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DEVELOPMENT OF THE METHOD FOR IDENTIFICATION OF THE UNKNOWN SHORT DURATION SOURCE IN URBAN ATMOSPHERIC ENVIRONMENT USING THE CFD MODEL

Ivan V. Kovalets[1,2]*, George C. Efthimiou*[3]*, Spyros Andronopoulos*[3]*, Alexander G. Venetsanos*[3]*,*
Konstantinos Kakosimos[4]*, Christos D. Argyropoulos*[4]

[1]Ukrainian Center of Environmental & Water Projects, prosp. Glushkova, 42, 03187, Kiev, Ukraine
[2]Institute of Mathematical Machines and Systems Problems NAS of Ukraine, prosp. Glushkova, 42, 03187, Kiev, Ukraine
[3]Environmental Research Laboratory, INRASTES, NCSR “Demokritos”, Patriarchou Grigoriou & Neapoleos Str., 15310, Aghia Paraskevi, Greece
[4]Chemical Engineering Department & Mary Kay ‘O Connor Processes Safety Center, Texas A&MUniversity at Qatar

Abstract: We recently developed the method for identification of location, start time, duration and release rate of an unknown short-duration source of airborne pollution in urban environment. The method has been integrated in the ADREA-HF CFD code and the testing has been carried out by performing series of source inversion runs using the data of 200 individual realizations of the puff releases as obtained in the wind tunnel CUTE experiment. The robustness of the developed source inversion approach was thus demonstrated. The developed algorithm could be potentially applied in real-time emergency response systems dealing with the releases of toxic hazardous substances.

Key words: *Inverse problem; CFD; Data assimilation; Urban atmospheric dispersion; Hazardous pollutant; Source inversion; CUTE experiment.*

INTRODUCTION

The source inversion problem - identification of the unknown source properties such as location, release rate, and others following plume detection by the monitoring network is of great practical interest (Hutchinson et al., 2017). This problem becomes even more important in case when hazardous toxic pollutants are detected in cities following accidental and/or deliberate releases because large density of urban population increases its vulnerability to such events. From the one side complex nature of atmospheric transport processes in urban atmospheric environment could be treated in the most comprehensive way by the CFD models. From the other - such models are usually time consuming and still their usage in the real-time emergency response systems is challenging (e.g. Kovalets et al., 2008).

The interesting practical case of transient dispersion problem is when time variability of concentration fields is caused by transient release i.e. instantaneous or finite-duration source acting in stationary meteorological conditions. The time necessary for Source Receptor Function (SRF) calculations could be greatly reduced in such case and therefore below we consider the atmospheric dispersion problems characterized by small enough times (<1 hour) and spatial scales of up to about 10 km for which the assumption of stationary meteorological fields is frequently applied in practice. Another issue that arises in case of identification of transient releases is that in addition to source location and release rate which are the only unknowns for stationary release, in case of transient release time of release start and release duration are also unknown and release rate is variable. Thus the number of possible source configurations increases and hence it becomes much more difficult to find solution of the source inversion problem. The problem is simplified in case of short duration releases (~1 min) when the release rate could be assumed constant. Source identification problem in case of transient releases in urban atmospheric environments was previously considered in some works however usually essential simplifications had been made such as known source position (Salem et al., 2017) or limited number of known possible source positions (Vervecken et al., 2015).

The goal of our recent work was to develop the source inversion algorithm and to integrate it in CFD which allows for establishment of the unknown source parameters in case of the short duration release in urban environment and assuming stationary meteorological conditions and which is feasible for applications in real-time emergency response systems.

The present work is continuation of the previous works by Kovalets et al. (2011), Efthimiou et al., (2017a) in which the stationary release rate was considered and source inversion methodology was developed and implemented in ADREA-HF CFD code (Venetsanos et al., 2010). The newly developed algorithm was also implemented in ADREA-HF CFD model. Due to space limitations, the developed algorithm will be described in a journal paper. In this paper we present some details of implementation in ADREA-HD code as well as some results of its testing against measurement data of CUTE experiment.

DETAILS OF IMPLEMENTATION IN ADREA-HF CFD CODE

The ADREA-HF CFD code is a three dimensional transient fully compressible flow and dispersion CFD solver, able to treat highly complex geometries using the porosity formulation on Cartesian grids (Venetsanos et al., 2010). As far as inverse problem is formulated above only for the passive contaminant (which doesn't affect the wind flow) the wind field is pre-calculated, stored and then used for solving atmospheric dispersion problem.

