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CFD and Gaussian atmospheric dispersion models: A comparison for leak from carbon dioxide transportation and storage facilities

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ABSTRACT

Carbon Capture and Storage (CCS) is of interest to the scientific community as a way of achieving significant global reduction of atmospheric CO_2 emission in the medium term. CO_2 would be transported from large emission points (e.g. coal fired power plants) to storage sites by surface/shallow high pressure pipelines. Modelling of CO_2 atmospheric dispersion after leakages from transportation facilities will be required before starting large scale CCS projects. This paper deals with the evaluation of the atmospheric dispersion CFD tool Fluidyn-PANACHE against Prairie Grass and Kit Fox field experiments. A description of the models for turbulence generation and dissipation used (k–ε and k–l) and a comparison with the Gaussian model ALOHA for both field experiments are also outlined. The main outcome of this work puts PANACHE among the "fit-for-purpose" models, respecting all the prerequisites stated by Hanna et al. [Hanna, S.R., Chang, J.C. and Strimaitis, D.G., 1993. Hazardous gas model evaluation with field observations. Atmospheric Environment, 27, 2265–2285] for the evaluation of atmospheric dispersion model performance. The average under-prediction has been ascribed to the usage of mean wind speed and direction, which is characteristic of all CFD models. The authors suggest a modification of performance ranges for model acceptability measures, within the field of high pressure CO_2 transportation risk assessment, with the aim of accounting for the overall simplification induced by the usage of constant wind speed and direction within CFD atmospheric dispersion models.

1. Introduction

On a global scale, reserves of fossil fuels are far from exhausted, e.g. coal reserves are estimated to last several hundred years at the current production rate (Barrie et al., 2004). If the generated CO_2 can be prevented from reaching the atmosphere, future use of fossil fuels will remain viable. Hence the sequestration of carbon dioxide (CO_2) through injection into subterranean geological structures such as saline aquifers is of interest to the global community as part of continued efforts towards the reduction of greenhouse gas emissions (IPCC, 2005). Carbon dioxide would be captured at large point emission sources (e.g. power plants), and transported at high pressure ($\sim$10 MPa) via pipeline (on- and off-shore), sea-carrier (off-shore) or a combination of these (Svensson et al., 2004) to suitable locations where it can be sequestered underground.

If Carbon Capture and Storage (CCS) technology is to be widely introduced, then extensive networks of CO_2 transportation facilities will be needed (Gale and Davison, 2004). There is a possibility of leakage from this infrastructure through component failure or infrastructure damage. The failure probability of some parts of the high-pressure transportation system has been well documented in the oil industry literature (Burgherr and Hirschberg, 2005; Hirschberg et al., 2004; Townes et al., 2004), and the

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Nomenclature

P	pressure (MPa)
T	temperature (K)
u	fluid velocity ($m\,s^{-1}$)
v	wind speed ($m\,s^{-1}$)
g	gravitational acceleration ($9.8\ m\,s^{-2}$)
F_s	rate of momentum gain per unit volume due to pollutant emissions ($N\,m^{-2}$)
$F_{g/p}$	force due to: (g) gravitational acceleration, (p) interaction with droplets/particles ($N\,m^{-2}$)
I	specific internal energy ($J\,kg^{-1}$)
J	heat flux vector ($W\,m^{-2}$)
l	turbulent length scale (m)
k	thermal conductivity ($W\,m^{-1}\,K^{-1}$)
h_m	specific enthalpy of species m ($J\,kg^{-1}$)
$Q_{s/p/h}$	rate of specific internal energy gain due to: (s) pollutant emissions, (p) interaction with particles, (h) surface energy budget ($J\,kg^{-1}\,s^{-1}$)
u^*	friction velocity ($m\,s^{-1}$)
z_0	ground roughness parameter (m)
C_p	specific heat of air ($J\,g^{-1}\,K^{-1}$)
G	turbulence production rate by shear $= \sigma\nabla u$ ($m^2\,s^{-3}$)
W_p	turbulence production due to interaction with particles ($m^2\,s^{-3}$)
K	turbulent kinetic energy per unit mass ($m^2\,s^{-2}$)
C_1	k–ε turbulence model unitless constant equal to 1.44
C_2	k–ε turbulence model unitless constant equal to 1.92
C_s	unitless turbulence production factor equal to 1.5
C_E	unitless turbulence viscosity constant for the k–ε model, equal to 0.09
C_D	unitless turbulent energy dissipation constant for the k–l model, equal to 0.3
C_μ	unitless turbulence viscosity constant for the k–l model, equal to 0.1887
V_e	cloud travel speed ($m\,s^{-1}$)

