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EVALUATION OF FLACS CFD MODEL WITH MUST DATA

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1. INTRODUCTION

The FLACS (FLame ACceleration Simulator) model is a CFD model that is applied in this paper to simulate flow and dispersion of hazardous gases around obstacle arrays in the atmosphere. Results of its evaluation with the Mock Urban Setting Test (MUST) data are shown. The MUST experiment involved 120 shipping containers (2.4 m wide by 2.5 m high by 12.2 m long) installed in a rectangular array on the desert floor at Dugway Proving Ground, Utah (Biltoft, 2001). There were 37 tracer release trials analyzed, with monitors on four downwind arcs within the array.

CFD models are especially useful when the plume is dispersing within arrays of obstacles such as buildings in urban areas or industrial areas, which also can have many pipe racks, tanks, and other types of obstacles. Some CFD models are being run for specific urban building domains with links to urban neighborhood models and further links to mesoscale meteorological models (e.g., Brown et al., 2001). The FLACS CFD model is similar to many other CFD models but has a different approach in its use of a distributed porosity approach for parameterizing buildings and other obstacles. The porosity of a grid is represented as a fractional coverage of each grid volume and each grid face with sub-grid obstacles. Turbulence production terms are parameterized for sub-grid objects (Arntzen 1998). In the current paper, FLACS is evaluated with extensive field observations involving tracer gas releases in the MUST field experiment.

2. DESCRIPTION OF FLACS

FLACS was developed in the early 1980s to simulate the initial dispersion of gas leaks and subsequent explosions in offshore oil and gas production platforms. The conservation equations for mass, momentum, and enthalpy, in addition to conservation equations for concentration and for flammable gas effects, are solved on a Cartesian grid using a finite volume method. The equations are closed using the k-ε equations for turbulence. Hjertager (1985, 1986) describes the basic equations used in the FLACS model, and Hjertager (1988a, 1988b) present the results of several laboratory and field experiments used in the development of FLACS.

Because accidental explosions around oil platforms are normally preceded by the release and subsequent dispersion of flammable materials in the atmosphere in and around the platform, the FLACS CFD model contains algorithms for calculating the initial dispersion of flammable gas. The use of CFD models to calculate dispersion is widespread in explosion quantitative risk assessments (Hansen et al. 1999), and is required by industry standards in certain countries (NORSOK, 2001).

The proper representation of the obstacles was a key aspect of the development of the FLACS code. A so-called distributed porosity concept was developed, as a compromise between the need to characterize the geometric details and the need to have the code run in a reasonable time. Obstacles such as structures and pipes are represented as area porosities (the opposite of blockages) on Control Volume (CV) faces, and are represented as volume porosities in the interior of the CV. Each CV surface or each CV volume is either fully open, fully blocked or partly blocked. For the partly blocked surfaces or volumes, the porosity is defined as the fraction of the area/volume that is available for fluid flow. The resulting porosity model is used to calculate the flow resistance terms, the turbulence source terms from small objects, and the flame speed enhancement due to flame folding in the sub-grid wake. In FLACS, different drag coefficients are used for cylindrical and rectangular sub-grid objects, and significant drag and turbulence are generated only behind an object, and not along an object that partly blocks a CV. To handle all of these conditions within the porosity algorithm in FLACS, ten coefficients are calculated for each control volume. A comprehensive description of this concept is given in Hjertager (1985, 1986) and Arntzen (1998).

For the flow scenarios described in this paper, an important consideration is the drag formulation from the partly porous objects and the modeled turbulence production behind objects classified as sub-grid. For the smallest objects, the flow kinetic energy lost due to the drag is directly added as a production term for turbulent energy. With increased size of the sub-grid object relative to the grid size, the sub-grid turbulence production is gradually decreased. Objects with a

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dimension of 1.5-2.0 CVs (where the exact limit depends on position on grid) in both cross-flow directions are defined to be on-grid objects. For these objects, there is no sub-grid turbulence production, since the shear layers handle the turbulent production.

