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TWODEE-2: A shallow layer model for dense gas dispersion on complex topography ☆

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ABSTRACT

TWODEE-2 is a FORTRAN 90 code based on previous code (TWODEE). It is designed to solve the shallow water equations for fluid depth, depth-averaged horizontal velocities and depth-averaged fluid density. The shallow layer approach used by TWODEE-2 is a compromise between the complexity of CFD models and the simpler integral models. It can be used for forecasting gas dispersion near the ground and/or for hazard assessment over complex terrains. The inputs to the model are topography, terrain roughness, wind measurements from meteorological stations and gas flow rate from the ground sources. Optionally the model can be coupled with the output of a meteorological processor which generates a zero-divergence wind field incorporating terrain effects. Model outputs are gas concentration, depth-averaged velocity, averaged cloud thickness and dose. The model can be a useful tool for gas hazard assessment by evaluating where and when lethal concentrations for humans and animals can be reached.

1. Introduction

Many volcanic and non-volcanic areas in Italy emit huge amounts of gas into the atmosphere. One of the most frequent gases discharged from both volcanic (e.g., Solfatara Volcano) and non-volcanic sources (e.g., central Italy vents) is carbon dioxide (CO_2) which has a molecular weight greater than air. Under stable atmospheric conditions and/or in the presence of topographic depressions, CO_2 concentration can reach high values resulting in lethal effects to humans or animals. In fact, several episodes of this phenomenon were recorded at different areas in central Italy (Rogie et al., 2000) and worldwide. The most tragic example was the 1986 degassing of Lake Nyos, Cameroon, when a dense cloud of carbon dioxide hugging the ground suffocated more than 1700 people in one night (Clarke, 2001).

The cloud dispersion of gases denser than air released from natural sources is governed by gravity and by the effects of lateral eddies which decrease the cloud density through the incorporation of surrounding air. In the initial phase the negative buoyancy controls the gas dispersion and the cloud follows the ground (gravitational phase). In contrast, when the density contrast becomes less important, gas dispersion is mainly governed by wind and atmospheric turbulence (passive dispersion phase) (e.g., Costa et al., 2005). In principle, gas dispersion can be studied by fully solving the transport equations for mass, momentum and energy, but because the demanding computational requirements, different simplified models which describe only specific processes are commonly used. Approaches range from the simplest analytical Gaussian models to the more complex computational fluid dynamics (CFD) models (e.g., Macedonio and Costa, 2002). A compromise between the complexity of CFD models and the simpler integral models is given by the shallow layer approach which uses depth-averaged

☆ Code is available from server at http://www.iamg.org/CGEditor/index.htm.

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variables to describe gravity-driven flows of dense gas over complex topography (Hankin and Britter, 1999a; Venetsanos et al., 2003).

Here we describe TWODEE-2, a FORTRAN 90 code that solves a time-dependent model for dispersion of a heavy gas based on the shallow layer approach. TWODEE-2 is derived from the optimization and improvement of a previous FORTRAN 77 code (TWODEE) developed by Hankin and Britter (1999a–c). In the manuscript, firstly we present the model equations and overview the resolution algorithm. Secondly we describe the code structure and the I/O files. Finally, we show an application example.

2. Heavy gas transport model

2.1. Model variables

TWODEE-2 is based on depth-averaged equations obtained by integrating conservation equations over the fluid depth. Such an approach is able to describe the cloud in terms of four variables: cloud depth, two depth-averaged horizontal velocities, and depth-averaged cloud density as functions of time and position. Since real clouds do not have a definite upper surface it is necessary to define cloud depth in terms of the vertical concentration distribution. In fact, we point out that the actual vertical concentration profile is not uniform as for fluids usually described by shallow water equations, but characterized by an exponential decay (Hankin and Britter, 1999a). In TWODEE-2, h is that height below which some fraction α of the buoyancy is located:

$$\int_{z=0}^{h} (\rho(z) - \rho_a)\,\mathrm{d}z \equiv \alpha \int_{z=0}^{\infty} (\rho(z) - \rho_a)\,\mathrm{d}z \tag{1}$$

where ρ and ρ_a are, respectively, the cloud and the ambient fluid (air) densities, z is the vertical coordinate, and α is a constant. The choice $\alpha = 0.90-0.95$ is normally adopted. Depth-averaged density $\overline{\rho}$ and velocity components $(\overline{u}, \overline{v})$ are defined as

$$h(\overline{\rho} - \rho_a) \equiv \int_{z=0}^{\infty} (\rho(z) - \rho_a)\,\mathrm{d}z \tag{2}$$

$$h(\overline{\rho} - \rho_a)\overline{u} \equiv \int_{z=0}^{\infty} (\rho(z) - \rho_a)u(z)\,\mathrm{d}z \tag{3}$$

$$h(\overline{\rho} - \rho_a)\overline{v} \equiv \int_{z=0}^{\infty} (\rho(z) - \rho_a)v(z)\,\mathrm{d}z \tag{4}$$

