5.11 FLACS CFD MODEL EVALUATION WITH KIT FOX, MUST, PRAIRIE GRASS, AND EMU L-SHAPED BUILDING DATA

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INTRODUCTION AND FLACS MODEL SUMMARY

Computational Fluid Dynamics (CFD) models are useful for simulating air flow and plume transport and dispersion within arrays of obstacles such as buildings or pipe racks and tanks. The FLACS CFD model (*Hansen, O. et al., 1999*) is being used by the authors to estimate flow and dispersion in the atmosphere around chemical processing plants. This paper contains the results of recent evaluations of FLACS with extensive field observations involving tracer gas releases in three independent field experiments (Kit Fox, MUST, and Prairie Grass) and wind tunnel data from the EMU L-shaped building.

FLACS started in 1980 as a result of an increasing focus on gas explosion hazards in the evolving oil and gas exploration in the North Sea (*Hansen, O. et al. 1999 and 2001*). Since the late 1990s, the model's dispersion capabilities have been improved, so that realistic gas cloud build-ups from leaks could be simulated. The physics of liquid particles (aerosols or sprays) have been recently included (*Hansen,O., 2003*), and currently there is a European Union - supported program to develop a dust explosion simulator based on FLACS. A distributed porosity concept is used in FLACS, where all objects are mapped to the grid using porosities (opposite of blockages). This concept was developed with the requirement that repeatable results should be obtained when changing the grid size, translating the grid, and other geometric modifications. Atmospheric boundary layer turbulence inputs to the FLACS model have also been recently improved. FLACS can parameterize the turbulence parameters based on input of Pasquill stability class or based on the Monin-Obukhov similarity theory for atmospheric boundary layers. Periodic fluctuations in wind direction have been further parameterized by imposing two sinusoidal periods (about 10-15 s and about 60-70 s).

Most FLACS model runs presented in this study were carried out in 2 to12 hours of simulation time on an ordinary PC, where the typical simulated experimental time was of the order 10 to 20 minutes. The strength of the porosity concept is that simulations are not slowed down as a result of increasing the level of detail in the geometry model.

MODEL PERFORMANCE EVALUATION METHODS

The statistical model performance approach used in the current paper is based on a methodology often discussed at previous Harmonization Conferences and described by *Hanna, S. et al. (1993)* and summarized by *Chang, J. and S. Hanna (2003)*. Because of interest in the model's ability to simulate the absolute maximum concentration, Max C, on the monitoring network during each experiment run, comparisons of the predicted and observed Max C are made. In addition, several statistical performance measures are calculated, including 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 factor of two of observations (FAC2):

$$FB = \frac{\left(\overline{C_o} - \overline{C_p}\right)}{0.5\ \left(\overline{C_o} + \overline{C_p}\right)} \quad (1) \qquad MG = \exp\ \left(\overline{\ln C_o} - \overline{\ln C_p}\right) \quad (2)$$

$$NMSE = \frac{\overline{\left(C_o - C_p\right)^2}}{\overline{C_o}\ \overline{C_p}} \quad (3) \qquad VG = \exp\ \left[\overline{\left(\ln C_o - \ln C_p\right)^2}\right] \quad (4)$$

$$FAC2 = \text{fraction of data that satisfy } 0.5 \le \frac{C_p}{C_o} \le 2.0 \quad (5)$$

where

C_p: model predictions of concentration,

C_o: observations of concentration,

overbar ($\overline{C}$): average over the dataset, and

The evaluations using equations (1) through (5) focus on the maximum concentration observed and predicted on a given arc during a given experimental trial. For the EMU L-shaped building (Hall, 1997), where there are not well-defined monitoring arcs, the evaluations focus on observed and predicted concentrations, paired in space and time, at several monitor locations

Based on extensive experience with evaluating many models with many field data sets, Chang and Hanna (2003) suggest that "acceptable" performing models have the following typical performance measures at research-grade experiments: FAC2 > 0.5, –0.3 < FB < 0.3 (or 0.7 < MG < 1.3), and NMSE < 4 (or VG < 1.6).