Greek letters

ρ	total mass density ($\rho_{CO_2} = 1.8\ kg\,m^{-3}$)
ρ_m	mass density of species m ($kg\,m^{-3}$)
ρ_{amb}	density of air ($1.2\ kg\,m^{-3}$)
$\delta_{s/p}$	source term for species due to (s) pollutant emission, (p) droplet evaporation/condensation ($kg\,s^{-1}$)
μ	primary (shear) viscosity of fluid ($kg\,m^{-1}\,s^{-1}$)
λ	secondary (bulk) viscosity of fluid ($kg\,m^{-1}\,s^{-1}$)
σ	Newtonian viscous stress tensor ($N\,m^{-2}$)
ε	dissipation of turbulent kinetic energy ($m^2\,s^{-3}$)
ζ	Monin–Obukhov similarity variable $= z/L$, dimensionless
κ	von Karman constant $= 0.41$, dimensionless
θ	potential temperature (K)
σ_h	turbulent Prandtl number, dimensionless
σ_k	dimensionless turbulence model constant for the k equation equal to 1.0
σ_ε	dimensionless turbulence model constant for the ε equation equal to 1.2
$\Psi_{(\varsigma)}$	similarity profile
ν_t	turbulent viscosity ($kg\,m^{-1}\,s^{-1}$)

principal causes of natural gas/CO_2 pipeline incidents have been classified – i.e. relief valve failure, weld/gasket/valve packing failure, corrosion and outside forces. In their study, Vendrig et al. (2003) reported an overall failure probability from a CCS transportation facility of about 0.37[1] per year, irrespective of its location (underground or above the surface) but with much higher likelihood for surface components (i.e. CO_2 recovery at source, booster stations and injection plants).

Gaseous CO_2 is an asphyxiant, a cerebral vasodilator and at high concentrations (i.e. >70,000 ppm) causes rapid circulatory insufficiency leading to coma and death (D.o.H., 2004). Carbon dioxide is about 1.5 times denser than air at ambient temperature and tends to remain close to the surface, posing a major health hazard. Moreover, an adiabatic (quasi instantaneous) pressure drop – as the ones expected from HP transportation facility failures – reduces the temperature by more than 100 °C (Joule-Thomson effect), raising its density to about 2.8 $kg\,m^{-3}$ (Mazzoldi et al., 2007). The tendency of the gas to stay close to the ground would be enhanced, amplifying the risk it poses to humans and the environment, particularly in situations of complex topography and low wind. Before CCS being developed, modelling of CO_2 atmospheric dispersion from proposed pipelines is critical. This modelling should be done using worst case leakage scenarios with the most sensitive receivers defined, if CO_2 transport facilities are located close to inhabited areas or an area with CO_2 sensitive receivers.

Air quality models are used to predict the transport and turbulent dispersion of gases released to the atmosphere. Several studies regarding potential atmospheric dispersion of CO_2 leaked from CCS transportation facilities have been drawn up in the last decade (Kruse and Tekiela, 1996; Turner et al., 2003; IEA, 2003; Vendrig et al., 2003). These investigations were carried out utilizing Gaussian/dense gas models.

Gaussian tools are widely used in risk analysis procedures, providing fast dispersion estimations and usually reliable results when describing unobstructed gas flow over flat terrain (Reynolds, 1992; Smith, 1999). Owing to the advance in computational power it is now practicable to apply Computational Fluid Dynamics (CFD) models for short- and medium-range gas dispersion scenarios. Although

[1] This result is valid for a modular pipeline system composed of CO_2 recovery at source, Converging pipelines, one Booster station, 10 km pipeline and one injection plant. Singular modules have lower probability but one integral transportation system would have a higher failure probability (it would consist of more than 10 km of pipeline and may be more than one booster station).

unworkable for real-time simulations because of the relatively long computational time and large scenarios set-up time needed, CFD is particularly useful when modelling plume dispersion on complex topography (McBride et al., 2001; Scargiali et al., 2005; Burman, 1998) and among buildings (Milliez and Carissimo, 2006; Yamada, 2004; Pullen et al., 2004; Tang et al., 2006).

The current paper describes the Fluidyn-PANACHE CFD model (hereinafter referred to as PANACHE) developed by Transoft International® (Venkatram and Tripathi, 1996). An evaluation predicting performance against a number of field observations from two independent release experiments (Prairie Grass and Kit Fox) has been carried out, discussing the turbulence models used for the two sets of trials. A comparison with the predictions of a Gaussian/dense gas model was carried out, taking the model ALOHA 5.4 as representative of this category, due to its wide usage history (D.O.E., 2004; Thoman et al., 2006; Alhajraf et al., 2005; Hanna, 2003).

2. PANACHE

Fluidyn-PANACHE (version 3.4.1) is a computer code for numerical simulation of atmospheric flows and pollution in short and medium-range scales. PANACHE uses Computational Fluid Dynamics tools (i.e. Navier-Stokes equations and turbulence models) in a finite volume-based approach, solving the differential equations governing mass, momentum, and energy transfer on discrete control volumes, provided by a non-uniform mesh generator that takes into account the presence of obstacles or topographical features (i.e. with generation of a finer mesh in critical areas).

2.1. Numerical scheme

The continuity equation for total fluid density is:

$$\partial\rho/\partial t + \nabla\cdot[\rho u] = \delta_s + \delta_p \tag{1}$$

where ∇ denotes the gradient of the considered quantity on the three dimensions, other symbols are as described in nomenclature. The appropriate SI units are implicitly assumed for all quantities.