The vertical distribution of density can be calculated from its depth-averaged value as (Hankin and Britter, 1999c)

$$\rho(z) = \rho_a + \frac{2}{S_1}(\overline{\rho} - \rho_a)\exp\left(-\frac{2}{S_1}\frac{z}{h}\right) \tag{5}$$

where S_1 is a shape parameter. The vertical concentration distribution c (in ppm) results:

$$c(z) = c_b + (10^6 - c_b) \times \frac{\rho(z) - \rho_a}{\rho_g - \rho_a} \tag{6}$$

where c_b is the background concentration (in ppm). Another useful quantity output by the model is the dose D, a temporal integrated variable defined as

$$D(t, z) = \int_0^t [c(z)]^n\,\mathrm{d}t \tag{7}$$

where n is the toxicity exponent.

2.2. Model equations

Assuming an homogeneous fluid and a hydrostatic pressure distribution, the shallow water equations for flows having a non-uniform vertical profile are given by (Hankin and Britter, 1999a)

$$\frac{\partial h}{\partial t} + \frac{\partial h\overline{u}}{\partial x} + \frac{\partial h\overline{v}}{\partial y} = u_{entr} + u_{sou} \tag{8}$$

$$\frac{\partial h(\overline{\rho} - \rho_a)}{\partial t} + \frac{\partial h(\overline{\rho} - \rho_a)\overline{u}}{\partial x} + \frac{\partial h(\overline{\rho} - \rho_a)\overline{v}}{\partial y} = u_{entr}\rho_a + u_{sou}\rho_g \tag{9}$$

$$\begin{aligned} &\frac{\partial h\overline{\rho}\,\overline{u}}{\partial t} + \frac{\partial h\overline{\rho}\,\overline{u}^2}{\partial x} + \frac{\partial h\overline{\rho}\,\overline{u}\,\overline{v}}{\partial y} + \frac{1}{2}S_1\frac{\partial g(\overline{\rho} - \rho_a)h^2}{\partial x} \\ &+ S_1 g(\overline{\rho} - \rho_a)h\frac{\partial e}{\partial x} + \frac{1}{2}\overline{\rho}C_D\overline{u}|\mathbf{u}| + V_x \\ &+ k\rho_a\left[\frac{\partial}{\partial t} + u_a\frac{\partial}{\partial x} + v_a\frac{\partial}{\partial y}\right][h(\overline{u} - u_a)] \\ &= u_{entr}\rho_a u_a \end{aligned} \tag{10}$$

$$\begin{aligned} &\frac{\partial h\overline{\rho}\,\overline{v}}{\partial t} + \frac{\partial h\overline{\rho}\,\overline{v}^2}{\partial y} + \frac{\partial h\overline{\rho}\,\overline{u}\,\overline{v}}{\partial x} + \frac{1}{2}S_1\frac{\partial g(\overline{\rho} - \rho_a)h^2}{\partial y} \\ &+ S_1 g(\overline{\rho} - \rho_a)h\frac{\partial e}{\partial y} + \frac{1}{2}\overline{\rho}C_D\overline{v}|\mathbf{u}| + V_y \\ &+ k\rho_a\left[\frac{\partial}{\partial t} + u_a\frac{\partial}{\partial x} + v_a\frac{\partial}{\partial y}\right][h(\overline{v} - v_a)] \\ &= u_{entr}\rho_a v_a \end{aligned} \tag{11}$$

where the meaning of all variables is given in Table 1. The equations above express, respectively, the balances of volume, mass and components of momentum. Terms in the left-hand sides of the momentum equations (10) and (11) include the temporal variation, the effect of convection, the pressure gradient for the case of hydrostatic but non-uniform density profile, the effect of ground slope, the surface shear stress (proportional to the drag coefficient C_D), the force per unit area exerted by turbulent shear stress and, finally, the leading edge terms that account for interaction among dense and ambient fluid. The latter gives a correction to the shallow water equations which give erroneous results for the leading edge as they assume that the pressure distribution is hydrostatic. This term is proportional to the semi-empirical coefficient k, evaluated in terms of the front Froude number Fr:

$$k = \frac{2}{(S_1\,Fr^2)} \tag{12}$$

The drag coefficient and the turbulent shear stress force are estimated as

$$C_D = \max\left(\min\left(\frac{2u_*^2}{|\mathbf{u_a}|^2}; 10^{-2}\right); 10^{-4}\right) \tag{13}$$

