1.38 INTER-COMPARISON OF THE AUSTAL2000 AND CALPUFF DISPERSION MODELS AGAINST THE KINCAID DATA SET

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INTRODUCTION

The two regulatory air dispersion models AUSTAL2000 (henceforth AUSTAL; VDI 3945, 2000) and CALPUFF (Scire *et al*., 2000) are compared using the Model Validation Kit (hereafter MVK; Olesen, 1994). AUSTAL is a Langrangian particle-tracking dispersion model recommended by the German UBA while CALPUFF is a Gaussian puff model recommended for certain regulatory applications by the US EPA. AUSTAL incorporates a diagnostic model to reconstruct the 3D wind field over complex terrain, whereas CALPUFF may utilize discrete station met file data or gridded diagnostic output from the CALMET meteorological processor. Because of the fundamentally different algorithms used by these models, it is useful to inter-compare them and assess model variability using the MVK data sets provided by the Harmonisation Committee.

In this study, the model predictions of arc-wise maximum concentrations at various distances downwind of a point source release are compared with the Kincaid tracer data set contained in the MVK. The Kincaid experiment features relatively homogeneous physical conditions. Therefore, it was suitable to run the "CALPUFF Lite" model, which uses hourly meteorological data files directly, without using the CALMET pre-processor. Since the transport time between the stack and the outermost receptor arcs frequently exceeds one hour, the tracer gas release was initiated several hours before sampling. Thus, it is necessary to employ continuous records of emission and meteorological conditions for each complete day of the experiment, which includes the emission period before the sampling network started to operate (Strimaitis et al., 1997).

MODEL CONFIGURATIONS

Several model configurations are examined in this study. The performance of the models for these various setup states is judged using the standard statistical measures recommended in the MVK.

AUSTAL

A time series that includes wind direction and speed, Monin-Obukhnov length, stack exit velocity and thermal flux, and emission rate of the tracer gas is prepared for each AUSTAL dispersion calculation. AUSTAL allows a maximum of 10 discrete monitors. Thus, we set an array of discrete monitors at downwind distances: 1, 2, 3, 5, 7, 10, 15, 20, 30, and 50 km (tracer results at 0.5 and 40 km, although provided in the MVK, are excluded). Wind direction was fixed during the AUSTAL simulations.

Since the tracer emission is from an elevated stack, the highest level of wind tower data at 100 m is the most representative for input to AUSTAL. The required Monin-Obukhov length,was computed using the meteorological processor from CTDMPLUS (U.S. EPA, 1989), based on the onsite tower wind data. The thermal flux from the stack was derived from the wind tower data according to

$$Q_q = c_p \rho (T_q - T_\circ) S v_q , \qquad (1)$$

where Q_q is the thermal flux associated with an exhausted gas of density, ρ, the excess temperature above ambient is $T_q - T_o$, v_q is the stack exit velocity, S is the stack cross-sectional area, and c_p is the specific heat capacity at constant pressure. An approximation suitable for calculating the thermal flux of a power plant according to the VDI document is given by

$$Q_q = 1.36 \times 10^{-3} (T_q - 283.) S v_q \qquad (2)$$

where Q_q is measured in units of MW and all other variables measured in SI units. Equation (2) provides a slightly higher estimate than (1) (assuming dry air), and may be necessary to account for humidity in the exhausted gas from the power plant. Lastly, the stochastic variability of AUSTAL is controlled by setting the integer quality factor QA between -4 and 4. Increasing QA by 1 doubles the rate of particles released and reduces statistical uncertainty (scattering) by a factor of $\sqrt{2}$ - at the expense of doubling the computational time. The default QA is zero.

The Monin-Obukhov length derived from 100-m level onsite data, along with the thermal flux for dry air (Equation (1)), and the default quality factor, constitute a baseline AUSTAL run. Using this configuration as a baseline, three other configurations are also considered (see Table 1). These are: (A) using the 10-m wind instead of the 100-m wind; (B) using the VDI thermal flux instead of Equation (1); and, (C) using the highest value of QA(4) instead of the default zero. Table 1 summarizes the configurations of AUSTAL and CALPUFF examined in this study.

Table 1. A summary of the four AUSTAL model configurations studied: AUSTAL (A,B,C,D) and the CALPUFF configuration (CPF).

Model	Wind Levels	Thermal Flux Equation	Quality Factor
(A)	Onsite 100 m	Dry Air	0
(B)	Onsite 10 m	Dry Air	0
(C)	Onsite 100 m	VDI Equation	0
(D)	Onsite 100 m	Dry Air	4
CPF	Onsite 100 m	N.A.	N.A.

CALPUFF

For comparison purposes, the CALPUFF configuration uses single level winds at 100 m and discrete Turner stability classes (*N*) for dispersion calculations. The Turner class is computed by PCRAMMET (U.S. EPA, 1999) based on the onsite 10-m wind data and off-site cloud cover.

COMPARISON RESULTS

Table 2. Performance statistics obtained using Kincaid data of quality 2 and 3. The Sigma (standard derivation), Bias = C_{OBS} - C_{MOD} , and other variables are explained in the text.