RESULTS OF EVALUATIONS

The major interest was on field experiments involving obstacles. For this reason, the MUST (*Biltoft, C., 2001*) and Kit Fox (*Hanna, S. and J. Chang, 2001*) experiments were chosen. Also, because of concerns about CFD models' abilities to maintain the proper atmospheric turbulence levels over an open field in the absence of buildings, the well-known Prairie Grass field experiment (*Barad, M., 1958*) is included. Finally, to demonstrate the FLACS model's capabilities at close distances from a single building, the EMU L-shaped building data set (*Hall, R.C., 1997*) is used.

MUST The Mock Urban Setting Test (MUST) field experiment consisted of 37 releases of propylene tracer gas in an array of 120 obstacles at the Dugway Proving Ground desert site (*Biltoft, C., 2001*). The obstacles were shipping containers with dimensions 12.2 m long by 2.42 m wide by 2.54 m high (see Figure 1). The release locations were altered slightly from trial to trial, but were always near the first three rows of obstacles in the foreground. There were four sets of downwind monitoring arrays (at downwind distances of about 25, 60, 95, and 120 m), and the maximum observed and predicted concentrations on each array were compared. It is found that there is an approximate factor of two under prediction for Max C and about a 35 % under prediction on average. The relative scatter is about 1.5 times the mean. 64 % of the predictions are within a factor of two of the observations. These numbers are within the range of acceptable model performance.

Kit Fox The Kit Fox field experiment took place at the Nevada Test Site, where two types of "billboard" obstacle arrays were used – the larger ERP array with height 2.4 m, and the smaller URA array with height 0.2 m (*Hanna, S. and J. Chang, 2001*). There was a total of 52 experiments: 6 ERP trials with "plume" releases (duration of 120 s or greater), 13 ERP trials with "puff" releases (duration of 20 or 25 s), 12 URA trials with "plume" releases, and 21 URA trials with "puff" releases. CO_2 gas was released at ground level from a 1.5 by 1.5 m square opening near the middle of the obstacle array. In all experiments, the maximum observed and predicted concentrations on each of the four monitoring arcs (at 25, 50, 100, and 225 m) were evaluated. The FLACS model performs quite well, with a relative mean bias less than ± 20 % and a relative scatter of 50 % or less. Over 90 % of the model predictions are within a factor of two of observations.

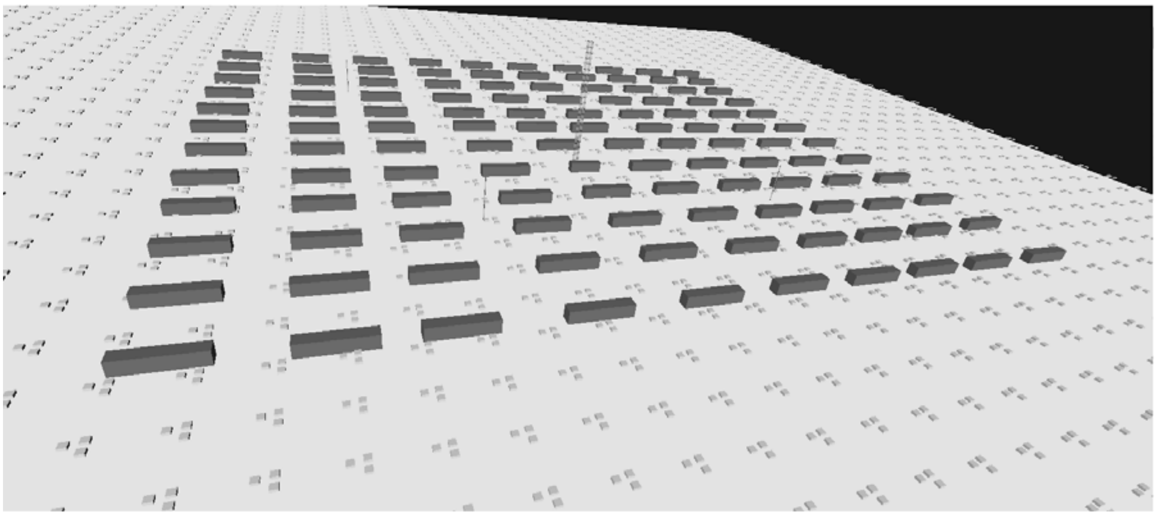

Figure 1. Locations of 120 obstacles (2.54 m high) in MUST experiment (from Biltoft, 2001). The obstacles are 2.54 m high. The numerous groups of three smaller obstacles represent bushes. Tracer gas was released from locations between the first and third rows in the foreground. Four monitoring "arcs" were between rows 3 and 4, 5 and 6, 7 and 8, and 9 and 10, at downwind distances averaging about 25, 60, 95, and 120 m.