Table 1
List of symbols

Symbol	Definition
b	Entrainment velocity empirical coefficient. See Eq. (15). Usually set to 0.11
c	Cloud dense gas concentration in ppm
c_b	Dense gas background concentration in ppm
C_D	Skin friction (drag) coefficient. See Eq. (13)
Cr	Courant number. Usually set to 0.25
D	Dose. See Eq. (7)
$e = e(x, y)$	Terrain elevation
Fr	Front Froude number. See Eq. (12). Usually set to 1
g	Gravity acceleration
$g(\overline{\rho} - \rho_a)$	Cloud buoyancy
h	Cloud depth
K	Von Karman constant. Usually set to 0.4
L	Monin–Obukhov length
n	Toxicity exponent. See Eq.(7)
P	Pressure
Ri_b	Bulk Richardson number
S_1	Shape parameter. See Eq. (5). Usually set to 0.5
t	Time
T	Temperature
$\mathbf{u} = (\overline{u}, \overline{v})$	Depth-averaged velocity
u_{entr}	Air entrainment velocity. See Eq. (15).
u_{sou}	Dense gas inflow velocity
u_*	Friction velocity
$\mathbf{u}_a = (u_a, v_a)$	Ambient fluid velocities along (x, y), respectively
U_a	Ambient fluid velocity modulus
$\mathbf{V} = (V_x, V_y)$	Turbulent shear stress force (per unit area)
w_*	Atmospheric convective velocity
(x, y)	Horizontal spatial coordinates
z	Vertical coordinate
$z_0 = z_0(x, y)$	Roughness length
z_{ref}	Reference height
α	Constant. See Eq. (1). Usually set to 0.90–0.95
α_2	Entrainment velocity empirical coefficient. See Eq. (15). Usually set to 0.7
α_3	Entrainment velocity empirical coefficient. See Eq. (15). Usually set to 1.3
α_7	Entrainment velocity empirical coefficient. See Eq. (15). Usually set to 0.45
Δt	Time step
Δx	Spatial discretization along x
Δy	Spatial discretization along y
k	Semi-empirical parameter. See Eq. (12)
$\overline{\rho}$	Depth-averaged cloud density
ρ_a	Ambient fluid density
ρ_g	Dense gas density
ψ_m	Atmospheric stability function. See Eq. (16)
ζ	Constant for turbulent shear stress. See Eq. (14). Usually set to 0.0

$$\mathbf{V} = \zeta h \overline{\rho} \nabla (h |\mathbf{u}| \nabla \mathbf{u}) \tag{14}$$

where ζ is a small constant of proportionality. On the other hand, the air entrainment velocity u_{entr} is calculated using empirical formulations (Hankin and Britter, 1999a):

$$u_{entr} = \frac{K}{1 + bRi} \times \sqrt{u_*^2 + (\alpha_2 w_*)^2 + \frac{1}{2} C_D \alpha_3^2 |\mathbf{u}|^2 + \alpha_7^2 |\mathbf{u} - \mathbf{u_a}|^2} \tag{15}$$

where b, α_2, α_3, and α_7 are empirical constants. Eq. (15) reflects the top entrainment of ambient fluid through the incorporation of eddies into the body of the cloud (edge entrainment is not currently considered). TWODEE-2 is based on the numerical solution of the governing equations (8)–(11) together with the closure relationships (12)–(15) using the algorithm described in Hankin and Britter (1999b).

2.3. Wind model

Concerning definition of the wind field TWODEE-2 admits two options, uniform wind or spatially variable wind which allows to incorporate terrain effects. For the first option, when the wind is considered horizontally uniform, meteorological data at a height $z = z_{ref}$ are directly read from a wind data file, commonly provided by a ground-based station. For the second option, when the wind is spatially variable, data at height $z = z_{ref}$ are provided by the program DIAGNO. The program DIAGNO, also included in the TWODEE-2 package, is a meteorological processor based on the Diagnostic Wind Model (Douglas et al., 1990). The DWM generates a quasi-steady-state gridded wind field from input data ("observations") at a point of the domain. The model adjusts the domain-scale mean wind for terrain effects and then performs a divergence minimization to ensure mass conservation. In both cases, uniform or spatially variable wind field, TWODEE-2 reads temperature and wind velocity at $z = z_{ref}$ as inputs and uses these data to calculate the vertical wind profile according to the Monin–Obukhov similarity theory (e.g., Jacobson, 1999):

$$U_a(z) = \frac{u_*}{K}\left[\ln\left(\frac{z}{z_0}\right) - \psi_m\left(\frac{z}{L}\right) + \psi_m\left(\frac{z_0}{L}\right)\right] \tag{16}$$

L and u_* are estimated using the non-iterative method of Louis (1979) based on the bulk Richardson number Ri_b:

$$Ri_b \approx \frac{g[\theta(z_{ref}) - \theta(z_0)](z_{ref} - z_0)}{\theta(z_0)[u_a^2(z_{ref}) + v_a^2(z_{ref})]} \tag{17}$$

The stability function ψ_m is evaluated from the Businger–Dyer relationship (e.g., Dyer, 1974) for unstable situations, i.e., $z/L < 0$, or in accord to Van Ulden and Holstag (1985) for stable situations i.e., $z/L > 0$ (for the details see, e.g., Jacobson, 1999).