One of the key issue in application of the CFD model for source term estimation is calculation of the source receptor function (SRF) which is obtained by integrating backward adjoint concentration equations. In case of stationary dispersion problem the number of adjoint equations to be solved is equal to the number of available measurement stations. In case of transient dispersion problem the number of adjoint equations to be integrated equals the number of available measurement values and thus is very large. However it is shown that if meteorological conditions are stationary the number of integrations of adjoint equations could be reduced down to the number of stations even in transient case. Indeed let simulated with forward model concentration following instantaneous ***unit*** release at time t_s at observation time t_o in point i is $c\left(t_o, \mathrm{r}_i; t_s, r_s\right)$. Here and below independent variables (time, position vector) of the forward and backward problem are listed in brackets before ";" and then parameters of the problem (time and spatial location of source) are listed. It is equal to solution of backward adjoint equation with instantaneous unit release of puff in observation point i at observation time t_o: $c\left(t_o, \mathrm{r}_i, t_s, r_s\right) = c^*\left(t_s, r_s; t_o, r_i\right)$. If meteorological fields (velocity, diffusivity) are stationary, then solution of adjoint equation apparently depends only on difference between time of observation and time of release:

$$c\left(t_o, \mathrm{r}_i, t_s, r_s\right) = c^*\left(t_s, r_s; t_o, r_i\right) = c^*\left(\Delta t_{so}, r_s; r_i\right)$$

$$\Delta t_{so} = t_s - \mathrm{t}_o$$

Thus calculation of source receptor function could be performed by N_o integrations of backward adjoint equations (N_o as in case of continuous release being number of observation locations) with instantaneous 'unit' releases at each point in the beginning of simulations (i.e. at t=T).

An adjoint equation is then solved by integrating non-stationary adjoint equation from sufficiently $t = T$ to $t = 0$. The adjoint equation is solved separately for each sensor and the obtained solution $c_n^*\left(x, y, z, \mathrm{t}\right)$ is stored in binary file.

With the aid of SRF the correlation function of simulated and measured concentrations is calculated in the loop spanning all sensors, all measurement times, and for each of the possible source locations (grid nodes), variants of the start time and duration of the release and finally the source parameters maximizing correlation function are evaluated.

It is important to note that reading of the binary files in which adjoint variables are stored (in total there are N_o such files) is time consuming procedure. Therefore ideally the loop is to be organized in such a way that the number of readings of binary files is minimized. However in such a case the algorithm could easily run out of memory (RAM). Therefore we used a suboptimal sequence of minimization procedure in which binary files are read $N_o N_\delta$ times but the amount of RAM required for running of the algorithm is significantly reduced. Following computational sequence the values of $J_{k,l,r}$ are obtained and direct minimization is done.

RESULTS

Model setup

Simulation of atmospheric transport for the conditions of CUTE experiment has been performed with ADREA-HF model by Efthimiou et al. (2017b). In present work we use very similar model setup in forward run following Efthimiou et al. (2017b). Two grids were used in simulations: fine grid – the same as in Efthimiou et al., (2017b) consisted of 157 × 129 × 25 control volumes (in the x-, y- and z-directions, respectively) and additional coarse used in this study had 72 × 61 × 14 control volumes.

The pre-calculated stationary meteorological fields (wind velocity components, turbulent diffusion coefficients) were used to drive the solution of backward adjoint equations. The adjoint equations were solved separately each sensor location and the time-integrated adjoint variables were stored in binary files. The following value of the time interval used for integration was used: $\Delta_{avr} = 10s$ which as it was described above coincided with the estimation of the minimum possible source duration interval $\Delta_{\min}^{s} = 10s$. The estimation for the maximum value of the source duration was twice the true release duration: $\Delta_{\max}^{s} = 60s$. The value of the time integration interval for backward adjoint equations was set equal to time integration interval of forward equations: T=1000 s.

For the calculation of the first guess estimations of the release start time the value for the threshold coefficient defining plume arrival time was set to 0.1. The wind speed at canopy height was estimated from the well known logarithmic velocity profile $u(z) = (u_*/0.4)\ln((z-d)/z_0)$. The canopy height was taken to average value of buildings: $H_c = 30$ m, the displacement height was estimated as $d = 0.8H_c = 24$ m, while roughness length was taken $z_0 = H_c/30 = 1$m. With using the above value of wind speed at reference height $U(z = 49m) = 6$ m/s the above estimations lead to estimation of the wind speed at canopy height equal to $U_c = 3.34$ m/s.

The CUTE-3 experiment was repeated multiple times in order to get information about the statistical properties of the highly fluctuating turbulent concentration signal. Such experimental setup is very convenient for testing of the source inversion problem, since it gives opportunity to solve inversion problem for each experimental case and to study robustness of the results of source inversion with respect to fluctuations caused by inherent uncertainty in turbulent concentration signal. Note that

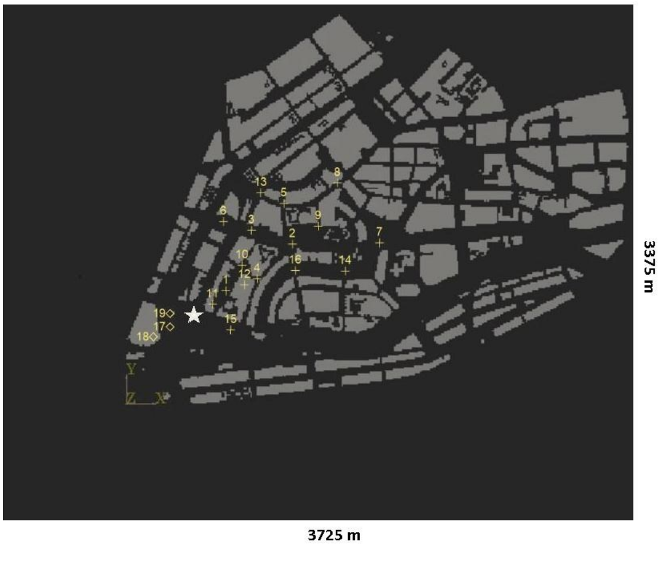

Figure 1. Geometry of the buildings in the area of the CUTE experiment and locations of sensors used in source inversion; source location is denoted by star; '+' — real sensors; ' ◇ ' — artificial sensors reporting zero values.

