SIMULATION DATABASE FOR ATMOSPHERIC DISPERSION OF POLLUTANT AND TOXIC COMPOUNDS DURING ACCIDENTAL FIRES

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Abstract: A preliminary implementation of a database (db) has been investigated as a tool for risk analysis and pollutants/toxics dispersion monitoring as a consequence of accidental fires. The db has been designed to offer a fast and clear modelling answer after the selection of a reduced number of input parameters describing: place and event intensity, weather conditions and time after the beginning of the event. In this earliest development and feasibility phase, the downwind maximum concentration ratio at different distances from the source are stored for more than 25000 different cases simulated with CALPUFF. Each record in the db is obtained by variation of wind intensity in the range between 1 and 5m/s, stability class between 1 and 6, initial temperature and velocity of the plume (varying respectively the values between 200 and 1200°C and from1 to 5m/s or changing the initial plume σ_z), equivalent diameter of the fire (from 1 to 100m), release height of the plume (from 1 to 50m). All the possible event cases have been simulated also considering the range from 1 to 8h after their beginning. The input variables describing plume initial temperature and velocity are calculated considering the heat release rates for different types of fuels as reported by the handbook for fire protection engineering (SFPE) and implemented in the Fire Dynamics Tools (FDTs) of the U.S.NRC. A prototype for data elaboration has been also developed, enabling the extraction of concentration profiles from the db, the partitioning of concentration ratios in three zones from the emission source and their visualisation with HTML code for web-based mapping resources.

Key words: *Calpuff, Atmospheric Dispersion Modelling, Accidental Fires.*

INTRODUCTION

Local administration and health authorities need to evaluate the extension of the area affected by harmful smoke pollution dispersion during accidental fires. These accidents encompass a very large number of possible events: e.g. industrial building fires, forest fires and pool fires involving different type of substances and fuel materials. In many cases during events only rough data for their characterisation are available causing high uncertainties in model calculation. The development of a static database of simulations has several advantages when a quick response is required: all data stored are always available and can be reached or elaborated by different software solutions, the input parameters of a specific event can be selected with filters or queries also by technicians not trained to apply atmospheric dispersion models. Moreover, the definition of standard queries can allow a combination between event parameters in case of high level of uncertainties as in risk analysis or during event evolution; the simulation results can also be shared between experts and validated before their practical utilisation.

DESCRIPTION AND PARAMETRISATION OF ACCIDENTAL FIRES

A set of parameters describing an accidental fire has been identified as model input parameters for describing a larger number of possible events. An accidental fire can be due to a combustion of pyrolysis gases from solids materials, evaporation of flammable liquids, release of pressurized gas or other complex release of liquid sprays and aerosols. All fires can be characterised by a first stage of ignition, where a buoyant gas stream undergoes combustion into a surround of basically uncontaminated air followed by a possible smouldering, by flaming and flashover. The buoyant flow including possibly also flames determines the fire plume, generally turbulent. As a matter of facts, considering also the inputs required by an atmospheric dispersion model, fire events can be characterised by virtual origin, diameter, height of flames, initial temperatures and velocities.

According to the Handbook of Fire Protection Engineering (SFPE, 2002), flame height L can be correlated to the diameter of fire source D and to the total heat release rate Q (L and D in m; Q in kW):

$$L = -1.02\ D + 0.235\ \dot{Q}^{\,2/5} \qquad (1)$$

The total heat release can be approximated to the total release rate obtained when the complete combustion of the burning material occurs. The Fire Dynamics Tools (FDTs) implemented by U.S.NRC reports the total heat release rate (HRR) specific per unit floor area (kW/m^2) for different materials. The ratio between flame heights and fire extension varies from 1-10 for pool fires up to 100-1000 for jet flames. In this preliminary work only reduced ratio between plume release height and fire extension have been considered. The specific heat release rate ranges between 81 kW/m^2, characteristics of flame retarded materials and up to 1,5 MW/m^2 of combustible polymers. Higher values are also reported for stacked materials of wood and cartons where the height of the stack assumes a controlling role. Considering building burnings, small fires are generally defined for total HRR lower than 1 MW, medium fires in the range of 1-5 MW and major fires when the HRR is higher than 5 MW (Armstrong, 2011). Considering the scientific literature, the accident in Buncefield Oil Storage Depots (B.O.S.D) in 2005 was represented by a fire diameter of 85m and an average HRR of 1,5 MW/m^2 due to liquid fuel combustion (Argyropoulos et al., 2010). This value correspond to the combustion of polymer like PE, PP and PS without presence of flame retardants.