2.4. Solving algorithm

TWODEE-2 is based on the numerical solution of the governing equations (8)–(11) together with the relations (12)–(15) and a set of boundary conditions. TWODEE-2 imposes different boundary conditions for outgoing and incoming fluxes: for outgoing flux, zero derivative conditions, whereas for incoming flux, null concentrations at boundaries (i.e., $h = 0$, $\overline{\rho} = \rho_a$, $\overline{u} = 0$, and $\overline{v} = 0$). The numerical method is based on the flux corrected transport (FCT) scheme of Zalesak (1979). This scheme combines the low numerical diffusion of high order schemes with the absence of numerical oscillations typical of low order schemes. Fundamentally, FCT calculates the fluxes between adjacent elements using a weighted average of flux as computed by a low order scheme and a high order scheme. The weighting is done in such a manner so as to use the high order scheme unless doing so would result in the creation of overshoots (that is, new extrema in the advected quantity) not predicted by the low order scheme. The stability of the numerical scheme is ensured by using a time step Δt equal to the critical:

$$\Delta t = \frac{Cr \min(\Delta x, \Delta y)}{|\mathbf{u}| + \sqrt{\dfrac{hg(\overline{\rho} - \rho_a)}{\overline{\rho}}}} \quad (18)$$

where Cr is the Courant number. For a detailed description of the solving algorithm see Hankin and Britter (1999b) and the references therein.

3. The TWODEE-2 set up

3.1. Installation and folder structure

- On a Unix/Linux/Mac X OS:
  (1) Decompress and untar the file `twodee2.tar.gz`.
  (2) Compile the program DIAGNO. Enter the directory `twodee2/Programs/Diagno/Sources`, then issue the command "`make`". You can edit the Makefile to select your favourite compiler.
  (3) Compile the program TWODEE-2. Enter the directory `twodee2/Programs/Twodee2/Sources`, then issue the command "`make`". You can edit the Makefile to select your favourite compiler.
- On a Windows OS decompress the file `twodee2.tar.gz` on your selected directory. The `twodee2.tar.gz` file already contains Windows executables for TWODEE-2 and DIAGNO programs.

Table 2 shows the TWODEE-2 folder structure. The directory `twodee2/Programs` contains the programs DIAGNO and TWODEE-2 with the corresponding source files. The directory `twodee2/Runs` contains the runs, each within its own folder. An example run named "Example" is provided with the installation.

Table 2
Directory structure of TWODEE-2

twodee2	**Programs**	**Diagno**	**Sources**	Source code files
			Diagno.win.exe	Windows executable
		Twodee2	**Sources**	Source code files
			Twodee2.win.exe	Windows executable
	Runs	**Example**	**infiles**	Example input files
			outfiles	Example output files
			Example.unix	Unix/Linux/Mac X script
			Example.win.bat	Windows (DOS) script
	README_Files.pdf			Description of I/O files

Directory names shown in bold.

3.2. Program run

TWODEE-2 and DIAGNO programs can be launched typing, respectively,

- "`Twodee2.exe problemname.inp problemname.log`"
- "`Diagno.exe problemname.inp problemname.log`"

where `problemname.inp` and `problemname.log` are the names (including paths) of the control input file and of the log file. Both file names are passed as a program call argument. However, it is highly recommended to launch the programs using the script files included in the package. For instance, to run the problem "Example":

- On a Windows OS enter the folder `twodee2/Runs/Example` and launch the script `Example.win`.
- On a Mac X/Unix/Linux OS enter the folder `twodee2/Runs/Example` and launch the script `Example.unix`.

Note: To create a new run simply create a new folder (with sub-folders `infiles` and `outfiles`), copy the input files and the script into it and modify the line of the script which defines the variable `problemname`.

4. The TWODEE-2 input files

TWODEE-2 needs the following input files:

- File `problemname.inp`—Control file that defines a TWODEE-2 (and a DIAGNO) run. Mandatory. This file is passed to the program(s) as a call argument and contains a set of blocks that define all the computational and physical parameters needed by the model(s).
- File `topography.dat`—Regional ground elevation file. Optional. The topography file specifies ground elevation e at a regional scale (i.e., in a region typically larger than the computational domain). Topography must be specified on a structured grid using arbitrary (but constant) grid spacing (e.g., 5, 10, 100 m, etc). Discretizations along x- and y-directions can be different. The only necessary requirement is that the computational domain must lay within the bounds of the region where topography is specified. TWODEE-2 reads the topography file and automatically interpolates elevations onto the nodes of the computational grid.
- File `terrain.dat`—Regional terrain roughness length file. Mandatory. The terrain file specifies the roughness length z_0 at a regional scale. The file format is analogous to that of the regional topography file. However, these two files can cover different regions and/or have different spatial discretizations.
- File `restart.dat`—Restart (initial conditions) file. Optional. The restart file can be used to start a new run from the end of a previous simulation. It is automatically created each time TWODEE-2 prints results

or at the end of a run. Any restart file previously created is destroyed whenever a new restart file is printed.