Modifications to the standard k-ε model that have been implemented in FLACS are described in detail by Hanna et al. (2004). In addition, it has been necessary to include algorithms that account for the effects of stability and for the effects of relatively low-frequency lateral meandering flow. Previously, a logarithmic stationary wind profile with a specific turbulence intensity and length scale was specified. This would typically lead to an over-prediction of the hazard distance (i.e., an over-prediction of concentrations) from a gas release, because the simulated atmospheric boundary layer turbulence was underestimated. Hanna et al. (2002) and Riddle et al. (2004) report similar results (i.e., underestimation of turbulence) with other CFD models. Using a method suggested by Han et al. (2000), FLACS was modified to estimate the turbulent kinetic energy and dissipation rate based on input of Pasquill stability class (from unstable A to stable F) or input of Monin-Obukhov length L.

It would be useful to account for the fact that the wind speed and direction in the atmospheric boundary layer vary with time and space over a continuous spectrum. Typical turbulence parameterizations in CFD models are primarily based on engineering approximations of sub-grid turbulence and may not be able to represent atmospheric eddies (fluctuations) with periods of 10s to 100s of seconds or more (the larger periods are associated with the so-called meandering flow field). If a CFD model does not satisfactorily account for the larger range of atmospheric eddies, it may therefore under-predict turbulence levels and consequently over-predict hazard distances. To better approximate the wide range of atmospheric eddy sizes in the version of FLACS used here, preliminary approximations of larger eddies with periods from 10 to 100 seconds have been implemented. In the current method, two harmonic waves with periods 10-15 s (slightly different for the three directions to avoid repetition) and 60-70 s (only for the two horizontal directions and also slightly different to avoid repetition) have been chosen to approximate the meandering flow. Based on standard assumptions in Arya (2001), the total magnitude of these velocity fluctuations is 2.4, 1.9 and 1.3 times the friction velocity, u*, in the along wind, cross wind, and vertical directions, respectively.

It was concluded from previous studies that the diameter of the cloud after expansion to ambient pressure must be resolved by at least 1 CV to obtain good results. For the MUST field data, described later, the small initial source diameter (about 1 cm) and the relatively large domains (about 100 to 1000 m) made it more difficult to follow this guidance, and much coarser grids than normally used were applied to ensure acceptable simulation times. Consequently, we have to accept the fact that the gas in the CVs near the source will be too dilute.

The question can be asked, if the FLACS system relies on high-resolution (e.g., 1 m resolution) geometric data to calculate the porosity values, will there be problems in urban areas because the data for large numbers of buildings are not sufficiently detailed? It is important to note that FLACS can use whatever data are available to approximate the porosity using empirical assumptions. If for instance, data on the smaller obstacles are lacking, an artificial congestion or porosity can be assumed. This method was used in the MUST runs described later, where sagebrush (0.40 m tall and shaped like wide porous boxes near the ground) was added to the domain. It was found that the small sagebrush obstacles did not significantly influence the results, since the MUST obstacles were much larger (about 2.5 m tall and 2.4 m wide and 12.2 m long) and there were 120 of them.

As for all numerical models, the run times for FLACS are roughly proportional to the number of grid cells times the number of seconds simulated times the number of time steps each second. The grids have been made relatively coarse in the current study, as the goal was to obtain relatively quick results. Within a few days, 40 or 50 tracer release trials in a field experiment could be simulated, with about ten 1 GHz Pentium 3 PCs available. The number of time steps each second depends on the time step criteria (i.e. the CFL number), the finest grid size, and the wind speed. If the grid is refined locally, then shorter time steps may be needed to satisfy the CFL criteria. For MUST, where the grid used for calculations contained 55,000-75,000 CVs and where there was 500 seconds of simulated time, the typical elapsed time on the PC for one run is six to ten hours (one case 15 hours).

The initialization of the wind field consumes a relatively small amount of time (about 10-50 seconds). The assumed initial wind field has a logarithmic mean wind profile at the upwind boundary, and subgrid plus larger turbulence components, as described earlier. Then, due to the generation of flows and turbulence by the presence of the obstacles, typically about 10-30 seconds are needed for the flow to adjust around the obstacles. The presence of obstacles will not significantly increase the requirement for simulation time for a given grid, because of the efficiencies offered by the sub-grid porosity assumption.