The momentum equation for the fluid mixture is:

$$\partial\rho u/\partial t + \nabla\cdot[\rho uu \quad \sigma] = \nabla P + F_s + F_g + F_p \tag{2}$$

where σ = Newtonian viscous stress tensor ($=\mu[\nabla u + (\nabla u)^T] + \lambda(\nabla\cdot u)i$, where μ,λ = first and second coefficients of viscosity, $\lambda = -2/3\mu$; T = matrix transpose; i = unit dyadic – product of vectors). Viscous forces in a fluid are function of the rate at which the fluid velocity is changing over distance, the Newtonian viscous stress tensor parts the stress field within the fluid molecules into (a sum of) a constant tensor (the rate-of-expansion tensor) and a traceless symmetric tensor (rate-of-shear tensor) – respectively, the term with μ and the term with λ.

The internal energy equation is:

$$\partial\rho I/\partial t + \nabla\cdot[\rho u \quad I \quad J] = \nabla\cdot u + \rho\varepsilon + Q_s + Q_p + Q_h \tag{3}$$

where J = heat flux vector $= k\nabla T + \rho\sum[h_m\nabla(\rho_m/\rho)]$.

PANACHE solves the governing equations described above both in three-dimensional space and in time. The spatial differentiation is done over a three dimensional mesh made up of arbitrary hexahedrons. Control-volume or integral-balance approach is used to construct the finite difference approximations for each of these control-volumes to preserve local conservation of differenced quantities. The time differentiation enables a unified approach towards both transient and steady state phenomena and is carried out over a sequence of time steps. An implicit procedure enables the use of unlimited time steps.

Two different approaches to compute the gravitational force in the momentum equation have been used for the trials:

- Buoyancy model, in which buoyancy terms due to density differences drive momentum:

$$F_g = (\rho - \rho_{amb})g \tag{4}$$

where ρ_{amb} = ambient density; g = gravitational acceleration vector.

This model was used for the Kit Fox experiment in which dense CO_2 was released.

- Full gravity model:

$$F_g = \rho g \tag{5}$$

This model was used for the Prairie Grass trials, together with the zero-gravity one – SO_2 at the test field was released in trace concentration and it can be considered as a continuous amount of neutrally buoyant gas, not affected by gravity. No relevant differences were noted between usages of these two.

2.2. Boundary conditions

Boundary conditions are specifications of properties on the surfaces of the domains and are required to fully define the flow simulation. Ambient mean wind speed and air temperature profiles are boundary conditions (supposing they are constant over the domain area) represented by logarithmic functions in these release trials. Specifically:

$$v(z) = u^*/\kappa\left[\ln(z/z_0)\Psi_{1(\varsigma)}\right] \tag{6}$$

$$\theta(z) = \sigma_h\theta^*/\kappa\left[\ln(z/z_0)\Psi_{2(\varsigma)}\right] \tag{7}$$

where θ^* = temperature scale; $\Psi_{1(\varsigma)}$ and $\Psi_{2(\varsigma)}$ = similarity profile.

The surface friction velocity, u^*, the temperature scale θ^*, and the Monin–Obukhov length, L are related by: $L = u^{*2}T/(g\kappa\theta^*)$ and $\theta^* = Q_h/(\rho C_p u^*)$. The micrometeorological parameters, u^*, θ^*, and L are evaluated for different atmospheric stability classes. For unstable and neutral conditions $u^* = U^*[1 + \text{a}\ln(1 + bQ_0/Q_1)]$, where $U^* = \kappa v/\ln(z_m/z_0)$ is the friction velocity for neutral conditions, $z_m = 4\,h_{an}z_0$, h_{an} = anemometer height, $Q_0 = Q_h/\rho C_p Q_1\theta U^{*3}/(\kappa g z_m)$,

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θ = potential temperature, a and b are constants dependent on z_0 and z_m (Transoft, 2006). For stable conditions Eqs. (6) and (7) are solved in L and the other parameters are found via their relations.

The ground roughness is another boundary condition discussed in Section 4 where the trials scenarios are described. In the Kit Fox trials PANACHE accounted for walls using the Log-Law condition within which the wall shear stress and heat transfer in the boundary layer are computed from the standard logarithmic law of the wall, and introduced into momentum and energy equations. It is assumed that neutral conditions prevail near ground. This assumption is reasonable as near the ground z is very low leading to low values of ζ – Eqs. (6) and (7).

It would be desirable to account for the fact that wind speed and direction vary with time and space over a continuous spectrum but, for the purpose of keeping the computational time tractable, mean values suggested by Hanna and Chang (2001) were used.

2.3. Turbulence models

In the two sets of release trials, both the turbulence models described below were used within PANACHE.

2.3.1. k–ε Model

The standard k–ε model is modified to include the effects of buoyancy and the stability condition of the atmosphere by means of Richardson number, the non-dimensional parameter characterizing the stability of the atmosphere in terms of temperature, defined as:

$$Ri = g/T(\partial\theta/\partial z)\rho/G \tag{8}$$

For unstable conditions Ri is negative and for stable conditions it is positive.

