- Successful evaluation of the model according to well-established case studies.
- Integration of the model with a new and custom mesh-generation algorithm.
- The new model puts forward the possibility of DES to be used in this field as a better alternative of LES and RANS.

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ABSTRACT

This paper addresses the current important problem of modelling the dispersion of toxic gases released in the urban terrains (i.e. neighbourhood scale) by the Detached Eddy Simulation (DES). This approach is a resolution that lays between the Reynolds Averaged Navier–Stokes and Large Eddy Simulation models and focuses especially on establishing a better balance between efficiency and accuracy. Herein are presented the theoretical approach of a new model, which is based on the DES and the Spalart–Almaras turbulent closure and a number of validation tests like the flow and the dispersion over and around a single building and an array of buildings. Overall, employed validation metrics were within the acceptable limits and the model demonstrated an acceptable agreement with the experimental datasets which confirms the use of this approach for the modelling and dispersion of gases in complex terrains like a city.

1. Introduction

The problem of toxic gas dispersion in a city is rather complex because the wind flow is fully separated and is characterized by vortex shedding and turbulent fluctuations throughout the fluid volume [1]. In this regime the simple fast approximate models (e.g. AERMOD, CALPUFF, OSPM) are not capable of reproducing the exact flow and providing reliable results, though some of them take into account the existence of buildings and other obstacles (e.g. Microswift-Spray, QUIC). This becomes particularly important in emergency planning, for instance in the case of a terrorist attack where we must consider the spread of highly toxic agents [2].

Therefore, there appears to be an obvious need for fully computational models that can predict details of the wind flow and the gas dispersion within an urban terrain. The majority of such models (Table 1) are based on the Reynolds Average Navier–Stokes equations (RANS) to predict the nature of the turbulent flow through the urban environment, which is in principle pre-requisite to the solution of the simpler – but itself complicated – problem of contaminant dispersion in the urban terrain [3–6]. Unfortunately, application of the RANS models have known drawbacks [3,7,8] like the need of special wall functions [9], the inacurate results when vortex shedding is involved etc. To resolve some of these issues Large-Eddy Simulation (LES) models have been successfully applied on the simulation of the wind flow and the dispersion of pollutants in urban terrains [5,10]. In LES, the equations are filtered so that the larger-scale motions are explicitly resolved and the smaller are represented by a subscale model (explicit LES) or by numerical methods to incorporate the subscale physics into the numerics (implicit LES). This method can produce results that are more accurate than RANS models, and that are less sensitive to the subscale model/numerics used. Unfortunately, the rigour associated with LES comes at the expense of a significant, usually excessive, computational requirement. For example, Chen et al. reported a

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Table 1
Indicative numerical neighbourhood scale atmospheric dispersion models.

Name	Type		Turbulence model	Developer	Reference
ADREA	RANS	FVM	zero, $k-l$, $k-z$, $k-\varepsilon$	NCSR & UoWM	[55]
CFD-Urban	RANS	FVM	$k-\varepsilon$	DTRA	[6]
Chensi	RANS	FDM	$k-\varepsilon$	Ecole Centrale de Nantes	[56]
Fast3d-ct	LES	FVM	MILES	Department of Defense USDoD	[2]
FEFLO-URBAN	LES	FEM	Smagorinsky	Naval Research Laboratory USNRL	[57]
FEM3MP	Hybrid RANS	FEM	eddy viscosity	DTRA	[58,59]
FLACS-URBAN	RANS	FVM	$k-\varepsilon$	GexCon	[60]
Fluent-EPA	RANS	FVM	$k-\varepsilon$	EPAEnvironmental Protection Agency, US	[61]
MISKAM	RANS	FVM	$k-\varepsilon$	Mainz University	[62,63]
MITRAS	RANS	FDM	$k-\varepsilon$	University of Hamburg	[64]
Urban-Stream	Hybrid PRANS	FVM	$k-\varepsilon$	DRD	[65]
VADIS	RANS	FDM	$k-\varepsilon$	University of Aveiro	[66]

RANS: Reynolds Averaged Navier–Stokes, LES: Large Eddy Simulation, MILES: Monotonic LES, FDM: Finite Difference Method, FVM: Finite Volume Method, FEM: Finite Element Method, DTRA: Defense Threat Reduction Agency US, DRD: Defense Research and Development Canada, NCSR: National Centre of Scientific Research, Greece, UoWM: University of Western Macedonia.

computational cost of 100 times greater than that incurred with the $k-\varepsilon$ RANS [11] for the prediction of flow over a matrix of cubes. While Vijiapurapu and Cui [12] reported just an increase with a factor of ~8 when they compared LES with $k-\varepsilon$ RANS for flow inside rough pipes. It is, therefore, necessary to seek a solution for the flow that is intermediate between the RANS and LES models in order to find a better balance between efficiency and accuracy. For example, Lien et al. [13] presented a form of hybrid RANS/LES utilizing the concept of a partially resolved numerical simulation to the simulation of an urban flow.