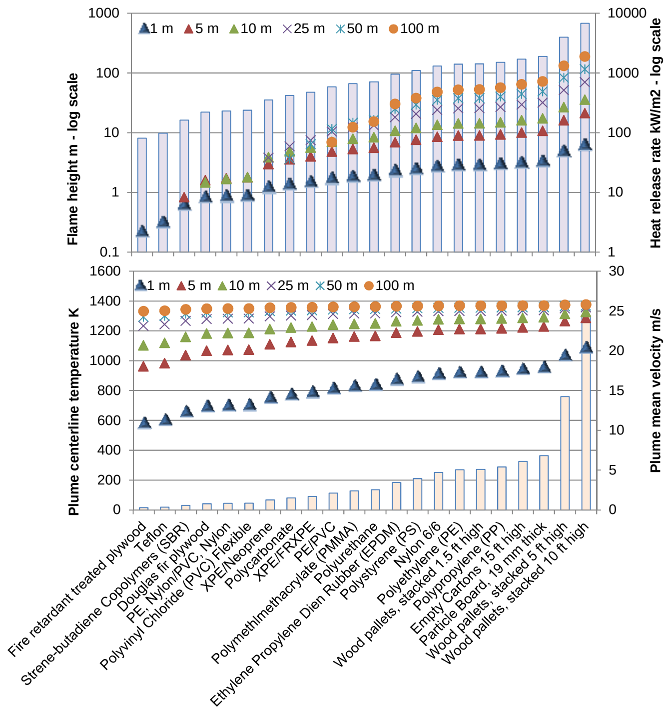

Figure 1. Parameters definition for accidental fires, according to the Handbook of Fire Protection Engineering (SFPE, 2002) and the Fire Dynamics Tools (FDTs) implemented by U.S.NRC (Marks: flame height and temperature, bars: HRR and plume velocity).

Figure 1 shows the possible theoretical flame heights for different burning material for fire sources in a range comprised between 1 and 100 m equivalent diameter. Very large fires involving crude oil in open sea has been investigated in the Newfoundland Offshore Burn Experiment (NOBE) and mathematically modelled by large eddy simulation (LES) model (Fingas et al., 1994, McGrattan et al., 1996). For the NOBE, an HRR of 200 MW was estimated considering an average burning surface of 100 m^2 with a specific heat release of 2 MW/m^2 and a particulate production rate of 0.78 kg/s. According to the procedures of US-NRC and the methodologies of the SFPE is possible to calculate for all the combination of the events the centreline plume temperature, at 1m distance above the plume origin and considering a referring atmospheric temperature of 25°C, according to the following equation (T_p in K, HRR in kW and h_0 in m):

$$T_p = 66.1764 \cdot (0.6 \cdot HRR)^{\frac{2}{3}} \cdot (1 - h_0)^{-\frac{5}{3}} + 298.15 \qquad (2)$$

Where the virtual origin of flames h_0 is obtained by:

$$h_0 = -1.02 \cdot D + 0.083 \cdot (HRR)^{\frac{2}{5}} \qquad (3)$$

The initial buoyant centreline plume velocity, w_0 in m/s, has been calculated according to the equation (Chang and Scire, 1999):

$$w_0 = 2.81672 \cdot 10^{-3} \frac{HRR \cdot T_p}{T_p - 298.15} \qquad (4)$$

In the second panel of figure 1 the possible ranges of plume temperatures and initial velocities are reported for different type of materials. The identified ranges confirmed previous and detailed analysis performed for an accident, where the dispersion modelling was performed considering a plume temperature variation in the range 200-1000°C and centreline velocity varying between 2.5 and 5m/s (Grimaldelli et al., 2005).

