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Simulations of the dispersion of reactive pollutants in a street canyon, considering different chemical mechanisms and micromixing

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ABSTRACT

The Stochastic Fields (SF) or Field Monte Carlo method has been used to model the dispersion of reactive scalars in a street canyon, using a simple chemistry and the CBM-IV mechanism. SF is a Probability Density Function (PDF) method which allows both means and variances of the scalars to be calculated as well as considering the effect of segregation on reaction rates. It was found that the variance of reactive scalars such as NO_2 was very high in the mixing region at roof-top level with rms values of the order of the mean values. The effect of segregation on major species such as O_3 was found to be very small using either mechanism, however, some radical species in CBM-IV showed a significant difference. These were found to be the seven species with the fastest chemical timescales. The calculated photostationary state defect was also found to be in error when segregation is neglected.

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1. Introduction

The street canyon has for many years been an active area of study in air quality modelling, both in terms of predicting actual roadside exposure to pollution and as a more theoretical test-case for using different numerical models. Experimental data has been obtained both from field studies (Rotach, 1995; Costabile and Allegrini, 2007) and from wind tunnel (Pavageau and Schatzmann, 1999) and water tank models (Caton et al., 2003). Computational modelling has been carried out in order to investigate the fluid mechanics and the dispersion of pollutants in and around the canyon (Chan et al., 2001; Baik and Kim, 2002; Jeong and Andrews, 2002). Work has also been carried out which attempts to quantify the exchange of mass and momentum at roof-top level using an exchange velocity in order to provide a model that can be applied to a real-world situations (Hamlyn and Britter, 2005). Walton and Cheng (2002) and Lui and Barth (2002) have used an LES calculation to predict the dispersion and fluctuation of an inert pollutant in a street canyon. Dixon and Tomlin (2007) have used a Lagrangian stochastic model for the same purpose.

Recent studies have focused on the turbulent dispersion of reactive pollutants in the street canyon setting. Baker et al. (2004) have carried out an LES study of a street canyon using a one-step, reversible NO, NO_2 and O_3 chemistry using a constant temperature in the canyon. They found that spatial variation of species within the canyon was significant. Baik et al. (2007), on the other hand, have used RANS modelling to predict the flow field in the canyon while using a similar chemistry to Baker et al. (2004). They performed a budget analysis of the terms in the advection–diffusion-reaction equation, which showed that the chemical reaction term is comparable to the advection and diffusion terms for O_3. Both these studies found that the air composition is close to chemical equilibrium within the canyon but is far from equilibrium where polluted air from the canyon is mixed with clean air at the top of the canyon.

Most reactive pollutant dispersion models so far have not included the effect of turbulence on reaction rates. Due

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to the non-linearity of the Arrhenius term and the effect of non-zero covariances between reactants evaluating mean reaction rates as a function only of mean concentrations and temperature may not yield a correct value. The fluctuations from the mean (either spatially or temporally) may need to be considered. The presence of fluctuations from the mean is known as segregation, while their decay due to molecular diffusion at the smallest scales of turbulence is often called micromixing. Whether the segregation has a significant effect on the reaction rate will depend on how rapidly micromixing destroys the segregation compared to the reaction speed. This is characterised by the Damköhler number, *Da*, defined as the ratio of mixing timescale to chemical timescale $Da = T_{\text{phys}}/T_{\text{chem}}$. For further discussion of this see Garmory et al. (2006). The above comments apply equally to RANS and LES calculations, the difference being that in the latter case the sub-grid segregation is expected to be smaller, but still not negligible in principle.

In this work we use the Field Monte Carlo method to simulate the dispersion of reactive pollutants within a street canyon and also to assess what effect segregation and micromixing have on the reactions. This is done using the simple NO, NO_2 and O_3 chemistry used in Baik et al. (2007) and also using the CBM-IV mechanism, which is a more complex chemistry comprising 28 species (Gery et al., 1989). The Field Monte Carlo method, also called the Stochastic Fields method, is a transported PDF method developed independently by Valiño (1998) and Sabel'nikov and Soulard (2005b). Rather than using the motion of notional particles through the flow this method solves stochastic partial differential equations (spde), derived from the modelled transported PDF equation (Fox, 2003), for a number of scalar fields extending across the spatial domain. A spde is solved for each scalar in each field, if the values for a particular scalar are taken at a point in space across all fields then the ensemble is statistically equivalent to the flow at that point. By doing this the effect of fluctuations on the reaction rates are calculated directly with no need for closure models for the mean reaction rate, which constitutes the greatest difficulty in turbulent reacting flows. The advantage of the field based method is that it is easily coupled with existing CFD techniques and is hence straightforward to implement in practical scenarios. In this work, the reactions have no effect on the density due to their negligible heat release, which allows us to pre-calculate the flow and then use a 'frozen' flow field for the subsequent reactive scalar calculations.