3. DESCRIPTION OF STATISTICAL MODEL PERFORMANCE EVALUATION METHODS

The FLACS model is evaluated following the approaches for model performance measures for air quality models suggested by Hanna *et al.* (1993) and summarized by Chang and Hanna (2004). The evaluations in this paper concern the 37 “continuous release” experiments during MUST (Biltoft, 2001). There were 48 tracer samplers or monitors installed on arcs at three specific downwind distances and on vertical towers. The emphasis here is on the 40 near-surface monitors and the data from the 8 monitors on the vertical towers are not analyzed. The evaluations in this paper focus on two outputs:

1) The maximum 60-sec average concentration observed and predicted on a given arc (i.e., unpaired in space at an arc distance) during a given experimental trial. Note that the location of the monitor with the observed maximum is not necessarily the same as the location of the monitor with the predicted maximum. The use of maximum concentrations on arcs for the model evaluation exercise is fairly standard for evaluations of dispersion models and field experiments in open terrain. Even though the MUST experiments involve obstacle arrays and tracer releases at heights less than the obstacle heights, the monitoring arcs were set up at distances beyond a few rows of obstacles. Consequently, for these experiments, the flow and dispersion around individual obstacles is not being investigated, and it is felt that the arc-maximum concentrations are appropriate for evaluation. However, the main use of a CFD model, and where it has advantages over more standard models such as Gaussian plume models or Lagrangian puff models, is to provide detailed three-dimensional, time dependent information in the area near (within one obstacle height) of the obstacle. Future evaluations of CFD models should focus more on the identification of important model outputs and development of methods to evaluate CFD models near obstacles.

2) The maximum 60-sec average concentration observed and predicted at each of the 40 monitors (i.e., paired in space) during a given experimental trial. This is a more stringent comparison than the unpaired comparison in number (1) above, since a slight (e.g., 10 degree) difference between the observed and predicted plume direction can cause major differences between predicted and observed concentrations at a given monitor location (Weil et al., 1992).

The following equations define the statistical performance measures that were used, 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 factor of two of observations (FAC2):

$$\mathrm{FB} = \frac{\left(\overline{C_o} - \overline{C_p}\right)}{0.5\ \left(\overline{C_o} + \overline{C_p}\right)} \qquad (1)$$

$$\mathrm{MG} = \exp\ \left(\overline{\ln C_o} - \overline{\ln C_p}\right) \qquad (2)$$

$$\mathrm{NMSE} = \frac{\overline{\left(C_o - C_p\right)^2}}{\overline{C_o}\ \overline{C_p}} \qquad (3)$$

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

FAC2 = Fraction of predictions that are within a factor of two of observations (5)

where

C_p: model predictions of concentration,

C_o: observations of concentration,

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

σ_C: standard deviation over the dataset.

A perfect model would have MG, VG, and FAC2 = 1.0; and FB and NMSE = 0.0. Of course, because of the influence of random atmospheric processes, there is no such thing as a perfect model in air quality modeling. In addition to the standard performance measures defined above, which use data from a large number of experimental trials, the simple ratio of the overall maximum observed concentration to the overall maximum predicted concentration on each arc can be listed. These two maxima may occur during different experiment trials.

Typical magnitudes of the above performance measures and estimates of model acceptance criteria have been summarized by Chang and Hanna (2004) based on extensive experience with evaluating many models with many field data sets. It was concluded that, for comparisons of maxima concentrations on arcs (i.e., output (1) listed above), and for research-grade field experiments such as the MUST experiment, "acceptable" performing models have the following typical performance measures. The fraction of predictions within a factor of two of observations is at least 50% (i.e., FAC2 > 0.5). The mean bias is within ± 30% of the mean (i.e., $-0.3 < \mathrm{FB} < 0.3$ or $0.7 < \mathrm{MG} < 1.3$). The random scatter is about a factor of two of the mean (i.e., $\mathrm{NMSE} < 4$ or $\mathrm{VG} < 1.6$). However, these are not firm guidelines and it is necessary to consider all performance measures in making a decision concerning model acceptance. Since most of these criteria are based on research grade field experiments, model performance would be expected to deteriorate as the quality of the inputs decreases.

