

multiSLAB: a wrapper for the SLAB heavy-gas dispersion model

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Abstract

The heavy-gas dispersion model SLAB has been extended in its functionalities in order to be easily run for multiple hours and to consider multiple sources, as well as plotting the results in a 2-D graph.

Keywords

Heavy-gas; SLAB dispersion model; multi-source; multi-hour; mapping

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1. Introduction

The choice of a dispersion model should take into consideration the pollutant emission conditions, its nature, the source's surroundings (simple or complex terrain topography, industrial or residential area, distance to the sea, ...) and the study's goal.

When the study's scope is a dense gas, a gas which is denser than ambient air and which, by its nature, requires a different atmospheric dispersion modelling approach [Puttock and Blackmore, 1982], a model, which is suitable to the situation and the pollutant's evaluation requirements should be used.

In this paper, we seek to implement a dense gas dispersion model, based on a model supplied by the US EPA (SLAB, 1990), but more versatile and appropriate to different conditions and scenarios.

Presently, the most common models dealing with dense gas dispersion are SLAB, FEM3, DEGADIS and GASTAR, though other programmes were produced, mainly in the 1980s [Koopman et al., 1989, Deaves, 1992]. The GASTAR model, developed by Cambridge Environmental Research Consultants Ltd.

[\[http://www.cerc.co.uk/environmental-software/GASTAR-model.html\]](http://www.cerc.co.uk/environmental-software/GASTAR-model.html), do not contemplate atmospheric chemical reactions and does not allow for complex terrain considerations, the altimetry being treated by simple slopes. The DEGADIS model, developed by Jerry Havens and Tom Spicer at the Arkansas University, U.S.A. [\[http://www.epa.gov/scram001/dispersion_alt.htm\]](http://www.epa.gov/scram001/dispersion_alt.htm), simulates the atmospheric dispersion at ground level, over flat terrain. The GASTAR and the FEM3 models have the limitation of being under commercial license and not available for modifications, while DEGADIS only simulates the release of zero-momentum gases. The SLAB model, which is the scope of this paper, and does not bear those limitations, was developed by the Lawrence Livermore National Laboratory, U.S.A. [\[http://www.epa.gov/scram001/dispersion_alt.htm\]](http://www.epa.gov/scram001/dispersion_alt.htm), which models the dispersion of dense gases solving the unidimensional equations of mass, species and energy conservation and the state equation. Although terrain sloping and obstacles are relevant to dense gas dispersion [Deaves and Hall, 1990, Nielsen, 1991, Roberts and Hall, 1994], SLAB, even only considering flat terrain, calculates concentrations for the half plane situated downwind from the source, and its results were considered satisfactory in the case of terrains with little complexity when computing concentrations at ground level [Hanna et al., 1993]. In this study, we are concerned with receptor heights between 1.5 and 4 meters, as indicated for the gas dispersion impact on human health and vegetation evaluation, as stated in the

2008/50/CE Directive, by the FAIRMODE group [FAIRMODE, 2011]. Nowadays, Computational Fluid Dynamics represents an upgrade for dense gas modelling [Tauseef et al., 2011], but also implies higher costs. This approach has been used for the VADIS code (developed at GEMAC/UA).

As available from the US EPA, SLAB requires an input file (INPUT) containing the dense gas and the atmospheric release characteristics, as well as meteorological data, referring to one or many hours.

After processing, SLAB provides the dispersion computation results in the PREDICT file (Figure 1), where the dense gas in the downwind concentration direction is given together with parameters for the concentration calculation at any point in the tridimensional space.

The model has some limitations regarding either the input file or the number of sources which may be considered. Only one source is modelled at a time, and there is no information provided on the long-term concentration of pollutants (for example, the annual average for purposes of comparison with legislated values), being the multi-hour run input file setup time-consuming.

Therefore, the work developed consisted in (1) the automation of the INPUT files production and SLAB runs and (2) the 2-D mapping of the results, with the visualisation of the average and maximum for different time-periods (for example, one year).