The equations for k (turbulence generation) and ε (turbulence dissipation) are given below:

$$\partial\rho k/\partial t + \nabla[\rho u \quad k - (\mu/\sigma_k)\nabla k] = 2/3\rho k\nabla\cdot u + G(lRi/\sigma_h)\rho\varepsilon + W_p \tag{9}$$

$$\partial\rho\varepsilon/\partial t + \nabla[\rho u \quad \varepsilon - (\mu/\sigma_\varepsilon)\nabla\varepsilon] = \varepsilon/\kappa[C_1G(lRi/\sigma_h) - C_2\rho\varepsilon + C_sW_p] \tag{10}$$

where σ_h is the Prandtl number which for the k–ε model = 1.11.

The turbulent viscosity is given by:

$$\nu_t = C_E k^2/\varepsilon \tag{11}$$

This model was used within PANACHE for the majority of Prairie Grass trials.

2.3.2. k–l model

This is a one-equation model where Eq. (9) for k is solved while the turbulent length scale is specified algebraically. σ_h in Eq. (9) for the present model is not constant but is a function of Ri. Eq. (10) is not solved and ε in Eq. (9) is defined as:

$$\varepsilon = C_D k^{3/2}/l \tag{12}$$

The length scale, l, is prescribed algebraically for different atmospheric stability conditions: stable (E, F) unstable (A, B) and neutral (C, D), (Transoft, 2006).

The turbulent viscosity is given as

$$\nu_t = C_\mu k^{1/2} l \tag{13}$$

As for all numerical models, the run times for PANACHE depend directly on the product of number of grid cells, the number of seconds simulated and the number of time steps per second. CFD-PANACHE was run on a single laptop provided with two 2.00 GHz Pentium 5 processors: within 4 weeks about 100 tracer release trials of the two field experiments described could be simulated. Representative computational times for the two experiments were: for Prairie Grass, with a grid consisting of 74,640 CVs and with 900 s of simulated time, it took between 1 and 3 h per simulation, with longer simulation times for unstable atmospheric conditions (classes A and B). For Kit Fox, with about 228,000 CVs and 300–1100 s simulated time, the elapsed time on the PC for one run varied from 3 to 10 h.

2.4. ALOHA 5.4

For the purpose of comparison, predictions by the CFD tool PANACHE have been compared to predictions from the Gaussian model ALOHA 5.4. A quick review of its main calculation equations is provided below. For further information see Reynolds (1992).

The classical Gaussian plume is a steady-state model that requires a continuous release of contaminant. The ensemble average (i.e. probabilistic) plume shape is approximated by time averages sufficient to smooth the effects of plume meandering. The equation for the Gaussian plume is a function only of the mean wind speed (assumed constant) and the crosswind and vertical standard deviations ($\sigma_y(x)$ and $\sigma_z(x)$). Source strength, Q, is mass of released material per unit time. The time averaged wind speed, v, is uniform everywhere. The contaminant concentration, $C(x, y, z)$, is given by:

$$C(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z v}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\exp\left[-\frac{1}{2}\left(\frac{z-h_s}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{z+h_s}{\sigma_z}\right)^2\right]\right\}$$

where σ_y is the standard deviation of $C(x, y, z)$ in the cross-wind direction and σ_z is the standard deviation of C in the vertical direction. These dispersion parameters are function only of the downwind direction, x. The z-dependent terms model the trapping effect of the ground by proposing a mirror source at distance h_s beneath the ground.

The heavy gas dispersion model in ALOHA is almost identical to the similarity model proposed by Colenbrander (1980). The plume is assumed to be composed of (i) a horizontally homogeneous core of width 2b which has vertical dispersion, and (ii) Gaussian-shaped edges (Colenbrander, 1980). The concentration is calculated as:

$$C(x,y,z) = \begin{cases} C_c(x)\exp\left[-\left(\frac{|y|-b(x)}{S_y(x)}\right)^2 - \left(\frac{z}{S_z}\right)^{1+n}\right] & |y| > b(x) \\ C_c(x)\exp\left[-\left(\frac{z}{S_z}\right)^{1+n}\right] & |y| \le b(x) \end{cases}$$

Four variables in the above equation are functions of x and must be computed for each downwind step: $C_c(x)$, the centerline ground-level concentration; $S_y(x)$, the lateral dispersion parameter; $S_z(x)$, the vertical dispersion parameter; $b(x)$, the half-width of the homogeneous core section.

A coupled set of parametric equations describing the effective cloud width, height and velocity and the mass and energy balance, approximating the mean density of the cloud gas mixture during the time, is described in the ALOHA theoretical description (Reynolds, 1992).

3. Statistical model performance evaluation method

The PANACHE model has been evaluated following the directives for atmospheric dispersion model performance measures suggested by Hanna et al. (1993) and summarized by Chang and Hanna (2004). The evaluation focussed on the maximum concentration observed and predicted on a given arc during a given experimental trial. The use of maximum concentration on arcs for the model evaluation exercise is standard for evaluations of dispersion models and field experiments in open terrain (Hanna et al., 2004).

