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Modelling reacting localized air pollution using Computational Fluid Dynamics (CFD)

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ABSTRACT

A Computational Fluid Dynamics (CFD) approach is used to model reacting NO_2 dispersion of vehicle pollutants released from a dual carriageway in Maidstone, UK. The simulations are carried out over the course of one full day during January, 2008.

The developed CFD model utilizes a modified k-ε turbulence model and Arrhenius reaction kinetics with source terms for the reactions which include a photo-stationary set with peroxy radicals. An approach is taken whereby the reactions are solved specific to the rush hour period corresponding to the availability of certain hydrocarbons released from the vehicles.

The results of the simulation are compared with field measurements taken at the site which is made up of several, different sized buildings on varying terrain in Maidstone UK. The predictions and field measurements are considered over a 12 h period with averaged hourly results.

It was found that the reactive pollutant approach greatly improves the predictions as compared to the experiments. Furthermore the effect of peroxy radicals during rush hour periods is found to be a major disturbance to the photo-stationary set and its inclusion improved the predictions further.

1. Introduction

Typically, most localized air pollution studies employing Computational Fluid Dynamics (CFD) have involved passive dispersion of pollutants, the term passive relating to the assumption that no reactions take place. When simulating the dispersion of pollutants, such as carbon monoxide which typically reacts at a very slow rate (28 days), reaction modelling is unnecessary, however when modelling a secondary pollutant such as nitrogen dioxide the reactions should be considered.

Baik et al. (2007) and Baker et al. (2004) tackled the problem of reaction modelling for an idealized case emulating a typical street canyon. They modelled the photo-stationary reactions, however both these studies do not report direct comparisons with field measurements, instead some confirmation from previous studies indicates that the models behave correctly.

It should be noted that the simulation of passive pollutants has sometimes yielded reasonable results. This is most significant for pollutants such as NO_x which is highly dependent on the set of photolysis reactions. Kondo et al. (2006) managed to obtain comparable results by simulating the dispersion of NO_x from a suspended expressway when compared with field measurements, discrepancies were not associated with the lack of reactions' modelling but this may well have been the case.

Modelling reacting flows in combustion applications was one of the very early applications of CFD and indicates that it is possible to model extremely complex reaction processes which are dependent on temperature and pressure; however there is a lack of published studies in modelling reacting pollutants in the atmosphere. Nonetheless some of the methods used in combustion applications (ANSYS Fluent, 2008) may be applied, for example testing some of the existing modelling approaches for atmospheric problems as suggested by Mastorakos (2005) or coupling CFD codes with specialized chemistry models which are based on the volumetric reaction approach (Li et al., 2006 and Lee et al., 2003). However in the present case Arrhenius reaction kinetics are applied.

The NO_x pollutant and its reaction cycle are not fully understood. Many different pollutants can drastically affect its concentration levels due to countless reactions. These are controlled by many environmental variables such as sunlight, atmospheric stability, temperature, humidity, etc. Many of the problems relating to localized dispersion due to reactant concentrations have been addressed previously (Atkinson, 2000).

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Whether a reactant of a certain species is important or not in a particular model is dependent on both the concentration and the reaction rate. If the two parameters are small, it can be said that the reaction is unimportant, as long as they are expected to stay that way during the simulation (Jacobson, 2005).

The photo-stationary reaction set (made up of a set of three reactions; see equation (8)–(10)) is defined as the steady state approximation which governs the atmospheric flow reactions involving NO_2 for the majority of the time. It is widely believed to provide a good description of the atmospheric conditions. However, there exist reactions which have the ability to disturb this process, such as those derived from hydrocarbons. Arguably the most important of which is peroxy radicals which when added to the photo-stationary set (equation (11)) forms what has been described as the “urban reaction set” (Jacobson, 2005).

In the next sections, the NO_2 chemical reaction equations will be solved and discussed in detail. Initial simulations are carried out for vehicle pollutants from the A229 road in Maidstone, Kent used as a suitable test case for the model, to include the photo-stationary reaction set followed by the inclusion of an additional reaction involving hydrocarbons (i.e. an urban reaction set) for comparisons and analysis. The results of the CFD prediction are compared to measured NO_2 levels at the site during a full day.

2. The CFD modelling approach

In order to obtain the concentration of pollution the general flow equations must be resolved as well as a transport equation for the pollutant. The Reynolds Averaged Navier Stokes equations for continuity, momentum, and a standard scalar transport equation for the pollutant are defined as follows:

$$\frac{\partial\rho}{\partial t}+div(\rho\boldsymbol{U}) = 0 \tag{1}$$

$$\frac{\partial(\rho U)}{\partial t}+\mathrm{div}(\rho U\boldsymbol{U}) = -\frac{\partial P}{\partial x}+\mathrm{div}(\mu\,\mathrm{grad\,U}) + \left[-\frac{\partial(\rho\overline{u'^2})}{\partial x}-\frac{\partial(\rho\overline{u'v'})}{\partial y}-\frac{\partial(\rho\overline{u'w'})}{\partial z}\right]+S_{Mx} \tag{2}$$