Prairie Grass The Prairie Grass field experiment (*Barad, M., 1958*) has become the standard data base used for evaluation of models for continuous plume releases near the ground over flat terrain. The site consisted of an agricultural field where the grass had been cut. A continuous trace amount of neutrally-buoyant gas was released from a small tube at a height of 0.46 m. There were 43 trials in a variety of stability conditions. In all experiments, the maximum observed and predicted concentrations were evaluated at a height of 1.5 m on each of the five monitoring arcs (at 50, 100, 200, 400, and 800 m). FLACS shows a slight (20 %) average under prediction, with a relative scatter averaging about 70 % to a factor of two.

EMU L-shaped building wind tunnel experiment The Evaluation of Model Uncertainty (EMU) study involved a comprehensive evaluation of models in a European Commission – sponsored study described by *Hall, R. (1997)*. The current evaluation used only one of the EMU scenarios – a single L-shaped building located on a flat surface. Neutral ambient conditions were assumed and a continuous release of neutrally-buoyant gas took place from a "courtyard" door. Predicted concentrations at a few cross-wind locations on the cross-section at a distance H downwind of the lee edge of the L-shaped building were compared with the wind tunnel observations. Concentrations at 36 locations are compared (at y/H = -2.0, -1.5, -1.0, -0.5, 0.0, and 0.5; and at z/H = 0.16, 0.37, 0.67, 1.02, 1.47, and 1.99). Figure 2 shows the scatter plot of the data, indicating the good agreement but the slight under prediction tendency. In general 72 % of the predictions are within a factor of two of the observations and the cross-wind and vertical profiles were well-simulated. The median value of C_o/C_p is 1.55, implying about a 35 % under prediction. In addition, the dimensions of the predicted recirculation cavities are in agreement (± 50%) with known similarity relations based on wind-tunnel observations (*Hanna, S. et al., 1982*), where it is suggested that the length of the recirculation wake or cavity in the lee of the L-shaped building is about 1.0 to 1.5 times H, whereas the FLACS prediction for this length is about 1.5 to 2.0

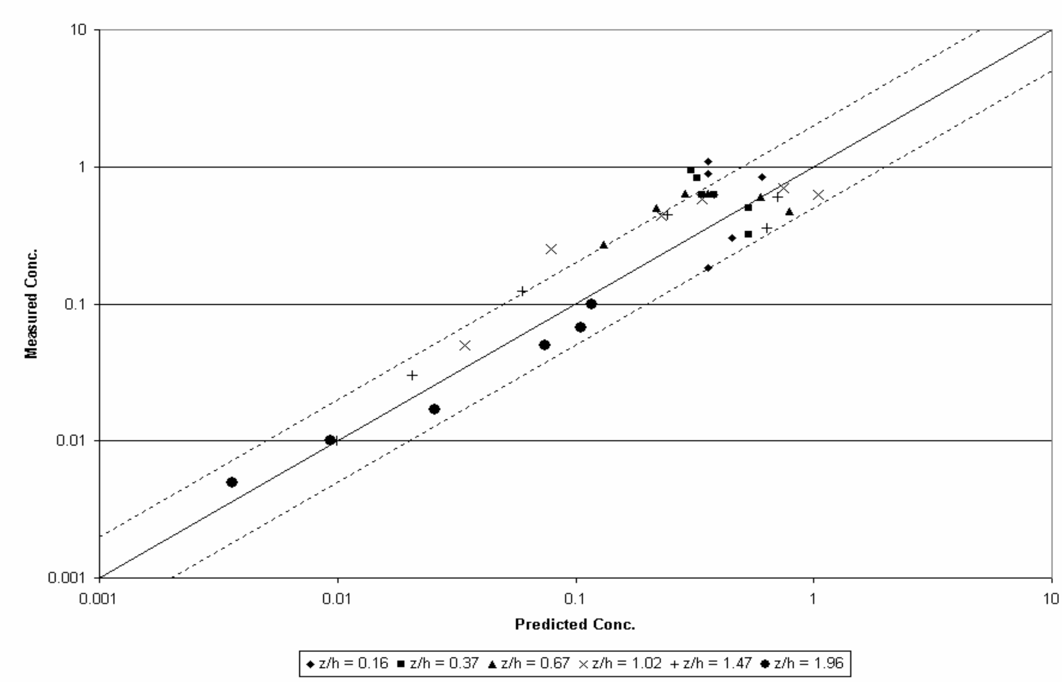

Figure 2. Scatter plot of FLACS predicted concentrations versus observed concentrations for EMU L-shaped building, at a distance of one building height, h, downwind of the lee of the building, for six different heights and six different lateral positions.