The following equations define the statistical performance measures, which include the fractional bias (FB), the geometric mean bias (MG), the normalized mean square error (NMSE), the geometric variance (VG) and the fraction of predictions within a fraction of two of the observations (FAC2) (Hanna and Chang, 2001):

$$\mathrm{FB} = \frac{(\overline{C}_o - \overline{C}_p)}{0.5(\overline{C}_o + \overline{C}_p)}, \tag{14}$$

$$\mathrm{MG} = \exp\left(\overline{\ln C_o} - \overline{\ln C_p}\right), \tag{15}$$

$$\mathrm{NMSE} = \frac{\overline{(C_o - C_p)^2}}{\overline{C}_o\overline{C}_p}, \tag{16}$$

$$\mathrm{VG} = \exp\left[\overline{(\ln C_o - \ln C_p)^2}\right] \tag{17}$$

$$\mathrm{FAC2} = \text{fraction of data that satisfy } 0.5 \le \frac{C_p}{C_o} \le 2.0 \tag{18}$$

where C_o = observations of concentration (highest value recorded); C_p = model predictions of concentration (highest value predicted); overbar ($\overline{C}$) = average over the dataset.

A perfect model would have MG, VG and FAC2 = 1; FB and NMSE = 0. Because of the influence of random atmospheric processes these values are not attainable, and the minimum performance measures for a model to be defined as "acceptable" (summarized by Chang and Hanna (2004), based on extensive experience with model evaluations) are as follow. The fraction of predictions within a factor of two from observations is about 50% (i.e., FAC2 > 0.5); the mean bias is within ±30% of the mean (−0.3 < FB < 0.3 or 0.7 < MG < 1.3); the random scatter is about a factor of two of the mean (NMSE < 4 or VG < 1.6). The listed acceptability criteria are for research-grade field experiment, with well-known controlled source term and many on-site observations of meteorology and concentrations.

4. Description of datasets and simulations results

In the current study, the focus was on evaluating the capabilities of PANACHE to predict atmospheric dispersion in the near and far field. It was used to simulate releases of a buoyant tracer gas (SO_2) on flat terrain (that is, the Prairie Grass field experiments) and releases of a dense gas (CO_2) on terrain with obstacles (the Kit Fox field trials). A brief description of the two scenarios is given below, together with performance evaluation.

4.1. Prairie Grass

The Prairie Grass field experiments (Barad, 1958) were conducted at O'Neill, Nebraska, during July and August 1956. The tracer consisted of small amounts of SO_2, released at an elevation of 0.45 m from a point source, with the duration of each release being about 10 min. Sulfur dioxide has a molecular weight which is more than twice that of ambient air, it could be considered a passive pollutant thanks to the very low concentration it was released at (Chang, 1998). Maximum concentrations were measured by samplers installed at a height of 1.5 m along five concentric arcs, located 50, 100, 200, 400 and 800 m downwind of the source. The wind measurements were taken by an anemometer 2 m above the ground, recording a wind speed ranging from 2 to 10 m s^{-1} over the entire set of trials; atmospheric stability covered the entire spectrum from A (unstable) to F (stable). Forty-three simulations were conducted with ALOHA and PANACHE representing each experimental condition for which the data were available. Within PANACHE the height of the domain for these trials was 100 m. The average wind speed and atmospheric conditions for each trial were taken from the work of Chang (1998).

4.1.1. Discussion of results

Eqs. (14)–(18) were applied to the dataset of observed maximum concentrations against PANACHE and ALOHA predictions. Results were divided into categories, each category referring to concentrations recorded at different arcs.

Fig. 1 represents observed values against predictions from the CFD model, the diagonal lines being the boundaries for model acceptability. PANACHE predictions at arc 1 underestimate the concentration values by about 33%. In

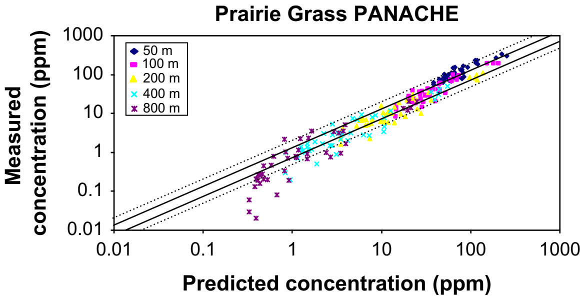

Fig. 1. PANACHE concentration predictions against observations for the Prairie Grass trials. Diagonal lines are boundaries for predictions acceptability, where dot lines are limits for $0.5 \leq C_p/C_o \leq 2.0$.

order to ensure acceptable simulation times, the small point source (about 1 cm diameter) and the relatively large domain ($\sim$1000 m) led the authors to opt for a coarser grid than normally used. Consequently, the model will overestimate the gas dilution in the CVs near the source. This accounts for the under-predictions at the nearest arc. Other modellers, coming across the same issue during Prairie Grass releases simulation, adopted the same strategy (Hanna et al., 2004).