	Mean	Sigma	Bias	NMSE	COR	FAC2	FB	FS
OBS	42.8	39.3	0	0	1	1	0	0
(A)	107.7	98.7	-64.9	2.8	0.35	0.26	-0.86	-0.86
(B)	122.4	120.2	-79.6	3.7	0.31	0.24	-0.96	-1.01
(C)	99.2	93.8	-56.3	2.6	0.32	0.26	-0.79	-0.82
(D)	107.5	80.0	-64.7	2.1	0.39	0.26	-0.86	-0.68
CPF	34.8	67.5	8.0	3.2	0.26	0.35	0.20	-0.53

Table 2 compares the model performance between AUSTAL (model configurations A,B,C and D) and CALPUFF (Model CPF) (arcwise maximal concentrations normalized by emission in units $10^{-9}sm^{-3}$). Concentrations at distances 0.5 km and 40 km are not considered in Table 2. A total of 557 observations are used from the Kincaid dataset, all of quality 2 or 3. The model performance is described in Table 2 by normalized mean square error (NMSE), linear correlation coefficient (COR), fraction within factor 2 (FAC2), fractional bias (FB), and fractional standard derivation (FS), as defined in Hanna et al. (1991).

From an examination of Table 2, CALPUFF outperforms the baseline AUSTAL (A) model configuration. CALPUFF has smaller mean error and higher correlation and a higher proportion of predictions within a factor of 2. The AUSTAL bias is relatively large and negative compared with that of CALPUFF. A negative bias implies overestimation of the ground level concentration (GLC). Although CALPUFF also overestimates the GLC for several arc-hour events, its average bias is positive and small in comparison to AUSTAL. This is because there are many more zero impacts predicted by CALPUFF, which produces the positive bias. A better way to see the trend of bias is through quantile-quantile plots, as discussed below and shown in Figure 1.

Among the AUSTAL configurations considered, configuration (D) features the best statistics, while those of (B) are the worst. Configuration (C) is somewhat better than the basis (A). In AUSTAL (D) the stochastic variability is reduced significantly because a much higher number of particles are being released during the model runs. This reduces the normalized mean squared error, increases the correlation between observation and prediction and substantially lowers the fractional standard deviation. However, the fraction within factor 2 and fractional bias for configurations A and D are the same, since the average predictions (*i.e.,* mean) are unchanged by the quality factor.

Configuration (B) has the greatest negative bias among the AUSTAL configurations considered. This implies that the wind profile extrapolation within AUSTAL under-predicts the wind speeds at elevated levels. The configuration (C) has the least bias among the group. We note that the VDI computed thermal flux is generally higher than that based on a dry air calculation, which explains why configuration (C) has the least degree of over-prediction. The thermal buoyancy of the plume from the power plant seem to be better represented by the VDI equation that that based on dry air assumption.

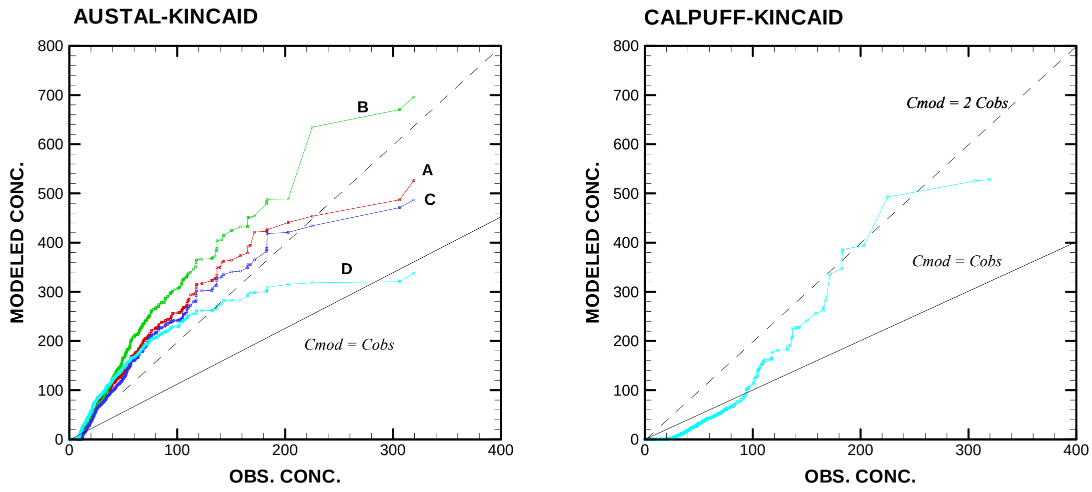

Figure 1. The quantile-quantile plots of AUSTAL (left) and CALPUFF (right) using Kincaid data of quality 2 and 3.

Figure 1 shows the quantile-quantile (QQ) plots for AUSTAL and CALPUFF comparing modeled data with observations. Figure 1 corroborates the conclusions drawn from analyzing the statistics in Table 2. AUSTAL is found to consistently overestimate the GLC by about a factor of 2 (dashed line). The predicted GLC's are highest with the AUSTAL configuration (B) and lowest with that of (D). The performance of AUSTAL (A, B, C) is similar to that of CALPUFF. All of them overestimate the GLC by approximately a factor of 2 over a range of observations. However, the use of higher quality factor in AUSTAL (D) decreases the degree of overestimation.

CONCLUSIONS

Given the same quality of meteorological data, the performance of AUSTAL is similar to that of CALPUFF when using the Kincaid data set. The AUSTAL predictions tend to be conservative, usually overestimating the Kincaid GLC by roughly a factor two. AUSTAL performance is strongly affected by the choice of "quality factor" parameter, which controls the stochastic variability through the number of particles released. AUSTAL also tends to underestimate the wind speed at elevated levels, but AUSTAL predictions are greatly improved when wind data at an elevated level (close to the elevated source in the Kincaid experiment) is provided. This study also showed that AUSTAL predictions are improved when the thermal properties of exhausted gas from a power plant are described by the VDI thermal flux equation.

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