2. Formulation

2.1. The stochastic fields method

The Stochastic Fields, or Field Monte Carlo, method is a transported joint composition PDF method developed for the simulation of turbulent reacting flows (Valiño, 1998; Sabel'nikov and Soulard, 2005b). A number of 'fields' extending across the whole spatial domain of the simulation are used which contain values for each scalar at every node on an Eulerian grid. The evolution of each field takes place according to a governing spde derived from the scalar PDF transport equation. The Ito SPDE as derived by Valiño (1998), using the Interaction by Exchange with the Mean (IEM) closure for micromixing, is

$$\mathrm{d}\tau_i^f = -U_k\frac{\partial\tau_i^f}{\partial x_k}\mathrm{d}t + \frac{\partial}{\partial x_k}\left(K\frac{\partial\tau_i^f}{\partial x_k}\right)\mathrm{d}t + \dot{w}\left(\tau_1^f,\tau_2^f,\ldots,\tau_I^f\right)\mathrm{d}t + (2K)^{1/2}\frac{\partial\tau_i^f}{\partial x_k}\mathrm{d}W_k^f - \frac{\tau_i^f-\overline{\phi}_i}{T_{\text{eddy}}}\mathrm{d}t \quad (1)$$

where τ_i^f is the value of scalar i in field f ($f = 1,\ldots,F$) and $\overline{\phi}_i$ is the local mean of scalar i. U_k is the mean velocity, K is the combined molecular and turbulent diffusivity, T_{eddy} is a characteristic timescale of turbulent scalar mixing used in the IEM model. As this is an Ito SPDE $(2K)^{1/2}(\partial\tau_i^f/\partial x_k)$ must be evaluated only once per timestep to ensure that it is independent of $\mathrm{d}W_k^f$ (Gardiner, 2004). The PDF is then represented by the ensemble of F stochastic fields τ^f which contain values for each scalar at each point throughout the flow. As this is a joint scalar PDF method and not a joint velocity-scalar PDF method (Pope, 1994) the velocity, turbulence and timescale must be provided from an external source, which in this case is a CFD solution. The SPDE solved here, Eq. (1), is in non-divergent form, Soulard and Sabel'nikov (2006) derive an SPDE in divergent form which gives results statistically equivalent to those used here. While not employed here it is thought that this divergent form may offer advantages in implementation using conservative numerical schemes. The Stochastic Fields method has to date been used to model combustion (Sabel'nikov and Soulard, 2005a; Mustata et al., 2006). We have previously used the method to simulate a NO_x/O_3 reacting plume in laboratory conditions (Garmory et al., 2006) and found excellent agreement with experimental data for mean and rms values. The method was also extended to the simulation of a jet engine exhaust plume in Garmory et al. (2008). The reader is referred to these papers for further discussion of the method.

2.2. Numerical methods

In this paper we use the same procedure for solving the Stochastic Fields equation as in our earlier paper Garmory et al. (2008). As a separate CFD calculation of the flow is required, we coupled our Field Monte Carlo method with a commercial CFD package, FLUENT. This was used not only to calculate the flow field, but also, by using an operator-splitting method, the spatial transport terms in (Eq. (1)) for each timestep. The advantages of coupling with a commercial CFD package are that there is no difficulty in exporting velocity field data to the reacting flow code and also that all the grid making and post-processing tools already available in FLUENT (or any other CFD code) can be used with this problem.

An operator-splitting procedure is used where in the first fractional step FLUENT's User Defined Scalars (UDS) option is used to solve for the transport terms in (Eq. (1)) for each scalar in each field using an iterative implicit method. The second step is to perform the random, or Wiener, step for each scalar in each field using $\Delta W_k^f = \xi_k^f \Delta t^{1/2}$ where ξ_k^f is a Gaussian random number with zero mean and unity variance (Gardiner, 2004). An independent value of ξ is

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