in ADREA-HF model we use Reynolds-averaged equations of fluid flow and concentration transport, therefore in the most ideal case (which could never happen in real applications) we should compare calculated results with ensemble-averaged results of measurements.

Since in case of CUTE-3 experiment we have many individual runs (ensemble members) carried out in the same experimental conditions we first of all performed source inversion runs with using respective results of ensemble-averaged measurements. The source receptor function calculated at this first stage was then used at the second stage of testing in which we performed source inversion with using measurements data from individual ensemble members of the CUTE-3 experiment. In total 200 source inversion runs were performed with using measurement data from individual ensemble members. Note that in CUTE-3 experiment there were 283 ensemble members. However many runs didn't contain data of all 16 sensors shown in Fig. 1. Therefore in our study we performed source inversion runs with using measurement data of those ensemble members which contained time histories of at least 70% of sensors. If particular ensemble member didn't contain time histories of the certain sensor then in source inversion run we used ensemble-averaged data of the respective sensor. Before the usage in source inversion runs the concentration measurements from individual ensemble members of the CUTE-3 experiment were time-averaged with 15-s time interval in order to reduce noise in the calculated correlation function due to the impact of the stochastic component of measurements. In addition as discussed below we used data of the 3 artificial sensors (Fig. 1) located upwind of the source and reporting just zero values.

Results of calculations

The results of source inversion runs with using the ensemble averaged measurements obtained in CUTE-3 experiment are shown in Table 1. In all cases reported in Table 1 achieved values of the correlation coefficient are higher than the corresponding values obtained in forward runs with the true source parameters. Thus there is some overfitting in source inversion runs, which is especially significant in case of the coarse grid. As it is seen from the Table 1 the results obtained with using only measurements from real sensors located downwind of the release are of poor quality on the coarse grid. The distance from the estimated release location to the true location is 265.6 m. The reason for this error could be understood by analyzing the calculated spatial distributions of the maximum correlation coefficient of model results as compared to ensemble averaged measurements achieved in source inversion algorithm for different assumed locations of the source.

Table 1. Source parameters used in CUTE experiment and obtained in source inversion runs using ensemble-averaged observations. r_h is horizontal distance from estimated to true source location.

Case	Obs.	Coarse grid-16 sensors	Fine grid-16 sensors	Coarse grid-19 sensors	Fine grid-19 sensors
r_h, m	0	265.6	72.2	54.1	53.3
Zs, m	0	13.5	6.	13.5	18
Qs, kg	50	219	117.6	97.5	116.1
ts,s	60	15.7	64.26	85.6	73.4
Δs, s	30	50	10	60	40
Cor. coef.	1	0.85	0.94	0.83	0.93

The estimated start times of the release presented in Table 1 mostly fall within the time interval covered by the true release. The estimated release durations in different cases vary in the wide range: from $\Delta^s_{\min} = 10s$ to $\Delta^s_{\max} = 60s$. Estimated release inventories in Table 1 exceed the true values in all cases by the factor of about 2. The most probable reason for this is that in all cases the estimated locations are situated upwind of the source and therefore increase in the released inventories compensates decrease in concentrations. In case of the fine grid the same 'compensation' effect takes place also because of the error in vertical position of the source.

CONCLUSIONS

In present paper the source inversion algorithm was developed and integrated in ADREA-HF CFD model which allows for establishment of the unknown source parameters (location, inventory, start time and duration of the release) in case of the short duration release in urban environment and assuming stationary meteorological conditions. It is shown that due to above assumptions the number of integrations of backward adjoint equations required for calculation of source receptor function could be reduced down to the number of available measurement stations. In result the computational effectiveness of the algorithm is close to real-time applicability. The algorithm is applicable to dispersion scenarios lasting up to 1 hour and to short duration releases lasting ~1 min when the release duration could be set approximately constant. The details of the method are described in the forthcoming paper (Kovalets et al., 2017).

It should be noted that even though the assumption of stationary meteorological fields restricts predictive capability of CFD model in our work the usefulness of the developed approach is justified by the robust performance of the algorithm as revealed in series of source inversion runs using the data of multiple individual realizations of the puff releases in the same average flow conditions. Real-time applicability of source inversion approaches based on more advanced CFD modeling tools such as LES is still limited (Mons et al., 2017) however the latter approaches remain interesting subject for further research.

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