APPLICATION OF THE ATMOSPHERIC DISPERSION MODEL

Simulations on pollutants atmospheric dispersion have been investigated with CALPUFF (TRC Companies, Lowell, MA), an advanced non-steady-state air quality-modelling framework developed by atmospheric scientists. CALPUFF can be applied on scales of tens to hundreds of kilometres. US Environmental Protection Agency lists it as the preferred system for assessing long-range transport of air pollutants. CALMET, a diagnostic 3-dimensional meteorological model, and CALPUFF system are used to simulate particulate matter dispersion from forest fires on the basis of MODIS products (Henderson et al., 2008). In a similar way to the definition of fire characteristics according to HRR, particulate emission rate are estimated from the fire radiative power (FRP) detected in specific pixels from MODIS and defined as the rate of release of the radiant component of the total heat energy generated by fire (Roberts et al., 2005; Wooster et al., 2005). In a first step of this activity, a recursive processor have been implemented. The system is able to launch a sequence of a huge number of simulation. Input parameters describing different meteorological conditions have been varied in combination with the possible ranges of fire parameters. Different fires are represented by circular area sources where the exit diameters, initial velocity and emission temperature are approximated to diameter of fire sources, centreline plume velocity at 1m above flame height and plume temperature. The releasing height can be considered as the minimum flame height as calculated in the fire parameterization. The emission source has been placed in a 12 x 12 km flat dominium and, for each fire scenario, simulations have been completed for 1, 2, 4 and 8 hours after the beginning of the event. For each simulation a default emission rate of 1 g/s of non-reactive particulate matter has been set. Combining different fire event parameters (equivalent diameter and average plume velocity) the pollutant concentration C_0 has been calculated as stack exit concentration. Results for the maximum downwind hourly ground concentration *C* have been stored for each simulation.

Architecture of the simulation database

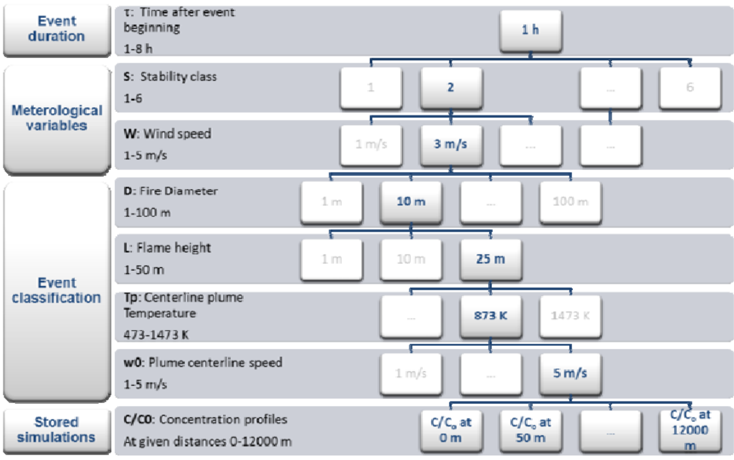

Figure 2. Simplified architecture of the simulation database.

By the combination of all the possible parameter ranges CALPUFF has simulated around 25000 different cases. All the records obtained from INPUT/OUTPUT parameters of the simulation can be stored in a table with a similar structure as reported in figure 2. One or more cases are selected according to event duration, meteorological variables, fire characteristics. In the elaboration of complex scenarios database queries can be defined considering average or statistical profiles defined on ranges of variation for meteorological and fires variables. The modelling system has shown its difficulty to simulate very large fires for equivalent diameter of 50m and above. For these cases test runs with emission sources approximated to buoyant area sources have been performed setting a default emission rates of $1g/s/m^2$. Also in these cases some limitation have been detected, thus claiming for further analysis by considering the possibility of subdividing larger fires into a set of smaller point emission sources.

