DISPERSION MODEL VALIDATION ILLUSTRATING THE IMPORTANCE OF THE SOURCE TERM IN HAZARD ASSESSMENTS FROM EXPLOSIVE RELEASES

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Abstract: This paper validates the explosion module of the ADMS-STAR2 atmospheric dispersion model against deposition data from the Operation Roller Coaster Double Tracks and Clean Slate I trials. The dispersion models HPAC, Hotspot and DIFFAL have also been included in this study to compare and contrast with the ADMS-STAR2 code.

The models were compared against arc-wise maximum (maximum value along each arc) and arc deposition data for both the Double Tracks and Clean Slate I trials. They were run using varying complexities of meteorological data, terrain and land cover.

ADMS-STAR2 run with no knowledge of the particle size distribution under estimates the deposition by about 2 orders of magnitude, however when it is run with an AWE adaptation of HPAC's particle size distribution it does significantly better and is comparable to the other models included in this study.

Key words: ADMS-STAR2, HPAC, Hotspot, DIFFAL, Operation Roller Coaster, Double Tracks, Clean Slate I, explosion module, particle size distribution.

INTRODUCTION

The Atmospheric Dispersion Modelling System Short Term Atmospheric Release 2 (ADMS-STAR2) atmospheric dispersion model has been developed from the extant Atmospheric Dispersion Modelling System (ADMS) model by Cambridge Environmental Research Consultants (CERC) for the Food Standards Agency (FSA) (CERC, 2009). ADMS-STAR2, together with a number of other dispersion models have been compared against experimental data from trials from the Operation Roller Coaster operation.

Operation Roller Coaster was a joint US/UK series of four experiments studying the results of (nonnuclear) detonation of nuclear weapons in support of the transport and storage of such weapons. The four experiments (Double Tracks, Clean Slate I, II and III) took place in May and June of 1963 at the Tonopah Test Site in Nevada, US. The aim of the experiments was to study the dispersal of weapons grade plutonium (Pu) from a detonation of the high explosive (HE) in the weapon(s) (Stewart, K.,1963).

The Double Tracks trial studied the dispersal of weapons grade plutonium from a high explosive detonation from a single weapon, whereas Clean Slate I studied the dispersal of weapons grade plutonium from a high explosive detonation from a number of weapons, arranged in a typical storage configuration of the time. Clean Slate II and III where not included in this study because the weapons were positioned in earth-covered bunkers which adds to the complexity of the calculation.

Deposition values were recorded on a number of arcs downwind for each of the four experiments. Each experiment had its own configuration, with different numbers of samplers and different levels of instrumentation. Double Tracks and Clean Slate I had the largest amounts of deposition data recorded of the four experiments.

This paper focuses on the deposition values recorded from the alpha survey on each of the arcs for Double Tracks and Clean Slate I (Johnson, W. S., 1963). There were 17 arcs in the Double Tracks trial on which deposition data was recorded and 15 arcs in the Clean Slate I trial. The arcs ranged from ~800m and extended out to ~15km from the source for the Double Tracks trial and ranged from ~800m to ~11km for the Clean Slate I trial. The total amount of arc deposition data was ~650 values in the Double Tracks trial and ~350 in the Clean Slate I trial, giving a combined total of about 1000 values.

MODELS AND MODEL RUNS

Although ADMS-STAR2 is the primary model under consideration, the atmospheric dispersion models DIFFAL, Hotspot and HPAC have also been included in the study. Hotspot is publicly available and can be downloaded for free from the internet. HPAC may be obtained under licence with permission from the Defence Threat Reduction Agency (DTRA) in the US. DIFFAL is AWE's own emergency response and is not publicly available. The models and version numbers used in this study were:

(i) DIFFALSUITE v 1.029
(ii) ADMS-STAR2 v 2.0.2
(iii) Hotspot v 2.07.02
(iv) HPAC v 5.0

All the models use the same basic methodology to calculate the dispersion following an explosion. The initial buoyant rise from the explosion is treated separately from the subsequent advection and diffusion, though both of the phases use some common meteorological data.

The initial distribution of material from the explosive and the subsequent buoyant rise is modelled by considering the stabilised explosive cloud to be made up of a number of discrete releases, each characterized by its own location, size, mass and particle size. The advection and diffusion of each of these individual releases is then calculated separately and the results summed to give a total estimate. The models each use somewhat different parameterizations to characterize the explosive cloud but generally scale the release using the cloud top height (CTH). All the model runs here calculated the CTH by specification of the amount of HE in the weapon(s).