The results of the performance evaluations are given in the next section. Note that all performance measures are listed for output 1 (arc maxima), and only FAC2 is listed for output 2 (paired in space)

4. DESCRIPTION OF MUST DATA SET AND RESULTS OF EVALUATIONS

In order to demonstrate that a model is performing satisfactorily, it is best to evaluate the model using independent field experiments. Because the FLACS CFD model is intended for use at industrial sites and urban sites with numerous obstacles, such as buildings, storage tanks, and pipe racks, the focus should be on field experiments involving obstacles. For this reason, the Mock Urban Setting Test, or MUST (Biltoft, 2001) experiments were chosen. The MUST field experiment consisted of both continuous and puff releases of propylene tracer gas in an array of 120 obstacles at the Dugway Proving Ground desert site (Biltoft, 2001). The current paper concerns the 37 continuous release trials. The obstacles were shipping containers, which are about the size of the trailer in a tractor-trailer rig (12.2 m long by 2.42 m wide by 2.54 m high). Figure 1 shows the arrangement of the array of obstacles as simulated by FLACS. The wind speed assumed for each release trial was determined by averaging four wind observations at 6 m elevation near the corners of the obstacle array (only 2 or 3 were reported for each test). Average wind speed was 3 m/s and the wind direction generally blew from the foreground to the background of the array in Figure 1. The release locations were altered slightly from trial to trial, but were for most tests near the first three rows of obstacles (near the foreground of Figure 1). The first five tests had release location in the opposite end of the container array. There were four sets of downwind monitoring arrays (at downwind distances of about 25, 60, 95, and 120 m), and two types of comparisons were made – 1) the maximum observed and predicted 60-second average concentrations on each array, and 2) the observed and predicted 60-second average concentrations at each of the 40 monitor locations.

Table 1 summarizes the FLACS model performance for its predictions of maximum concentrations on each arc for the MUST obstacle experiments (i.e., the "unpaired in space" output (1) described above). The data in Table 1 suggests that there is an approximate factor of two under-prediction for Max C and about a 36% (i.e., (Mean C_o – Mean C_p)/C_o)) 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 or close to the range of acceptable model performance. There was little trend in model performance with downwind distance.

The FAC2 was calculated for each arc and experiment and for all 37 experiments for the "paired in space" output (2). Maximum 60-second average concentrations are compared at the 40 monitor locations. Table 2 provides an example of how FAC2 was calculated, using two of the 37 MUST experiments or runs (610731 and 610758). These experiments were selected because they show the large difference in FAC2 depending on whether the observed and predicted plume directions are close to each other or are different by 10 or 20 degrees. The observed plume direction is defined by the location of the maximum observed concentration on each distance arc, while the predicted plume direction is simulated by FLACS based on the observed wind directions on the four towers. Note that the four "arcs" are defined by monitors 1-12, 13-22, 23-30, and 31-40, respectively. For run 610731, the observed and predicted wind directions are different by about 20 degrees, leading to a very low FAC2 of 0.083. This is despite the fact that the unpaired arc maxima are predicted fairly well. For run 610758, the wind directions are lined up well, and the resulting FAC2 is much larger, 0.62. This phenomena has been pointed out by most persons evaluating dispersion models (e.g., Weil et al., 1992, and Chang and Hanna, 2004).

For all 37 experiments or runs and all monitors where either the observed or predicted concentration exceeds 0.2 ppm, the FAC2 equals 0.37 for the paired-in-space outputs. This value is almost half of the value (FAC2 = 0.62) found for the "unpaired-in-space" outputs described earlier. As pointed out earlier, the deterioration in FAC2 is due to the fact that sometimes observed and predicted wind directions are different by 10 degrees or more. The FAC2 values for the 37 experiments showed a wide range, from 0.0 to 0.83, with the 16th and 84th percentiles being 0.17 to 0.63. The extreme low value of FAC2 = 0.0 occurred in experiment 672003, when FLACS generally underpredicted the relatively high concentrations by an average factor of three or four. The extreme high value of FAC2 = 0.83 occurred in experiment 620246, where both the magnitude and the location of the predicted concentration lined up fairly well with the observed concentrations. These large variations in the FAC2 results for the 37 individual experiments in the "paired-in-space" outputs illustrate how it is important, in any model evaluation exercise with data, to have at least ten experiment trials, so that extreme results are averaged out and a better idea is obtained of overall model performance.