2. Development

The aim of the INPUT file production automation was to allow a single run for multiple sources and a long time period (more than one hour, usually one year) of meteorological data, and to produce results for different integration periods (hourly, eight-hourly, daily and annual), in order to be comparable with limit or reference values. On the other hand, mapping the dispersion modelling results allows for the visualization of the ambient concentrations resulting from the releases by all sources.

Thus, the multiSLAB tool was developed, using the perl programming language. This language was chosen for its ease in dealing with arrays and in manipulating ASCII files. The multiSLAB program contains four modules (Figure 2).

1. The first module runs the SLAB program from an INPUT file, created from source characteristics inserted in a multiSLAB input file (inSLABmhmf) and meteorological data, for the h hours and f sources

considered. Such results in the production of $h \times f$ PREDICT files, which are renamed according to the hour and the source. This first module is therefore an INPUT files generator followed by a wrapper, allowing for an automated sequential operation of the SLAB program, and a PREDICT files ordination tool.

The inSLABmhmf.txt input file is set up before running the multiSLAB program, containing various parameters to be inserted by the user:

- Sources' characteristics: constant or variable emission (in the case of variable or intermitting emission, a separate hourly emission has to be provided) and source localization;
- Dense gas characteristics: molar weight, vapour and liquid heat capacity, initial liquid mass fraction and liquid density of the source material;
- Spill characteristics: temperature of the source material, mass source rate, source height and area and continuous source duration;
- Grid characteristics: central point localization, domain dimensions, spacing between receptors (at this stage, the modelling guidelines from the European Air Quality Directive shall be taken into consideration);
- Other parameters: meteorological data measurement height and surface roughness of the area.

The multiSLAB model allows for the use of any Cartesian system coordinates expressed in meters. Sill at the preliminary stage, it is necessary to prepare the data for each hour to be considered. multiSLAB was designed so that it may accept, with small source code changes, meteorological data from various origins and in various formats.

2. The second module transforms the unidimensional SLAB output from each of the $h \times f$ PREDICT files (for every hour and every source) into a file with the concentrations for each receptor specified in the multiSLAB input file. The concentration at any point of the domain may be calculated using the following formula:

$$C(X, Y, Z, T) = CC(X) \cdot [\text{erf}(XA) - \text{erf}(XB)] \cdot [\text{erf}(YA) - \text{erf}(YB)] \cdot [\exp(-ZA^2) - \exp(-ZB^2)]$$

Where

$$XA = \frac{X - XC + BX}{\sqrt{2} BETAX}$$

$$XB = \frac{X - XC - BX}{\sqrt{2} BETAX}$$

$$YA = \frac{Y + B}{\sqrt{2} BETAC}$$

$$YB = \frac{Y - B}{\sqrt{2} BETAC}$$

$$ZA = \frac{Z - ZC}{\sqrt{2} SIG}$$

$$ZB = \frac{Z + ZC}{\sqrt{2} SIG}$$

erf is the non-elementary, sigmoid, Gauss error function $\text{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$

exp is the exponential function

Parameters $CC(X)$, $B(X)$, $BETAC(X)$, $ZC(X)$ and $SIG(X)$ depend on the downwind distance (X).

Parameters $XC(T)$, $BX(T)$ and $BETAX(T)$ depend on time (T). All these parameters are tabled in the PREDICT output file.

The coordinates of each receptor in the grid (X_G, Y_G) are transformed into a coordinates system which has the source as origin and the downwind direction as the positive x-axis by the following formula:

$$Y = [Y_G - Y_F - \frac{X_G - X_F}{\tan(WD)}] \times \sin(WD) \text{ and } X = \frac{X_G - X_F}{\sin(WD)} - \frac{Y}{\tan(WD)}$$

Where

X_F, Y_F Source coordinates

WD Wind direction

This step computes X and Y, to be related to the output data present in the PREDICT file.

At the end of this module's computations, $h \times f$ XYC (coordinates concentration) files are obtained.

3. The third multiSLAB module sums up, for each receptor and for each h hours, the contributions from the f sources. When these module's computations are completed, h XYC (coordinates concentration) files were produced.