Statistical values for PANACHE (Table 1) are all well within the limits for acceptable models: particularly, the fractional bias suggests that the mean value of model predictions matches with observations, while the proportions of the entities measuring the extent of the typical error (NMSE and VG) demonstrate an average scatter of less than half the mean of observations. For the two largest arcs (400 and 800 m), while the average values are acceptable, a proportionately larger deviation from observed value can be seen (Fig. 1). The results dataset shows a large over-prediction of concentrations at this arc for the trials with unstable atmosphere (classes A and B), with errors up to one order of magnitude. This may be due to the over-prediction of turbulence dissipation by the k–ε model and consequent over-prediction of gas concentration far from the source. Other modellers have reported this disagreement under unstable atmospheric conditions for the k–ε model (Sklavounos and Rigas, 2004).

For the trials with very stable atmospheric conditions (class F), on the other hand, the k–ε model under-predicted the concentration of SO_2 by up to a factor of five for each arc. For this reason the authors used the k–l model within the trials with very stable atmosphere (i.e. trials PG32, PG36, PG53, PG58 and PG59), which proved to perform much better for class F conditions.

The Prairie Grass field trials were also simulated using the Gaussian model ALOHA 5.4. ALOHA has got a heavy gas dispersion algorithm which has not been utilised for Prairie Grass because of the large over-predictions obtained by its usage in simulating the dispersion of a dense gas in very low concentration. The Gaussian model also gave good results, although it showed an average under-prediction at short distances and-over prediction at long distances for unstable atmospheric conditions (classes A and B), and an average over-prediction at short distances and under-prediction at long distances for stable conditions (classes E and F). These limitations are characteristic of Gaussian dispersion models that calculate the plume size and 2D concentration limits using algebraic equations (Dharmavaram et al., 2005). For neutral stability conditions, the fit showed to vary with wind speed, the model slightly over-predicting for high values of ambient velocity ($v > 6\ \mathrm{m\,s^{-1}}$) and under-predicting for low values ($v < 3\ \mathrm{m\,s^{-1}}$) (Fig. 2).

A summary of results and comparison between PANACHE and ALOHA can be seen in Table 1. For ALOHA, linear measures (FB and NMSE) are on the border of acceptability criteria, due to large errors within some trials, particularly for very stable and unstable atmospheric conditions and in case of very low wind speed. On the other hand, logarithmic measures compensate this trend, weighting extremely high errors.

Table 1
Comparison between PANACHE and ALOHA predictions within the Prairie Grass field experiment, using the statistical method suggested by Hanna and Chang (2001)

	FAC2	FB	NMSE	MG	VG
ALOHA	0.76	0.34	1.98	1.24	2.08
PANACHE	0.86	−0.03	0.23	0.93	1.49

4.2. Kit Fox

The Kit Fox experiment was carried out in summer 1995 at the US-DOE Nevada test site. A desert surface was artificially roughened using a combination of flat billboard obstacles in order to simulate the roughness of an industrial site and its surroundings at about 1/10 scale (Hanna and Chang, 2001). Pure gaseous CO_2 was released at ground level from a 1.5 m × 1.5 m square source placed near the middle of the obstacle array, for 2–5 min periods (continuous "plume") or for 20 s periods (transient "puffs"), including both neutral and stable atmospheric conditions.

Combinations of two types of flat "bill-board" shaped plywood obstacle arrays were used – the larger ERP (Equivalent Roughness Pattern) array (with height 2.4 m and installed in the inner 39 m × 85 m rectangle) and the smaller URA (Uniform Roughness Array) array (with height 0.2 m, in the outer 120 m × 314 m rectangle). The domain height for the Kit Fox trials was 100 m. Fig. 3 shows the arrangement of the test field as simulated by PANACHE (the URA obstacles array was substituted by an homogeneous

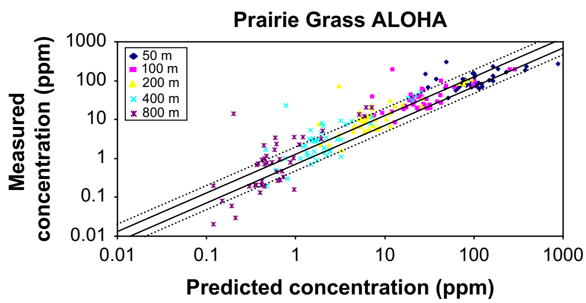

Fig. 2. ALOHA 5.4 predictions against observations for the Prairie Grass trials.