- File `source.dat`—Source term (dense gas fluxes) file. Mandatory. The source file specifies dense gas fluxes (in mass flow rate or mass flow rate per unit area) from different rectangular areas or point sources. TWODEE-2 reads this file and automatically calculates the upward source velocity u_{sou} (see Eqs. (8) and (9)) and interpolates the mass flow rate onto the nodes of the computational grid. Interpolation is done ensuring mass conservation. The advantage of this approach is that the source file becomes independent of the computational mesh (i.e., the source file is created only once and is the same regardless the location and/or the spatial resolution of the computational grid).
- File `winds.dat`—Meteorological data file. Mandatory. The wind data file contains meteorological data at different time slices. If the record `WIND_MODEL` in the control input file is `UNIFORM`, TWODEE-2 reads this file and estimates the atmospheric surface layer parameters. Otherwise, if the record `WIND_MODEL` is `DIAGNO`, this file is instead read by DIAGNO which uses values as input and TWODEE-2 simply uses the DIAGNO output (file `diagno.res`).
- File `points.dat`—File that defines the coordinates of the tracked points (points where time evolution of concentration is output). Optional.
- File `boxes.dat`—File that defines the coordinates of the tracked boxes (areas where evolution of averaged concentration is output). Optional.
- File `diagno.res`—DIAGNO output file. Optional.

For a detailed description on the formats and contents of the files above, see the file `README_Files.pdf` included in the TWODEE-2 package.

Note: File names are given just for illustrative purposes. Names and locations of TWODEE-2 I/O files are absolutely free and are defined by the user within the control file `problemname.inp`.

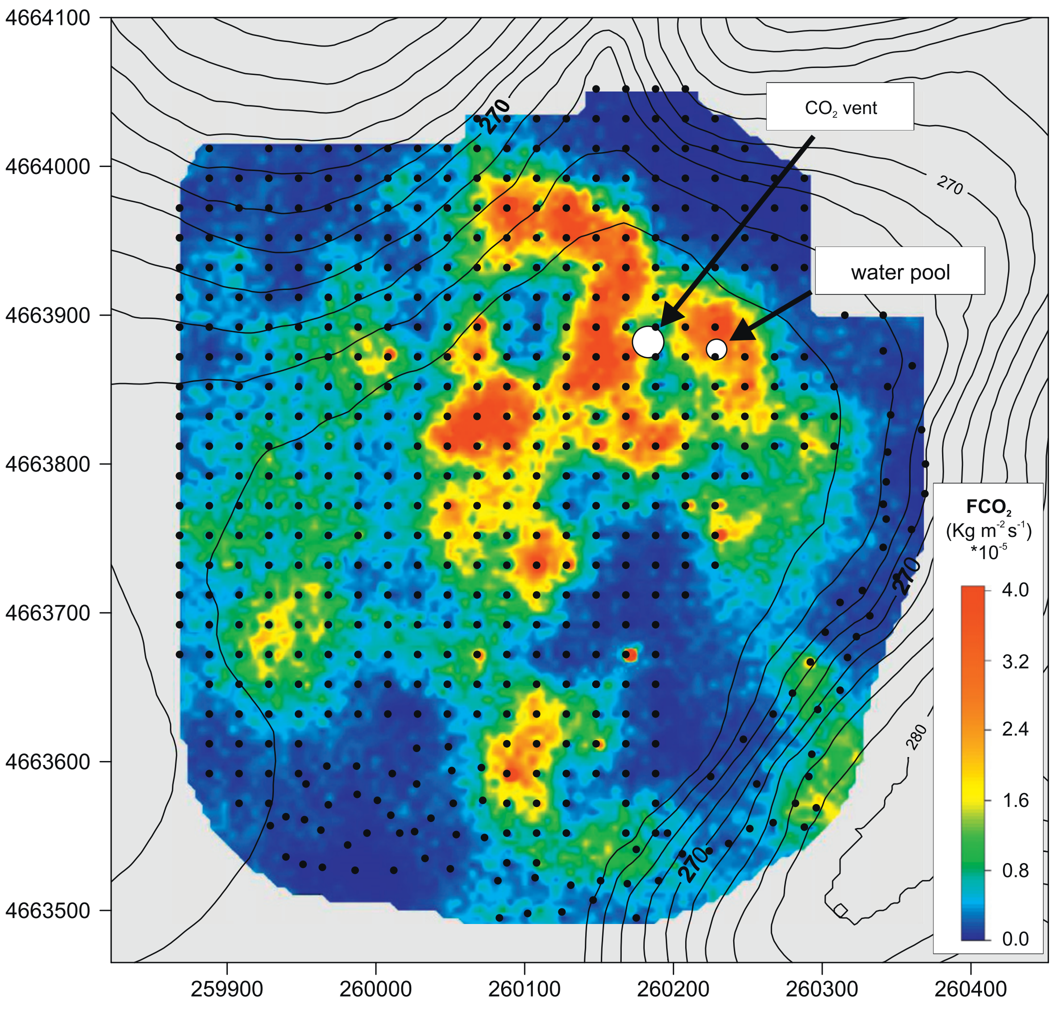

Fig. 1. Map of CO_2 flux at CdM. The measured CO_2 soil fluxes range from 2.3×10^{-8} to $2.8 \times 10^{-4}\,\mathrm{kg\,m^{-2}\,s^{-1}}$, with an average value of $7.7 \times 10^{-6}\,\mathrm{kg\,m^{-2}\,s^{-1}}$ or $160\,\mathrm{ton\,d^{-1}}$. The contribution from the focused vents is around $0.17\,\mathrm{kg\,s^{-1}}$ or $15\,\mathrm{ton\,d^{-1}}$ (Rogie et al., 2000). Axes show UTM coordinates in m (Costa et al., 2008).

