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Understanding the effect of the land use dry deposition scheme on predicted ozone concentrations

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Introduction

Feedback from Lucy Davis suggests that using the land use dry deposition scheme in the air quality set-up results in unrealistically high NAME predicted concentrations of ozone. To understand why this is the case, Lucy provided a test air quality run for February 2010. This note is a summary of the results of this investigation.

Case study

A six day air quality run for the period 00Z 11/02/2010 – 00Z 17/02/2010 was used as a case study. A coarse run with a horizontal output grid resolution of 0.5° by 0.5° and a high resolution run with a horizontal output grid resolution of 0.11° by 0.07° were both conducted. NAME predicted air concentrations of ozone from 0 m agl to 100 m agl are compared against hourly averaged observed ozone concentrations at a range of sites (rural, remote and urban background). The predicted air concentrations are 8-hourly averages for the coarse run and hourly averages for the high resolution run.

To begin the investigation, two NAME runs were conducted. The first run used the original dry deposition scheme. For ozone this used a fixed deposition velocity, v_d, of 7.0×10^{-4} m/s over sea (determined by the topography being less than 1.0×10^{-6} m) and of 4.0×10^{-3} m/s over land. The second run used the land use dependent dry deposition scheme which is based on the STOCHEM scheme and is described in Webster and Thomson (2012). For ozone, this considers uptake via the stomata, deposition via the cuticle and deposition to the underlying surface. Due to the solubility of ozone, the land use dry deposition parametrisation is dependent on soil moisture and whether the surfaces are wet or dry. Figure 1 shows a comparison of observed hourly averaged ozone concentrations (black dashed line) with NAME predicted ozone concentrations from the coarse run using the original dry deposition scheme (orange line) and using the land use dry deposition scheme (green line). Both NAME model runs show an over-prediction of ozone concentrations but the over-prediction is greater using the land use dry deposition scheme. A third NAME run was conducted. This used the land use dry deposition scheme except for ozone where the original dry deposition scheme was used. The blue line in Figure 1 shows the predicted ozone concentrations from this third NAME run. Predicted ozone concentrations from this NAME run are very similar to the NAME run using the original dry deposition scheme (shown in orange). This means that the increase in predicted ozone concentrations seen in Figure 1 is largely due to changes in the modelling of dry deposition of ozone rather than changes to ozone production or depletion concerned with changes in air concentrations of other species.