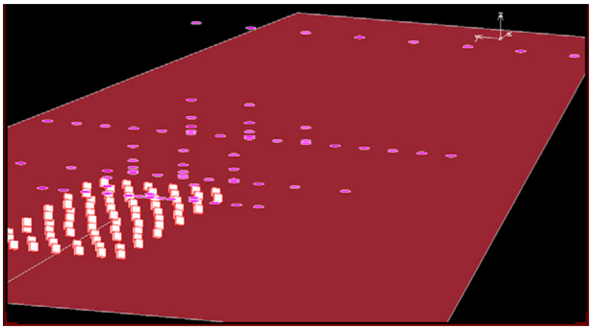

Fig. 3. Location of obstacles for the Kit Fox experiment: plot generated by PANACHE. White obstacles represent the URP array of 2.4 m high billboards, the red ground represents an urban area with a $z_0 = 0.01$ m. Purple dots are monitor points at different heights. (For interpretation of colour in the figure legend, the reader is referred to the web version of the article.)

urban area with average building height of 0.2 m, in order to have a surface roughness length z_0 between 0.01 and 0.02 m, as prescribed by Hanna and Chang, 2001). Eighty-four fast-response (one reading per second) concentration monitors were installed on the four downwind arcs (25, 50, 100 and 225 m), together with five meteorological towers recording wind speed and direction data each second[2] (WRI, 1998). There were a total of 52 release experiments, split into four sets for the statistical analysis: 6 ERP trials (with ERP and URA arrays present) with "plume" release (duration of 120 s or greater), 13 ERP trials with "puff" releases (duration 20 or 25 s), 12 URA trials (with only URA array installed) with "plume" releases and 21 URA trials with "puff" releases.

4.2.1. Discussion of results

Within PANACHE, the *k–l* model was used exclusively for evaluation of turbulence generation and dissipation. It performed slightly better than the *k–ε* model, the latter tending to under-estimate gas concentration to a larger extent at each arc.

Predicted values from PANACHE were compared with observations using Eqs. (14)–(18), as for the Prairie Grass trials. Table 2 shows the performance measures for the four sets of trials of the Kit Fox experiment, and Fig. 4 is a graphical display of results.

In terms of parameters ranges (outlined in Section 3, above) the model overall results show an average under-prediction which is particularly evident for continuous release trials. This tendency is justifiable keeping in mind that simulations were carried out using constant values for wind speed and direction, taking the average value of quotes recorded each second at the test field (Hanna and Chang, 2001). CO_2 is about 1.5 times denser than air ($\rho_{CO_2} = 1.8\ \mathrm{kg\ m^{-3}}$) and less viscous (Oldenburg and Unger, 2004), these differences keep the gas from mixing with the ambient air as much as a passive or buoyant pollutant would. Thus, the effect of a non-homogeneous wind on the gas dispersion could be seen as a differentiated impulse on diverse parts of the moving puff/plume, leading to an irregular concentration pattern within the cloud – the gas accumulating randomly inside the plume. Over the Kit Fox experiment, this is particularly evident for the trials with ERP obstacles present, the wakes behind the latter acting as preferential accumulation sites for the gas. The master dataset (WRI, 1998) reports that wind speed and direction values varied significantly during each experiment, by up to 5 m s^{-1} and 20° respectively, within a few seconds. It also reports cloud concentration values varying by up to 30,000 ppm in just one second (this is mainly true for the continuous release trials). Fig. 5 is a comparison of concentration values recorded by the monitor that read the highest concentration (P1911) with values calculated by PANACHE, during a Kit Fox trial (KF0404). From a risk analysis point of view predicted concentration values give a measure of the hazard affecting a person, hypothetically present – for CO_2 dispersion, this is dose of potentially inhaled gas over a certain time span. PANACHE gave a strong under-prediction for this trial (i.e. ~70%) but, as it is clearly shown in Fig. 5, the peak of MAX observed concentration represents an outstanding value, occurring naturally but diverging from the mean gas concentration. This maximum value could be used as a parameter for model performance evaluation but only as an upper limit. Models using constant wind parameters (i.e. giving fairly constant concentration predictions) would overestimate the overall hazard when used for risk assessment in the field of CO_2 transportation, if forecasting values higher than the short-term maximum. The authors suggest minimum ranges for model performance acceptability be adjusted to (e.g.): $0 < FB < 0.5$ and $1 < MG < 2$, when they are to be used in the field of risk assessment for CO_2 transportation.

The model PANACHE performed well for each of the four sets of trials, with a relative mean bias less than ±30% and a relative scatter of 60% or less. About 90% of predictions are within a factor of two of observations and the average

Table 2
Comparison between PANACHE and ALOHA predictions within the Kit Fox field experiment

	N	FAC2	FB	NMSE	MG	VG
ALOHA	18	0.76	0.16	0.76	1.26	2.91
PANACHE	52	0.89	0.3	0.32	1.3	1.29

Simulations from ALOHA only for continuous release trials.

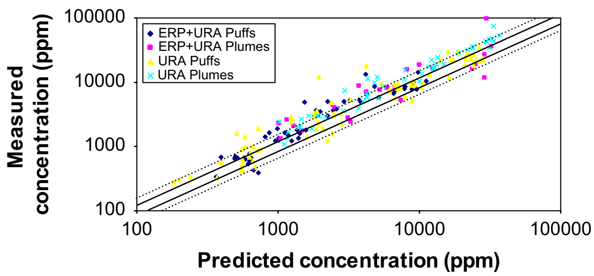

Fig. 4. PANACHE predicted against observed concentrations, different symbols represent results from different sets of trials.

[2] Within PANACHE simulations, only 77 monitor points have been used, the ones installed on MET towers in the real scenario were not present during computer simulations, as MET towers themselves.