5. The TWODEE-2 output files

TWODEE-2 outputs the following files:

- File `problemname.log`. This file, passed as a program call argument, contains information concerning the run (summary of input data, run time error messages, CPU time, etc.). It also outputs some basic indicators of the cloud evolution every minute.
- Files of results in GRD-format. For each user-specified time TWODEE-2 can generate 2D contour-files written in GRD-format for the following variables: h, $\overline{u}$, $\overline{v}$, $\overline{\rho}$, c, and D. These files can be read directly by several plotting programs like the commercial software Grapher©. Alternatively, the user may also generate its own plots using functions from several free packages (e.g., gnuplot).
- TWODEE-2 can also output comma separated variables (CSV)-format files with concentration at defined points and/or boxes every minute. The CSV is a free ASCII format in which variables are stored in columns separated by commas. It can be read by Excel© or by any text editor.

6. Application example

TWODEE-2 was applied to simulate dense gas dispersion episode from natural sources in central Italy. As an example, we report results for an experiment carried out in the area of Caldara di Manziana (CdM), Italy, a quaternary volcanic crater located 20 km NW of Rome

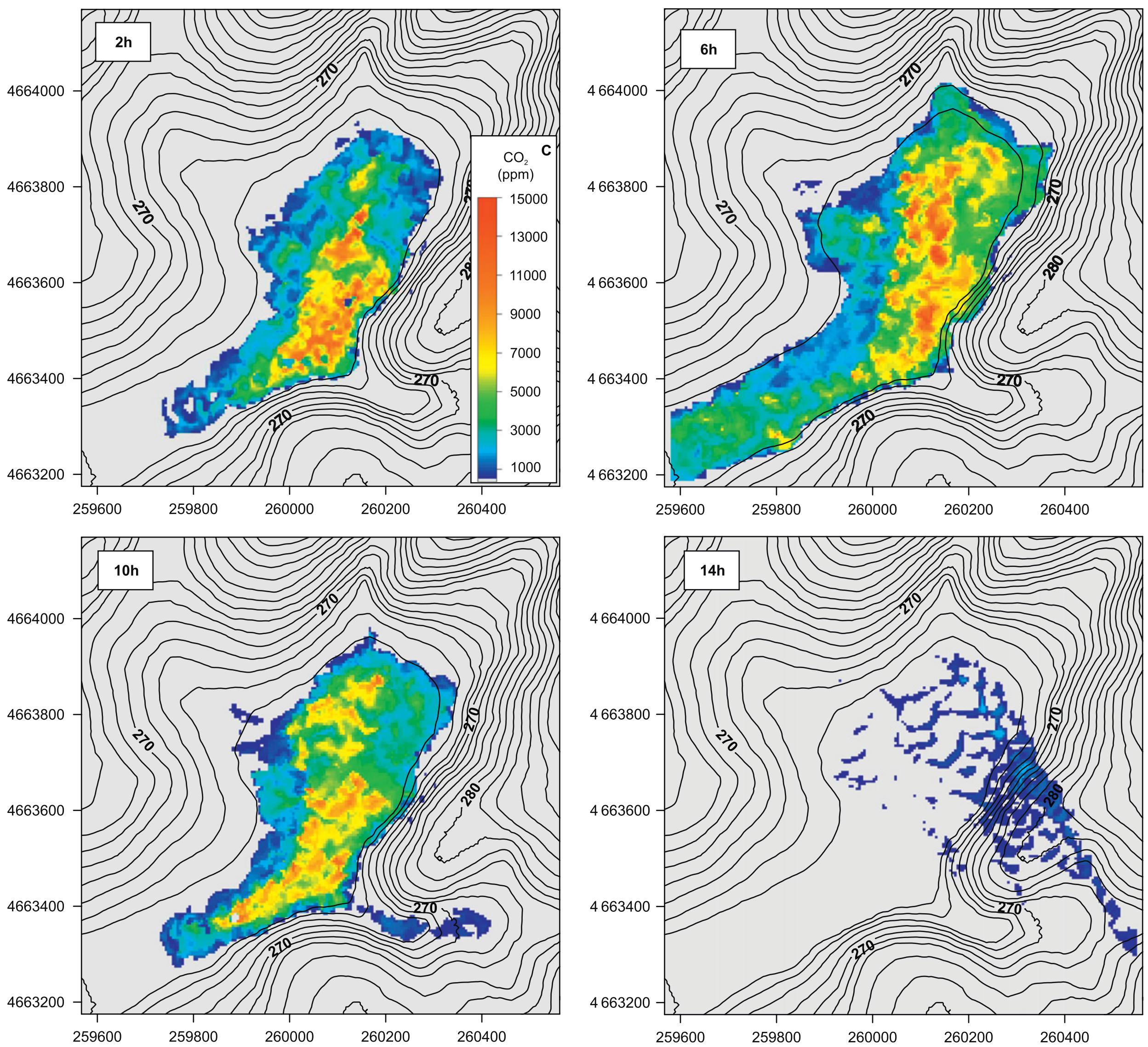

Fig. 2. Time evolution of concentration at 2.2 m height. Four different time slices at 2, 6, 10 and 14 h are plotted for illustrative purposes. Axes show UTM coordinates in m (Costa et al., 2008).

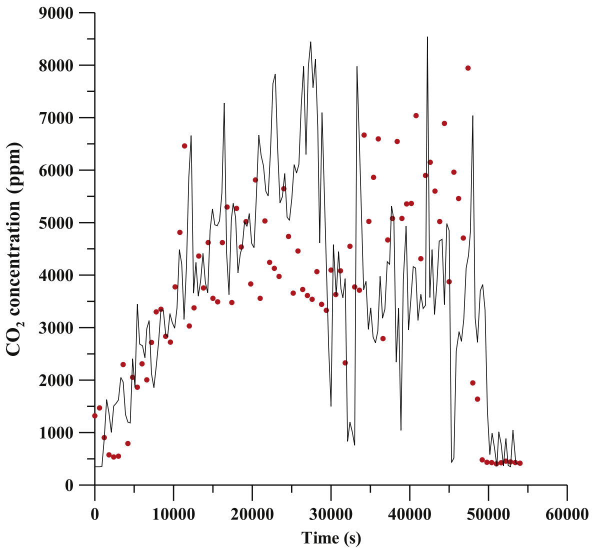

Fig. 3. Comparison between measured (red dots) and simulated (black line) concentrations averaged every 10 min. Point UTM coordinates are (260252, 4663873) (Costa et al., 2008).

(see Costa et al., 2008 for details). At CdM the emission of CO_2 occurs both as soil diffuse degassing and from two localized sources, a water pool and a vent (Fig. 1). During an experiment carried out on 5 and 6 February 2007 an open path infrared CO_2/H_2O analyzer measured CO_2 concentration at 2.20 m above the ground for 15 h, from 17:40 (local time, LT) of 5 February 2007 to 08:40 (LT) of 6 February 2007. During the same time span, a meteorological station placed at 3.45 m height acquired pressure, air temperature and wind speed. Both datasets were averaged every 10 min. The computational domain (1 km^2) was discretized using a grid of 125×125 points with a nodal distance of 8 m. Zero initial cloud depth and velocity were assumed. The averaged critical time step was around 0.3 s, implying almost 200 000 iterations to simulate the whole time interval (54 000 s). The CPU time required was less than 2 h on a standard Pentium IV desktop PC.