The evaluations reported in this paper suggest that FLACS is underpredicting, by a factor of two or more, the highest concentrations observed on the closest arc of MUST. Because the source aperture was relatively small (on the order of 1 cm), the FLACS simulation guidelines would require a much better grid resolution near the source than has been applied in the calculations reported in this paper. However, this increased resolution would have required very much longer simulation times on the PCs. The lack of local grid refinement may have been partly responsible for the slight underprediction tendency reported above. To improve the results, methods with local grid refinement near the source or analytical models for the initial plume development could be considered.

5. CONCLUSIONS

This paper describes the evaluation of the FLACS CFD model for transport and dispersion in obstacle arrays. The model was evaluated using the MUST data set and using quantitative performance measures, including the fractional bias (FB), the geometric mean (MG), the normalized mean square error (NMSE), the geometric variance (VG), and the fraction of data where predictions are within a factor of two of observations (FAC2). For the maximum concentration on an arc, FLACS is found to underpredict by about 36% on average. The relative scatter is about 1.5 times the mean. These numbers are mostly within the range of acceptable model performance. There was little trend in model performance with downwind distance.

The FAC2 performance measure (fraction of predictions within a factor of two of observations) is found to be 0.64 for the maximum concentrations on arcs, and was found to be 0.36 for the concentrations at all monitor locations (paired-in-space). As expected, the decrease in FAC2 for the paired-in-space comparisons is caused by slight differences (10 to 20 degrees) in predicted versus observed plume direction.

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Table

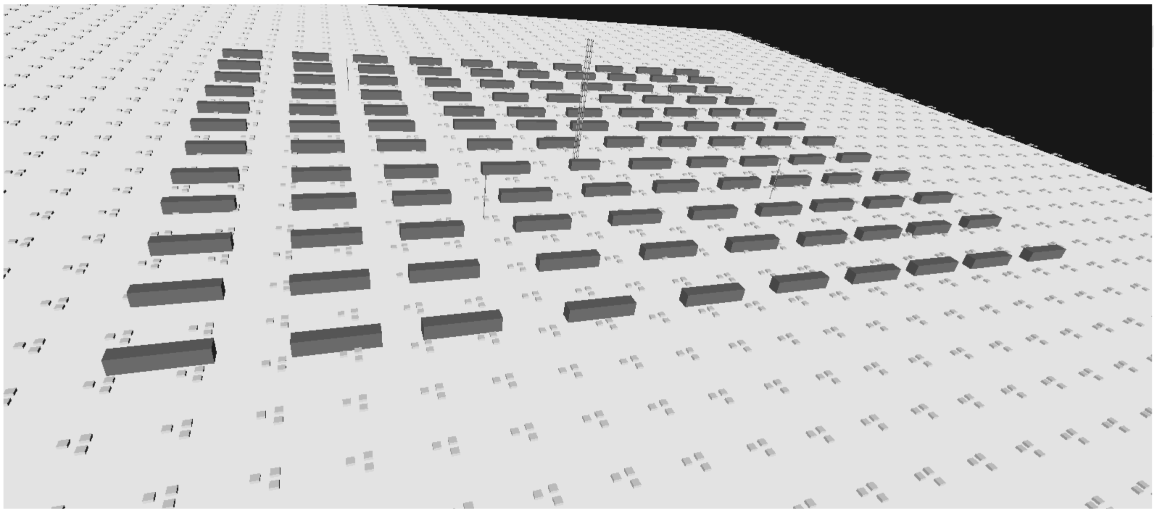

Figure 1. Locations of 120 obstacles in MUST experiment (described by Biltoft, 2001). This plot was generated by FLACS. The obstacles are 2.54 m high. The numerous groups of three smaller obstacles are intended to represent sagebrush and other bushes on the desert floor. Some towers are shown as vertical lines. The tracer gas was released from various locations between the first and third rows on the upwind (foreground) edge of the array. The four monitoring "arcs" were located between rows 3 and 4, rows 5 and 6, rows 7 and 8, and rows 9 and 10. Downwind distances of the arcs varied with release location but averaged about 25 m, 60 m, 95 m, and 120 m.