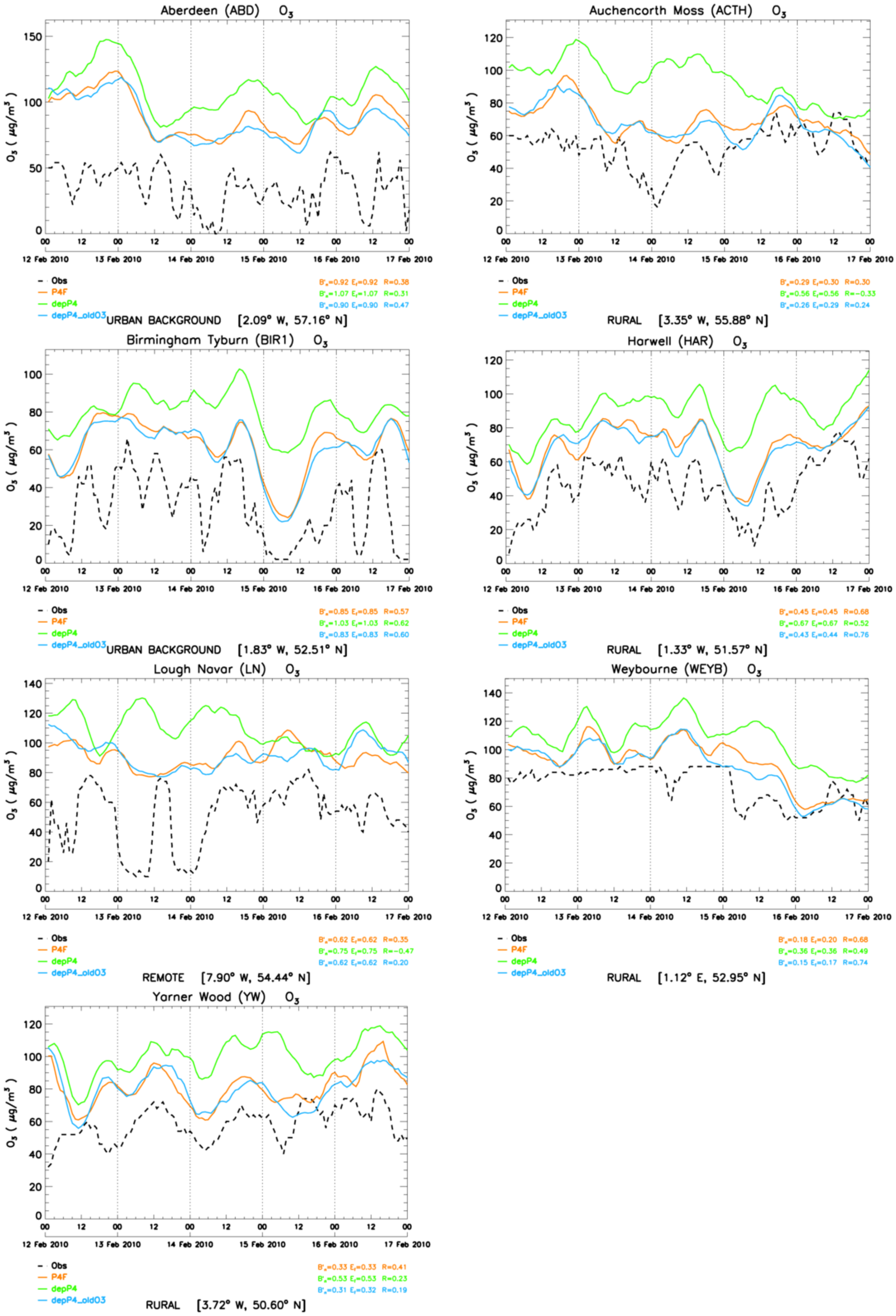

Figure 1: A comparison of observed ozone concentrations (black dashed line) and NAME predicted ozone concentrations from the course modelling run using the original dry deposition scheme (orange line), using the land use dry deposition scheme (green line) and using the land use dry deposition scheme with the original scheme for ozone (blue line).

We calculate average dry deposition velocities (v_d) for ozone over the 6 day period (518,400 seconds) from predicted total dry deposition over the 6 day period and predicted mean air concentrations,

$$v_d = \frac{dry\_deposition}{(518400 * air\_conc)}.$$

Figures 2 and 3 shows fields of average air concentrations, total dry deposition and average dry deposition velocities over the six day period for the NAME runs conducted using the original dry deposition scheme and using the land use dry deposition scheme, respectively. Overall with the original dry deposition scheme, air concentrations of ozone are lower, and dry deposition amounts and deposition velocities are larger. Figure 2(c) shows the two fixed dry deposition velocities used in the original scheme: 7.0 x 10^{-4} m/s over sea and 4.0 x 10^{-3} m/s over land. Figure 3 shows much more spatial variation in predicted air concentrations, and in dry deposition amounts and dry deposition velocities of ozone. Average dry deposition velocities range from 2.8 x 10^{-4} to 4.3 x 10^{-3} m/s with the smallest values over the sea and the largest values over land. Despite giving smaller dry deposition velocities overall, the land use dry deposition scheme appears to give an appropriate range of values comparing them with values given in the literature. For example, dry deposition velocities of ozone from field and laboratory measurements as given by McMahon and Denison (1979) are summarised in table 1. The highest dry deposition velocity listed by McMahon and Denison is 2 x 10^{-2} m/s measured over juniper bush. Whereas the smallest dry deposition velocity is 2 x 10^{-4} m/s measured over distilled water. The land use dry deposition scheme gives dry deposition velocities within this range and does, therefore, appear to be calculating realistic dry deposition velocities for ozone.