ANALYSIS OF THE PRELIMINARY RESULTS

The combination between all the possible fire types as described by diameter, height, plume centreline temperature and velocity combined with the possible values of meteorological parameters - stability class and wind velocity - determines a database of atmospheric dispersion profiles expressed in terms of concentration ratio referred to the fire origin. All the data stored in the database can be analysed varying the stored model input parameters. In figure 3, C/C_0 variation on fire distances are reported for 3 possible event configurations described by the model as point emission sources. In panel a) the simulations consider a fire diameter of 1m and a plume origin at 10m for an average temperature (range 200-1200°C) and velocity (range 1-5m/s) at the centreline origin of the plume. The different colours of the lines consider the possible meteorological stability classes from 1 to 6. The diagram reported below gives the correlation factor of concentration profiles at the variation of wind velocity, stability class and event duration, according to the following relation (where x can represent at different distances wind velocity W, stability class S, event duration τ, plume velocity w_0, plume temperature T_p and y is the concentration ratio C/C_0):

$$corr = \frac{\sum (x-\bar{x})(y-\bar{y})}{\sqrt{\sum (x-\bar{x})^2 \sum (y-\bar{y})^2}} \qquad (5)$$

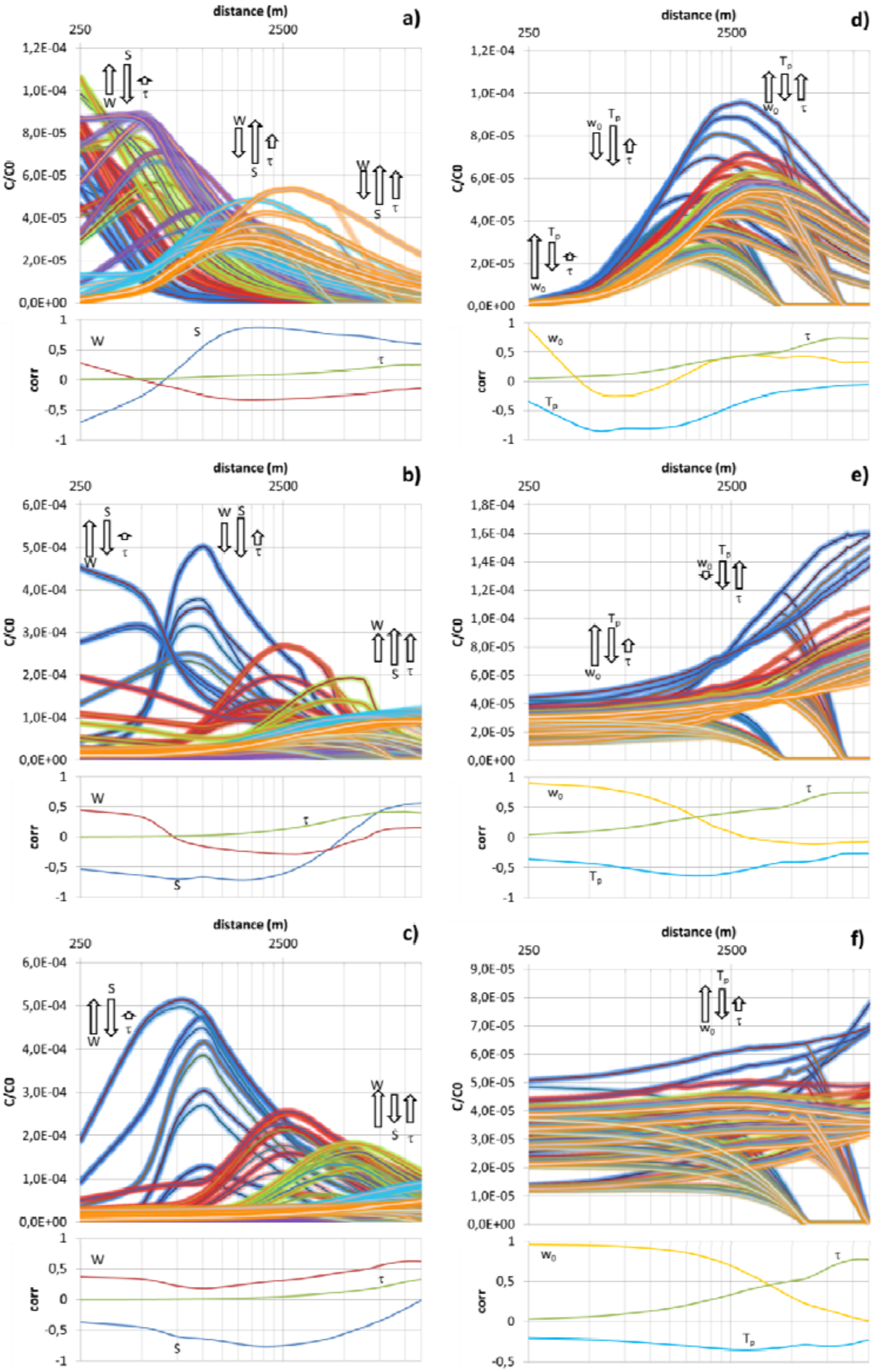

Figure 3. Effect of stability and wind velocity on average fire characteristic for three different geometry cases: a) 1m fire diameter and 10m release height, b) 10m fire diameter and 10m release height, c) 25m fire diameter and 25m release height. Effect of plume temperature and velocity at 1m/s wind and stability class F for three different geometry cases: d) 1m fire diameter and 10m release height, e) 10m fire diameter and 10m release height, f) 25m fire diameter and 25m release height. Arrows indicate the behaviour of C/C_0 when the corresponding parameter is varied accordingly.

By the combination of the two diagrams is then possible to identify a first area near the origin where an increase of wind intensity can determines an increase in concentration at the ground receptor. Complementarily, an higher stability class determines lower concentration. In a second area at about 2500 m from the origin, the correlation is opposite to the one in the first region and higher stability and lower wind intensity cause