4. In the fourth and last module the average and maximum concentration, for the integrating period

specified, are computed for each receptor, thus producing two files: mean.xyc and max.xyc.

A last tool lists, for a specified receptor, all the concentrations computed (the h modeled hours). Such a tool is useful to analyse the estimated concentrations distribution at a given receptor (in order to understand, for example, what is the amount of time the dense gas concentration is above a threshold value).

3. Case Study

As an example of the multiSLAB capabilities, the Bis(2-ethylhexyl)phthalate dense gas (used as a plasticizer in industrial processes) dispersion from a plant's 13 stacks was modeled using a year-long hourly meteorological data set (8760 hours). The plant is located at the centre of the domain shown in Figure 3.

Thus, module 1 runs the SLAB model (*number of sources × number of hours*) times, producing a same amount of PREDICT files, which are transformed into a same number of bidimensional concentration files (XYC type) by module 2, summed up into 8760 XYC files (one file for each modeled hour) by module 3.

Module 4 computes the annual average and maximum, for each receptor. Figure 3 shows the results (annual average and maximum) for the study domain.

Various tests were conducted as well, simulating the dispersion of a pollutant from a single source, under a SW wind, in order to compare the outputs from SLAB and multiSLAB. Figure 4 shows the results for four different averaging times. The direct comparison between the SLAB and multiSLAB results is not possible because the distances between points in the downwind direction for which SLAB outputs concentrations is irregular and therefore irreproducible in a Cartesian grid, as used by multiSLAB. Both SLAB and multiSLAB results may be fitted by a power law, as shown in Figure 4.

It may be seen that multiSLAB produces results similar to those from the original SLAB model provided by the US EPA. From Figure 4, it may be seen that a slight discrepancy (19% at most) is found when the averaging time is one hour. That difference is reduced when the averaging time is shorter. The origin of this disparity lies in the extrapolation of the time-dependent parameters in the concentration equation from the SLAB predict file. Indeed, those parameters are given only for short times, and their values for longer times are extrapolated, thus leading to discrepancies.

The original SLAB was evaluated using a wide amount of data obtained from field and laboratory

experiments [e.g. Ermak, 1982].

4. Concluding remarks and future work

With the goal to make the dispersion of dense gases possible for n point sources and an extended period of time (n hours), alterations to the SLAB model, developed by the US EPA, were implemented. Due to the restrictions of the SLAB model regarding the mapping of the results, other functionalities, allowing for the dispersion results mapping in a 2-D space within the domain, with the visualization of averages and maximums for different periods of time, were added.

The implemented alterations resulted into a model named multiSLAB. This model may be applied to a plant emitting a denser-than-air gas, at various emitting points, for a whole year meteorological data, producing results, presentable in dispersion maps, for the integration periods required and comparable with ambient air limit and/or reference values.

For validation purposes, the multiSLAB model was applied in parallel with the original SLAB model for the same conditions (one source), producing satisfactory results.

For future work, the following points will be considered:

- Validate multiSLAB using field data used to validate the original SLAB model (e.g. the Burro or Coyote series).
- Bypass the extrapolation of time-dependent parameters by calculating them directly using the original SLAB equations.

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Figure 1 - Original (as provided by the US EPA) SLAB functioning scheme