A view from above of the gas plume at 2.2 m height, showing the temporal evolution at different time slices, is plotted in Fig. 2. The cloud concentration reflects both wind intensity and direction. Wind blew SW during the first 2 h, then oscillated between SE and NE and, finally, shifted towards SSE in the last 2 h. Fig. 3 compares concentrations measured by the CO_2/H_2O analyzer at the point having UTM coordinates (260252;4663873;2.20) with the simulated concentrations averaged over an area of 25 m $\times$ 25 m centered at the same point. Note how TWODEE-2 tracks the evolution of concentration despite the turbulent nature of the flow, which produces a highly oscillatory behaviour.

7. Discussion, validity and limitations

TWODEE-2 is a FORTRAN 90 code for the dispersion of heavy gases based on the shallow layer approach. This approach is valid in the limit $H_*^2/L_*^2 \ll 1$, where H_* is the undisturbed fluid height and L_* the characteristic wave length scale in the flow direction (Ferrari and Saleri, 2004). The code is suitable for simulating the gravitational phase of gas dispersion when the negative buoyancy controls the transport and the cloud follows the ground. When the density contrast becomes less important ($\Delta\rho < 0.001$ kg/m^3 Mohan et al., 1995), a model based on the passive dispersion approximation is more suitable. TWODEE-2 removes several limitations of its parent FORTRAN 77 version:

- The computational grid is geo-referenced and can have an arbitrary number of nodes.
- Topography, terrain roughness, and dense gas fluxes for diffuse or punctual sources can be extracted from regional files.
- A non-uniform roughness height allows the user to simulate domains which contain zones with contrasted properties (e.g., a forest or a lake).
- The wind field is described through the similarity theory and can be both uniform and non-uniform. Time-dependent spatially variable wind fields accounting for terrain influence can be generated by the program DIAGNO by furnishing a domain mean wind value.
- Has multiple output possibilities. For example, TWODEE-2 can output the height at which a certain concentration value is achieved or can track the evolution of concentration at discrete points or at given areas.
- Improves code performance. TWODEE-2 solves the same governing equations using the same algorithm that its parent software. However, the implementation of the code is more efficient, a fact that reduces the computational times by a factor 2–5 depending on each particular run.