In the current paper, the well-known hybrid approach DES S-A (Detached Eddy Simulation Spalart–Allmaras) is introduced on the simulation of neighbourhood scale gas dispersion. This approach is based on the DES, which uses the one-equation closure S-A model [14]. The DES S-A approach has been mainly developed for aerodynamic studies and it has been successfully validated for similar problems [15–18]. One of the most important disadvantages of the DES S-A is the difficulty in generating a good grid to accommodate both RANS and LES [19]. Apart from that, DES S-A presents a number of advantages which affected its selection in the present research paper, these are listed below:

i) use of one hybrid approach for all transport scales (i.e. the S-A near the walls and the LES far away of the walls), which results in simplification of the calculation processes,
ii) the S-A is an one-equation model (turbulence closure; [20]), compared to typical two-equation RANS models (e.g. $k-\varepsilon$); this results in calculation time reduction, though probably not so large compared to not using LES everywhere,
iii) local type of the S-A model, for the turbulence viscosity.

For the implementation of the DES S-A model for the gas dispersion of gaseous pollutants, a new software, the Prognostic Model for Toxic Gas Dispersion (ProMTGD), has been developed on the .NET Framework. ProMTGD is based on an older 2D prognostic model [21] and the mesh generator HeMUT [22]. In the next sections, the theoretical model and the structure of ProMTGD are presented. Following that, the implementation of the software is examined by computing the wind flow and/or gas dispersion in a number of cases from peer-reviewed journals and the relevant VDI guideline 3783 [23], which is based on the CEDVAL dataset [24].

2. Model description

ProMTGD employs the finite element method in order to solve the necessary equations. This method provides greater flexibility [25,26] for the modelling of complex geometries than the finite difference and finite volume methods. In the next paragraphs the basis of the theoretical approach underlying the software is described.

2.1. Flow and dispersion – Reynolds averaged equations

The wind flow in an urban terrain is assumed to be an incompressible and neutrally-stratified fluid flow. Furthermore the atmospheric dispersion of a gaseous contaminant is assumed to be approximated as a passive dispersion. Thus the governing equations of mass, momentum and concentration based on the Reynolds-Averaged Navier–Stokes (RANS) approach are:

$$\frac{\partial \bar{u}_i}{\partial x_i} = 0, \tag{1}$$

$$\rho\left(\frac{\partial \bar{u}_i}{\partial t} + \bar{u}_j \cdot \frac{\partial \bar{u}_i}{\partial x_j}\right) = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) - \rho\overline{u'_i u'_j}\right] + \rho f_i, \tag{2}$$

$$\frac{\partial \bar{c}}{\partial t} + \bar{u}_i \cdot \frac{\partial \bar{c}}{\partial x_i} = \frac{\partial}{\partial x_i}\left(D\frac{\partial c}{\partial x_i} - \overline{u'_i c'}\right) + S_o, \tag{3}$$

where an over bar denotes the Reynolds averaging of a quantity and a prime on a quantity is used to denote the fluctuation of that quantity from its Reynolds-Averaged value. In more detail, $\bar{u}_i$ is defined as the mean velocity in the x_i-direction with $i = 1, 2$ or 3 representing the x-, y- and z-directions, t is time, $\bar{p}$ is the static pressure, μ and ρ are the viscosity and the density of the air respectively, f_i is the momentum source, $\bar{c}$ is the mean concentration of the gaseous contaminant, D is the molecular diffusivity and S_o represents the sources and sinks of the contaminant.

The Reynolds stresses and the turbulent scalar fluxes, required to close the transport equations for the mean momentum (Eq. (2)) and the mean concentration (Eq. (3)), are modelled using the Boussinesq hypothesis which is presented below:

$$-\rho\overline{u'_i u'_j} = \mu_t\left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i}\right) \tag{4}$$

and

$$-\overline{u'_i c'} = \frac{\mu_t}{\rho Sc}\frac{\partial \bar{c}}{\partial x_i}, \tag{5}$$

where μ_t is the turbulent viscosity and Sc is the turbulent Schmidt number (usually equal to 0.63). The Detached Eddy Simulation (DES) approach [14,18] in conjunction with the one-equation turbulence model Spalart–Allmaras [27] are employed for the calculation of the turbulence viscosity.