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DEVELOPMENT OF BUILD (BUILDING URBAN AND INDUSTRIAL LAGRANGIAN DISPERSION), A NEW OPERATIONAL DISPERSION MODEL FOR ACCIDENTAL OR DELIBERATE RELEASES IN COMPLEX AREA

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Abstract: The release of CBRN toxic substances (Chemical, Biological, Radiological and Nuclear) into the atmosphere is an important issue for the safety of people and the protection of infrastructures, more specifically in the case of accidental or deliberate release within an urban or industrial complex-built area. In order to be able to react quickly and take decisions, first responders, public authorities and industrial companies need operational simulation tools for emergency situations.

This paper presents the development and the physical parameterizations of a new operational dispersion model, called BUILD (Building Urban and Industrial Lagrangian Dispersion model), which is dedicated to simulate the transport of CBRN pollutants in complex built area. The BUILD model uses a geometrical preprocessor which converts 3D urban geometrical databases into 2D tiles of pre-calculated information on the street canyons, their connectivity and the recirculations in the wake of buildings.

The BUILD flow model is based on a "SIRANE like" parametrization for the dense part of an urban area (Soulhac et al., 2011, 2012). Nevertheless, the flow model has been enhanced to consider the recirculating transverse component of the flow in each street and a three-dimensional diagnostic flow model in the roughness sublayer, to take into account the deviation by buildings and obstacles. In order to represent obstacles and buildings in sparse areas (isolated roughness regime), the BUILD model uses an analytical building wake parametrization to describe the recirculating flow downwind of a building.

The transport and dispersion of pollutants are solved using a Lagrangian particles stochastic approach coupled with the simplified flow defined above. This new operational model is able to simulate the dispersion from a point source in a complex built area in a computational time less than one minute on a laptop.

The present paper describes the physical parameterizations of the model and their calibration. A companion paper (Slimani et al., Harmo20) presents in more detail the validation against wind tunnel data and CFD RANS and LES simulations on obstacles and streets network configurations.

Key words: Atmospheric dispersion modelling, emergency response, Lagrangian model.

INTRODUCTION

The release of CBRN toxic substances (Chemical, Biological, Radiological and Nuclear) into the atmosphere is an important issue for the safety of people and the protection of infrastructures, more specifically in the case of accidental or deliberate release within an urban or industrial complex-built area. In order to be able to react quickly and take decisions, first responders, public authorities and industrial

companies need operational simulation tools for emergency situations. Different simulation approaches have been developed and used for several decades to describe the transport and atmospheric dispersion of hazardous material emitted during short releases in urban environment, from the simplest Gaussian models, using specific parameterizations of the standard deviations of the cloud, up to the most detailed CFD approaches, such as RANS or even LES. In a crisis situation, the challenge for the models is to find the best compromise between the quality of representation of the physical processes (behavior of the plume, contour of the contaminated area, concentration decay with distance from the source), and the speed of execution of the code with the available IT resources.

To achieve this goal, operational models are generally based on a simplified description of the turbulent flow in the urban area or on pre-calculated flow fields stored in a database. "Database" approaches allow the use of detailed CFD-type flow models, but their limitation is that they can only be used over previously identified areas. Approaches based on a simplified description of the flow can be applied to an area that is a priori unknown, but their limitation lies in the simple parameterizations of the flow, which do not make it possible to describe all the complex urban geometrical patterns and which can lead to greater uncertainties.

In order to improve the existing set of available models for emergency response, this article presents the scientific formulations of the new atmospheric dispersion model BUILD (Building Urban & Industrial Lagrangian Dispersion). BUILD is a software developed for the simulation of atmospheric dispersion at the local scale, based on a simplified representation of the influence of buildings and obstacles, especially in urban or industrial environments. It is a rapid response operational software, which aims to provide time evolving concentration maps of a cloud of NRBC type hazardous materials, in the context of industrial accidents or malicious acts. It is developed in partnership between the Military Applications Department of the CEA and the Fluid Mechanics and Acoustics Laboratory of the University of Lyon.

The BUILD software is based on a parameterization of the flow in the atmospheric boundary layer, divided into several zones:

- Atmospheric boundary layer, including the surface inertial layer (between 50m and 1000m approximately): in this zone, the flow is assumed to be horizontal and dependent only on height. The vertical profile of the different characteristics of the flow is evaluated following classical boundary layer parametrizations (Fisher et al., 1998; Gryning et al., 2007).
- Roughness sublayer (between 20 m and 50 m approximately): in this zone, we propose a simplified flow model to take into account the disturbance induced by obstacles on the vertical profiles of velocity and turbulence parameters.
- Canopy of obstacles (between 0 m and 20 m approximately):
 - In dense urban areas, we consider a representation of the canopy as a network of interconnected streets, following the approach introduced by Soulhac (2000) and used in the SIRANE model (Soulhac et al., 2011).
 - In intermediate or sparse built environment, an analytical model of recirculation in the wake of obstacles is used.

The simulation of atmospheric dispersion is taken into account using a stochastic Lagrangian particles model, coupled with the parameterizations described above for the mean flow and the turbulence statistics. The following sections focus on the geometrical preprocessor, on the parameterization of the flow inside the canopy, on the Lagrangian dispersion model, and present some applications of the BUILD model in the cases of idealized geometries and real industrial sites.