The four models were run with varying complexity of meteorological data, land cover and terrain. All models were run with a single site 10m wind speed and direction. They were also run with profile meteorological data and/or 4D meteorological data if they allowed such data.

It should be noted that this validation measures the performance of the parameterisation of the initial explosive cloud <u>and</u> the subsequent atmospheric dispersion model together.

MODEL MEASURES

The results are presented in statistical and graphical form. The BOOT2 software (Chang, J.C and S.R. Hanna, 2005) has been used to calculate the basic statistical performance measures, which form a basis for air quality model evaluation. For the arc-wise maximum plots, as there is only one point for each arc (17 in the case of Double Tracks and 15 for Clean Slate I), these points are simply plotted on a graph against distance downwind. "Box plots" were used to summarise the full deposition datasets.

The BOOT2 fraction of predictions within a factor of 2 (FAC2) statistical measure is commonly favoured as it is not overly influenced by very low or high values, and is easily and immediately comprehensible to the non-expert, but it only provides a 'snapshot' of model performance at a factor of 2. Here the FAC approach has been extended to cover all factors. This gives a broader indication of model performance than just the FAC2 figure. A cumulative distribution function for FACn (i.e. MAX[Model/Observation, Observation/Model]) has been calculated. The results from an ideal model would lie on the line x=1 i.e. a line joining (1, 0) and (1, 100).

The degree of under and over prediction may also be of interest in some applications. However this information is lost when FAC is considered so the cumulative distribution function for the ratio of model prediction to observation is also displayed. This allows the user to easily ascertain the amount of under and over prediction. An ideal model would lie along the same line as in the FAC graphs (see Figure 3 for an example).

RESULTS

Figure 1 shows the model output for the arc-wise maximum comparisons with Double Tracks using simple meteorological data. It shows the normalised (the ratio of prediction to observation) arc-wise maximum deposition values (plotted on a log scale) against distance. Values greater than one show where models over predict and similarly values less than 1 show the ranges where models under predict deposition. It clearly shows that default ADMS-STAR2 vastly under predicts (by 2 orders of magnitude) at all ranges. The modified ADMS-STAR2 performs much better, although it does over estimate the deposition values by the greatest amount at short range. HPAC, Hotspot and DIFFAL also over predict the deposition values at short ranges (less than 3km from the source) to a lesser extent. All the models except Hotspot generally under predict the deposition at distances greater than 10km. Hotspot over predicts at all ranges.

There were 17 arcs in the Double Tracks experiment at which deposition values were recorded which extended out to about 15km. The maximum deposition value along each arc was identified and the

BOOT2 software run with the arc-wise maximum value produced by each of the models used in this study. Table 1 shows the results using the BOOT2 statistics package for Double Tracks. Based on the favoured FAC2 statistical measure, over 82% of HPAC's deposition predictions are within a factor of two of the observed values. A little under 30% of modified ADMS-STAR2 predictions are within a factor of two of the observed values. This factor is better than the other models. The very large value for the geometric variance for default ADMS-STAR2 is due to the near zero values produced by the model. Hotspot doesn't produce any false negative values (i.e. predicting a value less than the observed), indicating it has over estimated the deposition values for all the Double Tracks arc-wise maximum values.