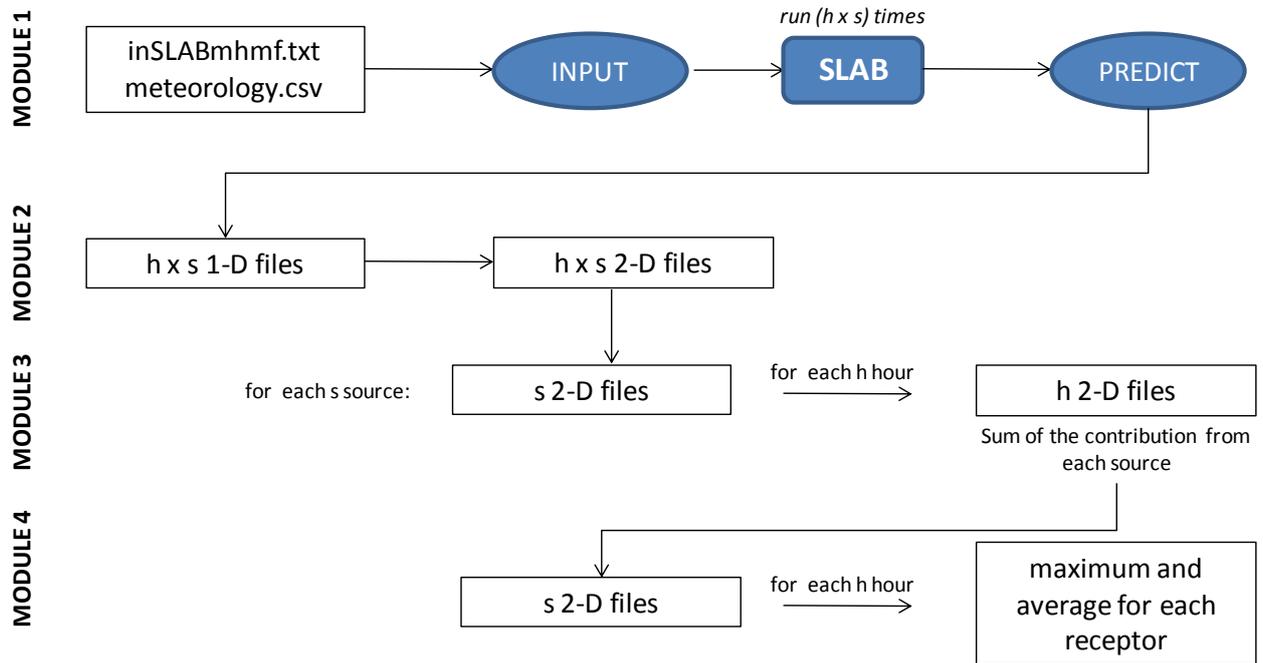


Figure 2 - multiSLAB working flowchart

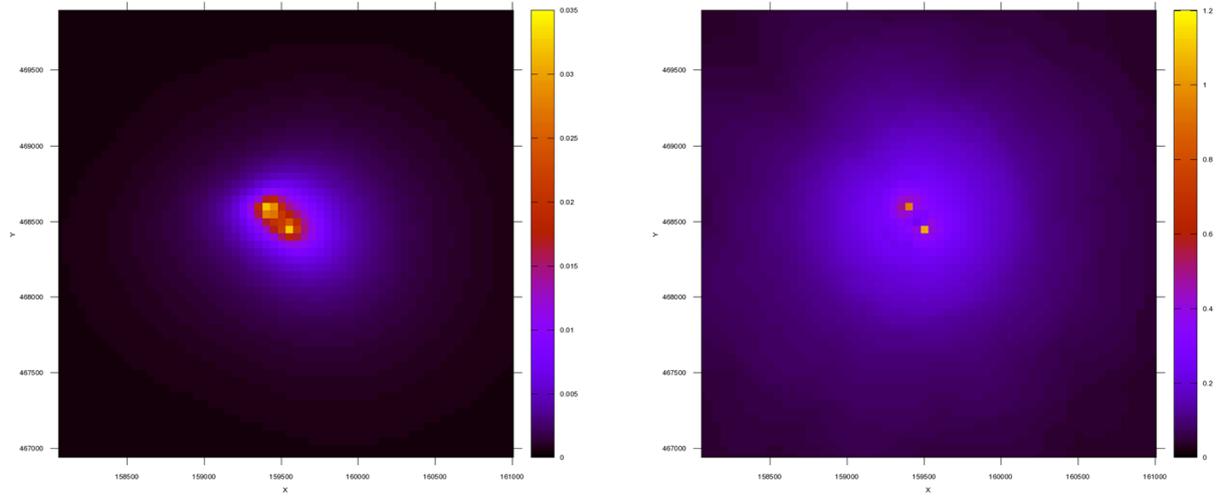


Figure 3 - DOP annual average and maximum concentrations (ppm)