CONCLUSIONS

Table 1 contains a summary of the performance measures for the FLACS model applied to the MUST, Kit Fox, and Prairie Grass field experiment data. The medians and ranges of the statistics were determined from the 25 sets of ranked numbers (4 arcs for MUST, 4 subsets of trials times 4 arcs = 16 arcs for Kit Fox, and 5 arcs for Prairie Grass). The medians for the max C_o/max C_p, FB, and MG suggest a general under prediction tendency of about 20 %. The medians for NMSE and VG suggest a relative scatter of about 50 %. About 86 % of the predictions are within a factor of two of the observations. The table also contains estimates of the range of the 25 ranked numbers.

Table 1. Median performance measures and range over Kit Fox, MUST, and Prairie Grass field experiments for FLACS CFD model.

	Median	Range
Max C_o/Max C_p	1.22	0.56 to 2.56
FB	0.18	-0.32 to 0.60
NMSE	0.29	0.07 to 2.03
MG	1.32	0.35 to 2.63
VG	1.28	1.07 to 17.9
FAC2	0.86	0.47 to 1.00

In addition, FLACS was evaluated with the wind tunnel observations of the EMU L-shaped building, showing that about 72 % of the predictions are within a factor of two of the observations, and that there is a tendency towards under prediction by about 35 %. The predicted dimensions of the recirculation cavity behind the building are within 50% of the known size of the cavity.

The performance of the FLACS model is well within the criteria for model acceptance, since about 86 % of the predictions are within a factor of two of the observations, the relative mean bias is about 20 % from the perspective of FB and about 30 % from the perspective of MG, and the relative scatter is about 50 or 60 %. The FLACS performance measures are consistent across the experiments.

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REFERENCES

Barad, M.L. (ed.), 1958. Project Prairie Grass. A field program in diffusion. Geophys. Res. Paper No. 59, Vols I and II, AFCRF-TR-58-235, Air Force Cambridge research Center, Bedford, MA.

Biltoft, C.A., 2001. Customer report for Mock Urban Setting Test (MUST). DPG Doc. No. WDTC-FR-01-121, West Desert Test Center, U.S. Army Dugway Proving Ground, Dugway, UT 84022-5000.

Chang, J.C. and S.R. Hanna, 2003. Air quality model performance evaluation. To appear in *Meteorol. Atmos. Phys.*

Hall, R.C. (ed.), 1997. Evaluation of Model Uncertainty (EMU) – CFD modelling of near-field atmospheric dispersion. Project EMU final report to the European Commission (Data CD also available with report) WS Atkins Doc No. WSA/AM5017/R7, WS Atkins, Woodcote Grove, Ashley Road, Epsom, Surrey KT18 5BW, UK.

Hanna, S.R., G.A. Briggs and R.P. Hosker, 1982. Handbook on atmospheric diffusion. DOE/TIC-11223 (DE82-002045). NTIS/USDOC, Springfield, VA

Hanna, S.R. and J. Chang, 2001. Use of the Kit Fox field data to analyze dense gas modelling issues. *Atmos. Environ*. 35, 2231-2242.

Hansen, O.R., 2003. Water deluge and influence on dispersion. FABIG Newsletter Art R485

Hansen, O.R., J. Renoult and J.R. Bakke, 2001. Explosion risk assessment, how the results vary with the approach chosen, Fall Symposium Proceedings, Mary Kay O' Connor Process Safety Centre, October 30-31, Texas USA, 395-410.

Hansen, O.R., I. Storvik and K. van Wingerden, 1999: Validation of CFD-models for gas explosions, FLACS is used as example. Model description, experiences and recommendations for model evaluation", Proceedings European Meeting on Chemical Industry and Environment III, Krakow, Poland, September 1999, 365-382.