a potential increase of concentrations. For all the receptors the effect of event duration increases progressively with distance. The effect of fire duration is similarly reproduced also for the other two cases reported in panel b) and c). They concern respectively fires of 10 and 25 m diameter and releasing height of 10 and 25m. Increases in concentration with stability increases are shifted to larger distances as the fire dimensions increase.

Also the area where wind intensity can produce a concentration reduction is progressively reduced as the fire dimensions increase. Panels d), e) and f) in figure 3 shows the effect of initial temperature and velocity of plume on pollutant dispersion ratio. The different colours of the lines consider plume temperature from 200 to 1200°C. They are obtained - as for the previous examples - considering three possible combination of fire diameters and release height, stability class 6 (F) and wind speed of 1m/s. The correlation analysis shows the same behaviour as for the analysis reported above. The increase of initial centreline plume temperature determines a decrease in dilution ratio. More complex behaviour is registered for plume velocity w_0. Only for the smallest fires it can be identified a region near 1000 m where an increase of exit velocity can decrease concentrations. For diameter of 10 and 25m higher plume velocity determines higher concentrations.

CONCLUSIONS

A recursive processor for an extensive launch of the atmospheric dispersion model CALPUFF has been implemented. As a theoretical case study, parameters range variation describing the largest number of possible accidental fires have been defined according SFPE and FDTs (SFPE, 2002 and Fire Dynamics Tools FDTs); fires have been modelled as stacks. The recursive processor has allowed to create a database prototype encompassing more than 25000 different possible scenarios. The impacts of event parameters have been investigated as function of ground distances from the emission sources. Analysis on statistical description of concentration profiles have been presented, though further analysis are still required, in particular for larger diameter fires, considering the possibility of partitioning them into a combination of smaller diameter stacks. A prototype for data elaboration has been also developed, enabling concentration profiles visualisation with HTML code for web-based mapping.

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