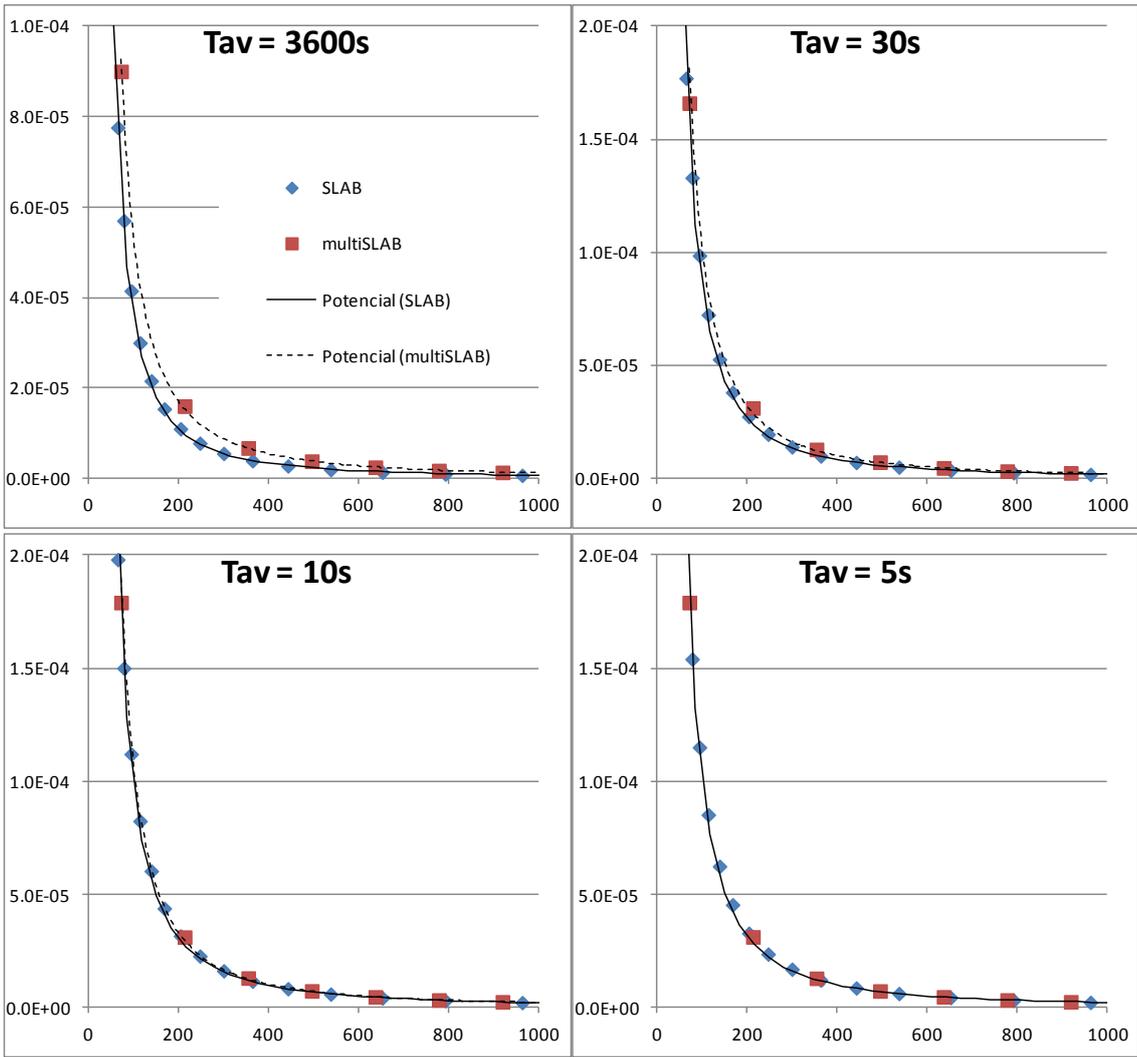


Figure 4 - SLAB and multiSLAB output (x-axis: distance from source, y-axis: concentration in ppm, T_{av} = averaging time)