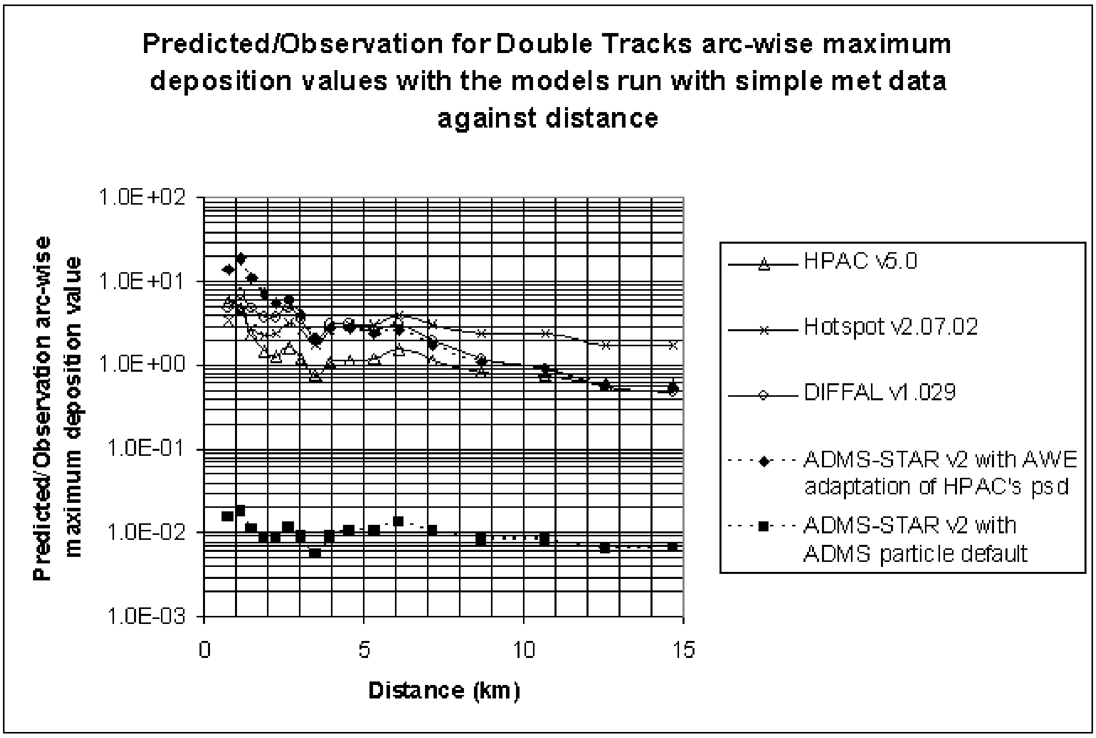

Figure 1. Prediction/Observation arc-wise maximum deposition values with the models run using simple meteorological data against distance for Double Tracks.

Measure	Ideal	HPAC	HOTSPOT	DIFFAL	ADMS-STAR2 with AWE adaptation of HPAC's particle size distribution	ADMS-STAR2 with ADMS particle default
FBFN	0	0.029	0.000	0.009	0.004	1.958
FBFP	0	0.808	0.961	1.176	1.526	0.000
FB (=FBFN-FBFP)	0	-0.779	-0.961	-1.167	-1.522	1.958
AFB (=FBFN+FBFP)	0	0.837	0.961	1.185	1.530	1.958
MGFN	1	1.115	1.000	1.088	1.076	104.280
MGFP	1	1.472	2.686	2.644	3.265	1.000
MG (=MGFN/MGFP)	1	0.757	0.370	0.411	0.330	104.28
NMSE	0	4.610	2.030	4.420	17.86	129.55
VG	1	1.590	2.860	3.880	9.670	0.261×10^{10}
R	1	0.769	0.912	0.923	0.832	0.885
FAC2	1	0.824	0.176	0.235	0.294	0.000
MOEFN	1	0.952	1.000	0.980	0.982	0.011
MOEFP	1	0.418	0.351	0.257	0.133	1.000

Table 1. BOOT 2 statistics using the arc wise maximum deposition data for Double Tracks with the models run with simple meteorology (17 points).

Figure 2 shows the box plots for all the models using simple meteorological data using all the normalised (the ratio of prediction to observation) deposition data from the Double Tracks trial. It shows the under estimations of deposition by 2 orders of magnitude produced by default ADMS-STAR2 (see figure 2c). Most models have difficulty on the 3.5km arc (where the boxes go off-scale).

The data points that cause this correspond to the receptor points that are on the edge of the arc (i.e. at the furthest points from the centre-line). This is on the edge of the plume predicted by the models where they produce some near zero values. HPAC does well at most ranges but does particularly well at predicting deposition values at mid-ranges i.e. ~1.5km to ~7km (with the exception of the 3.5km arc) as the median value (the line at the centre of the box) is very close to 1 and the boxes are fairly compact about that line. The plots show that most models (except the default ADMS-STAR2) tend to over predict deposition values close to the source and under predict at longer ranges. Modified ADMSSTAR2 tends to over predict the deposition values up to about 7km after which it tends to under predict but the under prediction at these longer ranges is to a lesser extent than all of the other models.

