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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).