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Table 1. Performance measures for the 37 experiment trials in the MUST obstacle array, where maximum observed and predicted concentrations (in ppm) on four monitoring arcs are compared.

	Median over 4 arcs	Arc 1 25 m	Arc 2 60 m	Arc 3 95 m	Arc 4 120 m
Max C_o (ppm)		99.5	35.7	17.2	10.1
Max C_p (ppm)		47.2	13.9	7.73	10.0
Max C_o/Max C_p	2.15	2.08	2.56	2.22	1.01
Mean C_o (ppm)		25.5	8.9	5.5	4.2
Mean C_p (ppm)		14.6	5.3	3.0	3.7
FB	0.53	0.55	0.51	0.60	0.45
NMSE	1.64	2.03	1.85	1.44	1.24
MG	1.57	1.44	1.43	1.72	1.70
VG	1.69	1.71	1.44	1.67	2.65
FAC2	0.64	0.68	0.60	0.78	0.59

Table 2. Example of “paired in space” comparison of observed and predicted 60-s average concentrations (in ppm) for two (610731 and 610758) of the 37 MUST experiments. The predicted concentrations use the wind velocity information from the first several minutes of the experiment, while the observed concentrations represent the maximum 60-s average concentration during the entire experiment. The “FAC2 ?” column indicates whether (Y) or not (N) the predicted concentration is within a factor of two of the observed concentration, for cases where either concentration is 0.2 or larger. The four “arcs” are defined by monitors 1-12, 13-22, 23-30, and 31-40, respectively. The effect of wind direction differences can be seen, where the observed and predicted plumes are shifted in space for the data on the left, and are in approximate agreement for the data on the right.

	OBS RUN	PRED		OBS RUN	PRED	
MONITOR	610731	FLACS	FAC2 ?	610758	FLACS	FAC2 ?
1	0	0		0	0	
2	0	0		0	0	
3	0.092	0.02		0	0	
4	0.11	1.3	N	0	0.02	
5	1.259	5.21	N	0.241	1.14	N
6	8.175	22.69	N	15.344	20.9	Y
7	20.372	14.13	Y	23.923	26.47	Y
8	8.687	0.08	N	10.19	8.14	Y
9	22.593	0	N	4.685	2.32	N
10	14.063	0	N	0.1	0.04	
11	8.166	0	N	0.008	0.01	
12	1.875	0	N	0.001	0	
13	0	0.02		0	0	
14	0.136	0.3	N	0	0	
15	0.516	2.71	N	0	0	
16	3.582	11.87	N	0.124	0.12	
17	8.2	10	Y	4.682	2.58	Y
18	6.221	0.04	N	12.605	13.87	Y
19	1.209	0	N	7.535	8.05	Y
20	10.621	0	N	0.77	1.13	Y
21	9.245	0	N	0.063	0.11	
22	0.019	0.27	N	0	0	
23	0.199	1.74	N	0	0	
24	1.348	5.88	N	0	0	
25	5.268	4.64	Y	0.247	0.05	N
26	5.843	0.18	N	2.873	2.14	Y
27	0.946	0	N	5.992	7.73	Y
28	5.227	0	N	1.521	4.42	N
29	7.617	0	N	0.133	1.14	N
30	0	0		0	0.05	
31	0	0.6	N	0	0	
32	0.475	3.21	N	0	0	
33	1.732	5.07	N	0	0	
34	4.657	1.84	N	0	0.01	
35	4.873	0.47	N	0.139	0.1	
36	3.497	0.07	N	0.771	0.6	Y
37	0.505	0.01	N	2.524	2.06	Y
38	0.369	0	N	3.055	4.32	Y
39	1.813	0	N	1.782	4.99	N
40	5.531	0	N	0.032	2.46	N