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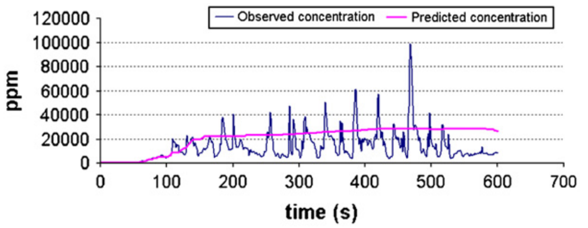

Fig. 5. Kit Fox trial KF0404. Concentration values read each second during the first 10 min of the trials at monitor point P1911 ($x = 25$ m) against values calculated by PANACHE.

under-prediction of gas concentration over the dataset is caused by the over-simplification induced by the use of an average value for wind speed and direction. There is little trend with atmospheric stability or downwind distance, while data suggest the best predictions to be at higher average values of wind speed – WRI (1998) reports less wind speed and direction variations within trials with higher average values.

The CFD model has been compared with predictions from the dense gas algorithm of ALOHA 5.4. As it can be seen from Table 2, the Gaussian model performed well. Good performance was also achieved for the Kit Fox trials, although there are some limitations within simulations set-up. The minimum release duration computed by ALOHA is 1 min, so that the puff releases (20 s duration) could not be modelled. ALOHA can account for only one surface roughness per scenario, so that for the ERP + URA continuous releases the simulations have been worked out with the ERP value for z_0 taken as constant over the domain. Moreover, ALOHA can account for continuous releases only from point sources, thus, the 1.5 m side square ground source effect could not be evaluated within the trials.

Nevertheless, its results are well within the range for model acceptability.

4.3. Cloud travel speeds V_e

Cloud travel speeds V_e were estimated for all Kit Fox trials, at all the arcs. Speeds were assumed to equal monitoring arc distance divided by time of travel, from the source to the monitor points that recorded maximum concentrations at each of the four distances. The values reported in Table 3 are ratios of predicted against observed speeds (m s^{-1}). Speed was calculated using the arc distance from the source divided by the first arrival time of the 50% MAX concentration of the cloud, at the monitor point where the maximum concentration was recorded for the particular arc, both for observed and predicted concentrations. As described in the previous paragraph, the maximum concentration values of the cloud are the product of random accumulation of the heavy gas: using the first arrival of the 50% MAX concentration for speed estimation makes clear that what is calculated is the velocity of the arriving, thickening cloud, regardless of the short-term concentration fluctuations. This technique is suggested by Hanna and Chang (2001).

Table 3
Ratios between predicted against observed cloud speed values (m s^{-1}) for the different trials, recorded at each of the four arcs within PANACHE

	25 m	50 m	100 m	225 m
ERP puff	0.71	0.86	1.15	0.84
ERP cont.	0.91	0.82	1.25	0.94
URA puff	1.1	0.85	1.57	1.06
URA cont.	0.7	0.53	1.13	0.74

As observed during the experiment (Hanna and Chang, 2001), due to the vertical dispersion of the cloud as it moves downwind from the 25 m arc to the 225 m arc, the puffs/plumes were seen to accelerate by a factor of up to three or four. This is due to the cloud being brought under the influence of higher wind speeds at greater heights. PANACHE gave estimations of cloud speed with an average error of about 20% (Table 3), accounting for its acceleration further downwind (i.e. there is no evident discrepancy of speed ratios among the four arcs, for any of the subset). From the values reported in Table 3, no particular trend for the predicted velocity can be seen – accounting for presence/absence of obstacles and puff/plume releases.

5. Conclusions

The modelling software Fluidyn PANACHE has been evaluated against the Prairie Grass and Kit Fox field experiments, involving about 100 trials. The statistical model performance evaluation method suggested by Hanna and Chang (2001) for the evaluation of atmospheric modelling software has been applied to the results: outcomes put the model performances well inside the limits of acceptability for atmospheric dispersion software. The average under-prediction of results within Kit Fox trials is due to the extreme short-term variation in wind speed and direction during the field experiment. It is evident that CFD models may only under-predict results. Not accounting for processes leading to the generation of highly differentiated gas concentration in clouds over time and space, CFD tools give an accurate description of average gas concentration omitting the naturally occurring short-term concentration peaks. The authors suggest accounting for this issue when evaluating a CFD model to be used in the analysis of risk posed by gases for which exposure is a parameter of concern (e.g. CO_2).

Fluidyn PANACHE is a CFD tool, developed solely for the purpose of atmospheric dispersion modelling and its relative ease of use makes it a good choice for future CO_2 dispersion modelling in hazardous locations. The only difficulty may be the choice of the turbulence prediction model for different atmospheric stability conditions: this paper may be of advantage for PANACHE users when dealing with this issue.

The model performances have been compared with the results of a Gaussian plume dispersion model (ALOHA 5.4). The latter also gave fairly good results. The basic knowledge needed for setting up model runs and the short computation times give these models priority over all other dispersion tools in accident situations, when rapid responses are required for starting emergency procedures or alerting rescue teams.

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