$$\frac{\partial(\rho V)}{\partial t}+\mathrm{div}(\rho V\boldsymbol{U}) = -\frac{\partial P}{\partial y}+\mathrm{div}(\mu\,\mathrm{grad\,V}) + \left[-\frac{\partial(\rho\overline{u'v'})}{\partial x}-\frac{\partial(\rho\overline{v'^2})}{\partial y}-\frac{\partial(\rho\overline{v'w'})}{\partial z}\right]+S_{My} \tag{3}$$

$$\frac{\partial(\rho W)}{\partial t}+\mathrm{div}(\rho W\boldsymbol{U}) = -\frac{\partial P}{\partial z}+\mathrm{div}(\mu\,\mathrm{grad\,W}) + \left[-\frac{\partial(\rho\overline{u'w'})}{\partial x}-\frac{\partial(\rho\overline{v'w'})}{\partial y}-\frac{\partial(\rho\overline{w'^2})}{\partial z}\right]+S_{Mz} \tag{4}$$

$$\frac{\partial(\rho\Phi_\mathrm{i})}{\partial x}+\mathrm{div}(\rho\Phi_\mathrm{i}\boldsymbol{U}) = \mathrm{div}(\Gamma_\Phi\,\mathrm{grad}\,\Phi_\mathrm{i}) +[-\frac{\partial(\rho\overline{u'\Phi'_1})}{\partial x}-\frac{\partial(\rho\overline{v'\Phi'_1})}{\partial y}-\frac{\partial(\rho\overline{w'\Phi'_1})}{\partial z}]+S_{\mathrm{R_i}} \tag{5}$$

Where:

U, V, and *W* are the mean velocities in their corresponding direction *x, y,* and *z U* is the average velocity.

P is the pressure field.

ρ is the density of the main fluid.

u', v' and w' are the instantaneous velocities in their corresponding direction *x, y,* and *z*.

Φ is the pollutant mass fraction.

Φ' is the instantaneous pollutant mass fraction.

Γ_Φ is the Molecular and Turbulent diffusion.

SR is the source term from reactions.

In the present case the Etling and Detering (1985) turbulence model is used which closes off the equations.

$$\frac{\partial(\rho k)}{\partial t}+\mathrm{div}(\rho kU) = \mathrm{div}\left[\frac{\mu_t}{\sigma_k}\mathrm{grad}k\right]+2\mu_t E_{ij}\bullet E_{ij}-\rho\varepsilon \tag{6}$$

$$\frac{\partial(\rho\varepsilon)}{\partial t}+\mathrm{div}(\rho\varepsilon U) = \mathrm{div}\left[\frac{\mu_t}{\sigma_\varepsilon}\mathrm{grad}\varepsilon\right]+C_{1\varepsilon}\frac{\varepsilon}{k}2\mu_t E_{ij}\bullet E_{ij}-C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} \tag{7}$$

E_{ij} is the mean deformation of the fluid elements (strain rate).

$\mu_t = \rho C_\mu k^2/\varepsilon$ is the turbulent viscosity.

σ_k, σ_ε, $C_{1\varepsilon}$, $C_{2\varepsilon}$, C_μ are all constants.

Etling and Detering conducted numerical calculations utilizing the standard *k*-ε model with standard coefficients on a neutrally stratified (dry adiabatic) boundary layer and made comparisons of turbulent kinetic energy, turbulent dissipation and velocity with observed data. The compared velocity profile showed distinct deviations between the *k*-ε model and observed results. Also the results showed over-predicted eddy viscosity and friction velocity. The discrepancy is due to the fact that the development of the model was based on non-rotating turbulent boundary layer (B.L) flows whilst atmospheric B.L's do inherently contain highly rotating flow. Etling and Detering propose modifications to the constants as follows: $C_\mu = 0.0256$, $\sigma_k = 0.74074$, $\sigma_\varepsilon = 1.298701$, $C_{1\varepsilon} = 1.13$, $C_{2\varepsilon} = 1.90$ which yield predictions closer to the experimental data.

A Schmidt number of 1.3 was used in this study, this was determined from preliminary trial simulations. Tang et al. (2006) and Riddle et al. (2004) found that reasonable pollutant concentration results were only achievable when the Schmidt number was varied and a range of values was used from 0.7 to 1.3. They state that the value used is highly dependent on the particular problem and probably the stability of the atmosphere.

Tang et al. (2006) compared centreline and crosswind concentrations in a street canyon and generally observed that a Schmidt number of 1 gave the best results. However the concentrations they measured included distances from 50 m through to 800 m from the source, it was observed that at the 50 m mark a Schmidt number of 1.3 gave the best results.

The density of the fluid is calculated in the usual manner, that is mass fraction weighted average of the densities of all the species, based on ideal gas law for each.

The following reactions are considered in this present work

$$NO_2 + h\nu \rightarrow NO + O \tag{8}$$

$$O + O_2 + M \rightarrow O_3 + M \tag{9}$$

$$O_3 + NO \rightarrow NO_2 + O_2 \tag{10}$$

$$RO_2 + NO \rightarrow RO + NO_2 \tag{11}$$

Seven transport equations for NO, NO_2, O, RO, RO_2, O_2 and O_3 are solved with source terms for the reactions. The source terms are a function of the pollutant concentration in each cell for each pollutant and the reaction or photolysis rate (N.B $h\nu$ represents an incident photon, M is a third body). The species N_2 is not solved and