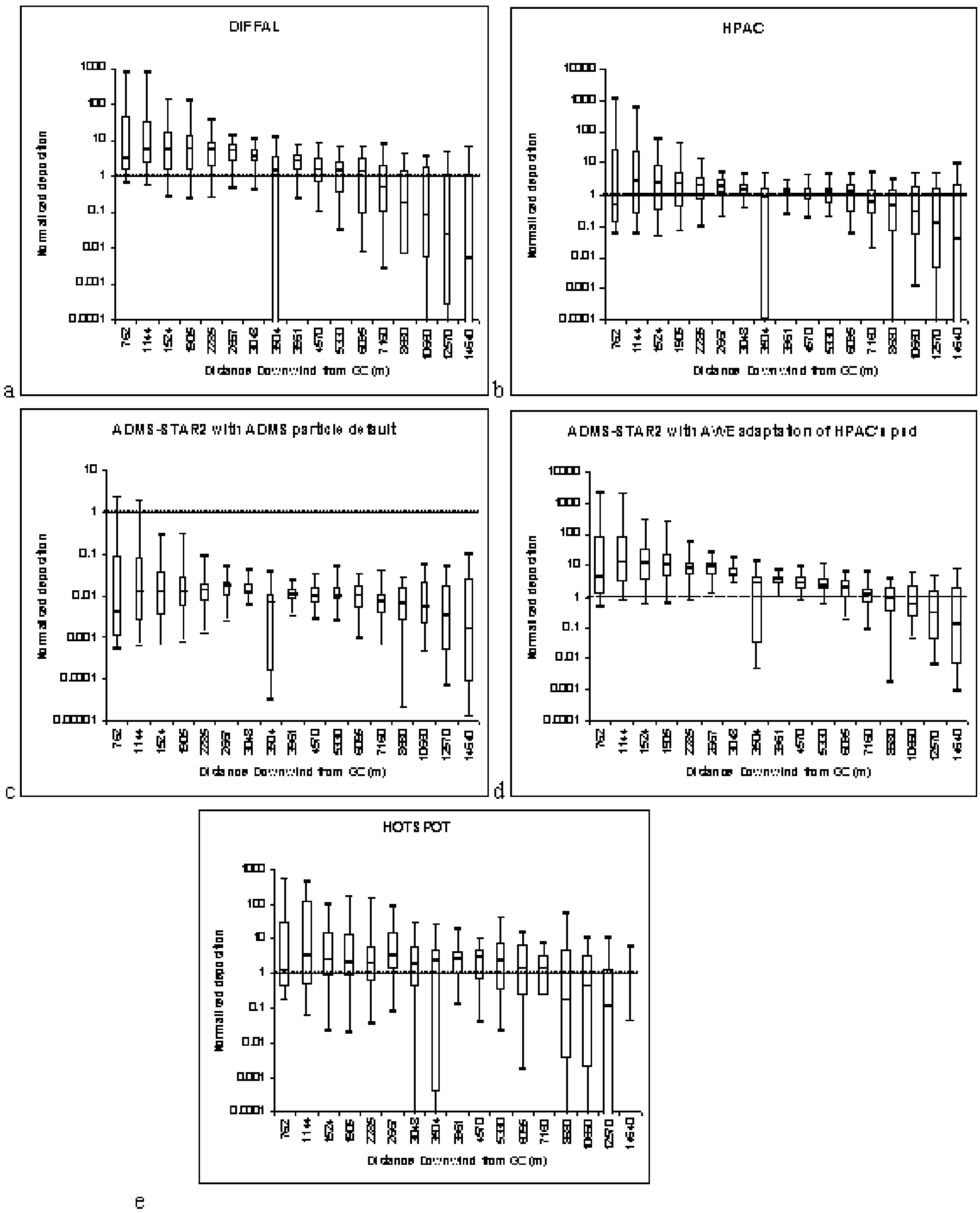

Figure 2. Box plots showing normalised deposition against downwind distance produced by the models run with simple meteorological data for Double Tracks with all the arc deposition data.

Figure 3 show the cumulative distribution function for FAC for all of the model runs with varying amounts of meteorological, terrain and land cover data for the Double Track trial. Again it shows the poor performance of ADMS-STAR2 with it's own default particle and it's improved performance with a better representation of the particle size distribution. HPAC run with profile meteorological data performs best of the model/meteorological data combination for Double Tracks.