URBAN GEOMETRICAL PREPROCESSOR

BUILD is based on a simplified description of the geometry of the site considered. The area is divided into 1km x 1km tiles and each tile is described with a resolution of 1 meter. Obstacles and buildings are initially given by their contours and heights. This input data is converted to an image where the gray level represents

the height of the wall. Different image processing algorithms are then applied in order to simplify the geometry of the buildings and to identify the topology and characteristics of the network of streets (see **Figure 1**) so that each pixel in a tile can be located precisely in streets, according to the walls.



Figure 1. Steps of the URBAN geometrical preprocessor.

WIND FLOW AND TURBULENCE PARAMETERIZATION IN THE BUILDING CANOPY

Network of streets model

From the geometrical preprocessor, each pixel of the domain is positioned in relation to the streets and its coordinates in the local coordinate system are determined: $\eta = 2y/W$ et $\zeta = 2z/H - 1$. The mean longitudinal velocity in each street is assumed uniform and parameterized following the approach implemented in the SIRANE model (Soulhac et al., 2008, 2011). The transverse velocity field is defined with linear profiles, in agreement with the experimental data of Salizzoni et al. (2011) (see **Figure 2**-c):

$$\begin{cases} \overline{v}(\eta,\zeta) = v_{\text{street}} f_v(\eta) g_v(\zeta) \\ \overline{w}(\eta,\zeta) = w_{\text{street}} f_w(\eta) g_w(\zeta) \end{cases} \text{ with } \begin{cases} f_v(\eta) = 1 - \eta^2 \\ g_v(\zeta) = \zeta \\ f_w(\eta) = \eta \\ g_w(\zeta) = 1 - \zeta^2 \end{cases}$$
(1)

 $\langle C(\lambda) \rangle = 1$

where v_{street} is calculated as proportional to the perpendicular component of the friction velocity of the overlying surface boundary layer and w_{street} deduced from the continuity equation ($w_{\text{street}} = H/W \cdot v_{\text{street}}$). Similarly, the turbulent kinetic energy field in each street is assumed to be uniform, with a value related to the external friction velocity: $k_{\text{street}} = 0.5u_*$ (see **Figure 2**-d,e).

Building wake model

In the case of low building density, the BUILD model represents the main feature of the flow around each obstacle, i.e. the large recirculation area downwind of the obstacle (Hosker, 1985). To characterize the geometry of the recirculation zone, an advection-diffusion process of the velocity defect in the wake of the obstacle has been implemented and emulated by an image processing algorithm, using translation-blurring of the image of each building (see **Figure 3**). The recirculation limit is defined by thresholding the grayscale velocity defect field, adjusting the threshold to get the recirculation length provided by empirical rules (Hosker, 1985). Once the shape of the recirculation is known, parameterizations similar to equations 1 are used to get the velocity field inside each recirculation (see **Figure 4**).



Figure 2. Parameterization of the flow in each street: a) local coordinate system, b) longitudinal mean velocity with numerical profiles of Soulhac et al. (2008), c) transverse mean velocity field, d) and e) turbulent kinetic energy, with experimental profiles from Salizzoni et al. (2011).





Figure 4. Velocity field in the building recirculation area.

LAGRANGIAN DISPERSION MODEL

In the BUILD model, turbulent dispersion is simulated using a stochastic particle approach, based on the tracking of Lagrangian trajectories of individual particles in the velocity and turbulence field defined above. The temporal evolution of the *i*th component of the Lagrangian velocity of each particle is estimated with the equation:

$$U_{i}(t) = \overline{U}_{i}(t) + U_{i}'(t) \text{ with } U_{i}'(t+dt) = U_{i}'(t) + dU_{i}'$$
(1)

where the mean Lagrangian velocity \overline{U}_i is equal to the local Eulerian velocity \overline{u}_i . The evolution of the fluctuating velocity U'_i is determined by the stochastic differential equation (Thomson, 1987):

$$dU'_{i} = a_{i}(\boldsymbol{X}, \boldsymbol{U}', t)dt + \sum_{j} b_{j}(\boldsymbol{X}, \boldsymbol{U}', t)d\xi_{j}$$
⁽²⁾

where a_i and b_j are expressed in terms of standard deviations of the velocity fluctuations σ_{u_i} and of the Lagrangian times $T_{L,i}$. Once the cloud of particles has been transported using the previous equations, the

concentrations are calculated by dividing the sum of the mass of all the particles present in a grid cell, by the volume of this grid cell.

VALIDATIONS AND APPLICATIONS OF THE BUILD MODEL

A companion paper (Slimani et al., 2021) presents in detail the validation of the BUILD model against wind tunnel data and CFD RANS and LES simulations on an isolated obstacle and on a streets network configurations. In the present article are only illustrated on **Figure 5** some concentration fields calculated with BUILD model in various build-up area types: network of streets, isolated obstacle, real industrial area.



Figure 5. Application of the BUILD model on various build-up area types.

CONCLUSION

This article presents the main features of a new operational model for the simulation of atmospheric dispersion at the local scale, based on simplified parameterizations of the influence of buildings and obstacles, especially in urban or industrial environments, and its application on various build-up area types.

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