Potential applications of the model include CO_2 concentration distribution under a variety of atmospheric conditions and assessment of environmental hazards from potential leakage and seepage related to accumulation of large quantities of injected CO_2 in geologic sequestration sites (e.g., Oldenburg and Unger, 2003, 2004). The results obtained in test applications (Costa et al., 2008) show the high performance of the model when the input parameters are correctly furnished. However, the code still has some limitations to be corrected in a future. Improvements should include:

- The possibility to use non-uniform and/or non-structured computational meshes.
- The edge entrainment term to simulate the introduction of ambient fluid not only from the top of the cloud but also from the edges.
- To allow DIAGNO to read data from more than one meteorological station.
- To account for thermodynamic effects such as gas condensation by introducing an additional equation for gas enthalpy.

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References

Clarke, T., 2001. Taming Africa's killer lake. Nature 409, 554–555.

Costa, A., Macedonio, G., Chiodini, G., 2005. Numerical model of gas dispersion emitted from volcanic sources. Annals of Geophysics 48, 805–815.

Costa, A., Chiodini, G., Granieri, D., Folch, A., Hankin, R., Caliro, S., Avino, R., Cardellini, C., 2008. A shallow layer model for heavy gas dispersion from natural sources: application and hazard assessment at Caldara di Manziana, Italy. Geochemistry Geophysics Geosystems 9, Q03002, doi: 10.1029/2007GC001762.

Douglas, S., Kessler, R., Carr, L., 1990. User's Manual for the Diagnostic Wind Model. Volume III, U.S. Environmental Protection Agency, Report No. EPA-450/4-90-007C. Systems Applications Inc., San Rafael, CA.

Dyer, A., 1974. A review of flux-profile relationships. Boundary Layer Meteorology 7, 363–372.

Ferrari, S., Saleri, F., 2004. A new two-dimensional shallow water model including pressure effects and slow varying bottom topography. ESAIM: Mathematical Modelling and Numerical Analysis 38, 211–234.

Hankin, R., Britter, R., 1999a. TWODEE: the Health and Safety Laboratory's shallow layer model for heavy gas dispersion. Part 1. Mathematical basis and physical assumptions. Journal of Hazardous Materials A 66, 211–226.

Hankin, R., Britter, R., 1999b. TWODEE: the Health and Safety Laboratory's shallow layer model for heavy gas dispersion. Part 2. Outline and validation of the computational scheme. Journal of Hazardous Materials A 66, 227–237.

Hankin, R., Britter, R., 1999c. TWODEE: the Health and Safety Laboratory's shallow layer model for heavy gas dispersion. Part 3. Experimental validation (Thorney island). Journal of Hazardous Materials A 66, 237–261.

Jacobson, M., 1999. Fundamentals of Atmospheric Modelling, first ed. Cambridge University Press, New York, p. 656.

Louis, J., 1979. A parametric model of vertical eddy fluxes in the atmosphere. Boundary Layer Meteorology 17, 187–202.

Macedonio, G., Costa, A., 2002. Finite element modeling of gas dispersion in the atmosphere. In: Buccianti, A., Marini, L., Ottonello, G., Vaselli, O. (Eds.), Proceedings of the Arezzo Seminar in Fluids Geochemistry. Pacini Editore, Ospedaletto (Pisa), Italy, pp. 147–159.

Mohan, M., Panwar, T., Singh, M., 1995. Development of dense gas dispersion model for emergency preparedness. Atmospheric Environment 29, 2075–2087.

Oldenburg, C., Unger, J., 2003. On leakage and seepage from geological carbon sequestration sites: unsatured zone attenuation. Vadose Zone Journal 2, 287–296.

Oldenburg, C., Unger, J., 2004. Coupled vadose zone and atmospheric surface-layer transport of carbon dioxide from geologic carbon sequestration sites. Vadose Zone Journal 3, 848–857.

Rogie, J., Kerrick, D., Chiodini, G., Frondini, F., 2000. Flux measurements of nonvolcanic CO_2 emission from some vents in central Italy. Journal of Geophysical Research 105 (B4), 8435–8445.

Van Ulden, A., Holstag, A., 1985. Estimation of atmospheric boundary layer parameters for diffusion applications. Journal of Applied Meteorology and Climatology 24, 1196–1207.

Venetsanos, A., Bartzis, J., Wurtz, J., Papailiou, D., 2003. DISPLAY-2: a two-dimensional shallow layer model for dense gas dispersion including complex features. Journal of Hazardous Materials A 99, 111–144.

Zalesak, S., 1979. Fully multidimensional flux-corrected method transport for fluid. Journal of Computational Physics 31, 335–362.