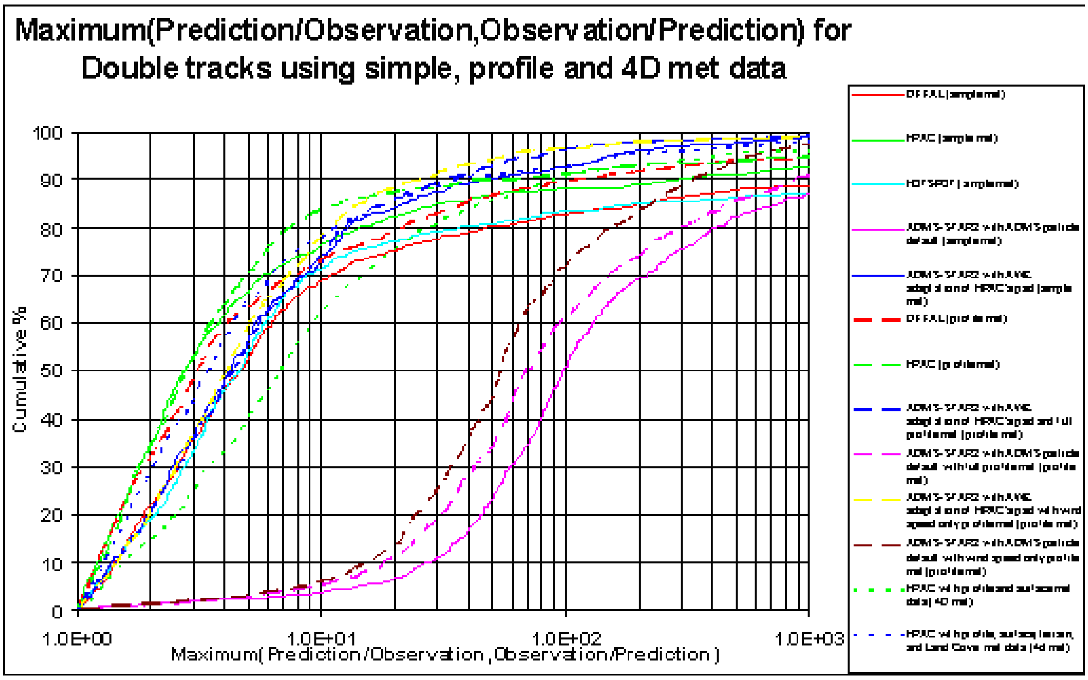

Figure 3. FAC cumulative distribution function for the arc deposition data of Double Tracks using Simple, Profile and 4D meteorology.

CONCLUSIONS

All the models do better at modelling arc-wise maximum deposition values compared to predicting all deposition values across the plume. In general HPAC is the best performing model, if there is no preference for under or over predictions.

Although the explosion module in ADMS-STAR2 does estimate the final dimensions of the initial buoyant cloud, it does not offer default values for either the release fraction or particle size distribution which would be applicable in all scenarios and is the major difference between ADMS-STAR2 and the other models. It is therefore essential that the user has information on both of these parameters before using the model. Lack of knowledge of these parameters can significantly affect the results, as shown throughout this paper.

ADMS-STAR2 augmented by the input of a pertinent release fraction and particle size distribution compares reasonably well against the other models, although ADMS-STAR2 run times were significantly longer than any of the other models.

REFERENCES

CERC, 2009: ADMSSTAR2 User Guide Version 2.0, Cambridge Environmental Research Consultants Ltd., 3, King's Parade, Cambridge, CB2 1SJ.

Stewart, K., 1963: AWRE Report No. T6/69. Roller Coaster. Summary Report. Unpublished AWE report.

Johnson, W. S., 1963: Roller Coaster Report No. POR-2505. Project Officers Report – Project 2.5, Alpha Survey. Unpublished US Department of Defence report.

Chang, J.C.[1,2] and S.R. Hanna[3], 2005: Technical Descriptions and User's Guide for the BOOT Statistical Model Evaluation Software Package, Version 2.0, [1]Comprehensive Atmospheric Modelling Program, School of Computational Sciences, George Mason University, 4400 University Drive, MS 5B2, Fairfax, VA 22030-4444, [2] also affiliated with Homeland Security Institute, 2900 South Quincy Street, Suite 800 Arlington, VA 22206-2231, [3] Harvard School of Public Health, Landmark Centre, Room 404J, 401 Park Drive, Boston, MA 02215-0013.