Figure 4 shows a comparison of hourly observed ozone concentrations and hourly NAME predicted ozone concentrations from the high resolution runs for the three model set-ups described above (using the original dry deposition scheme, using the land use dependent dry deposition scheme, and using the land use dry deposition scheme except for ozone where the original dry deposition scheme is used). Despite there being more noise in the results, the overall story is the same as that obtained from the course runs. This is a consistent result throughout and hence further model predictions from the high resolution runs are not shown.

Analysis of ozone concentrations predicted by NAME and AQUM show that both models have a positive bias, indicating that both models over-predict ozone concentrations. AQUM, which has a similar land use dependent dry deposition scheme, has a larger bias than NAME (with the original dry deposition scheme) which is in keeping with the findings here (personal communication, Paul Agnew).

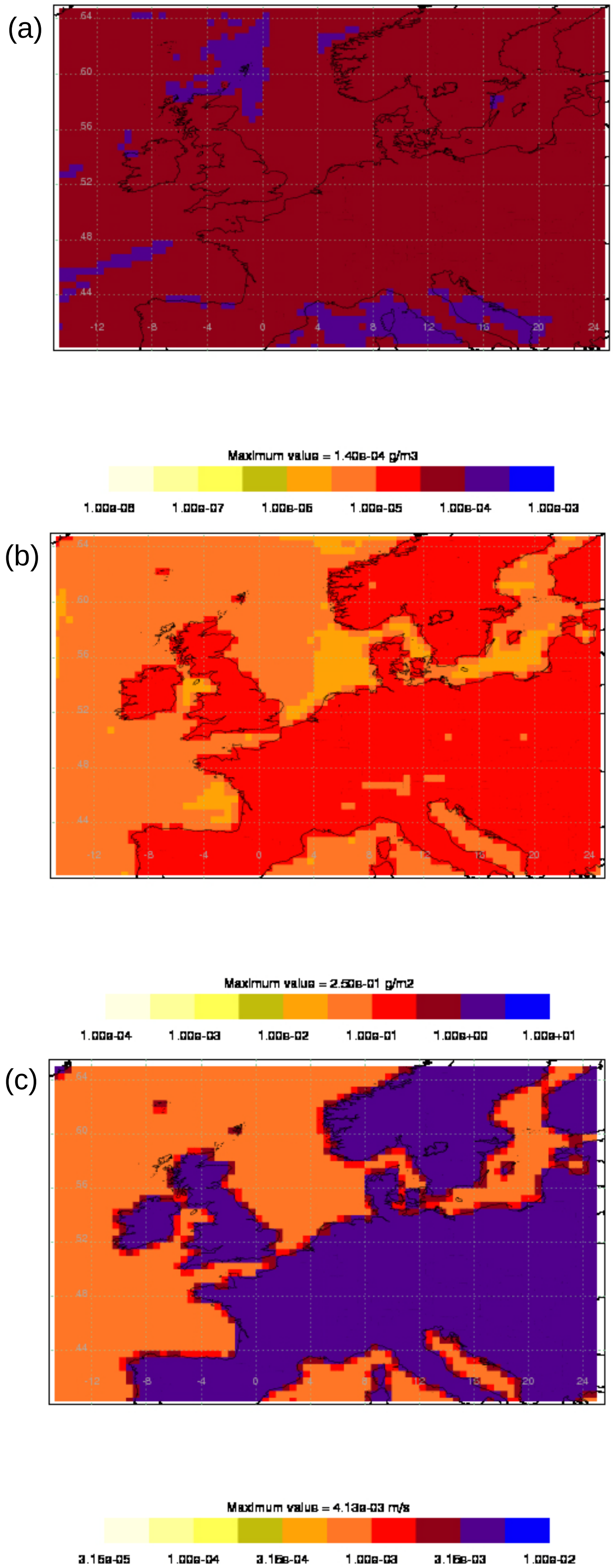

Figure 2: (a) NAME predicted boundary layer average air concentrations, (b) NAME predicted total dry deposition, and (c) NAME predicted average dry deposition velocity of ozone over 6 days using the original dry deposition scheme.

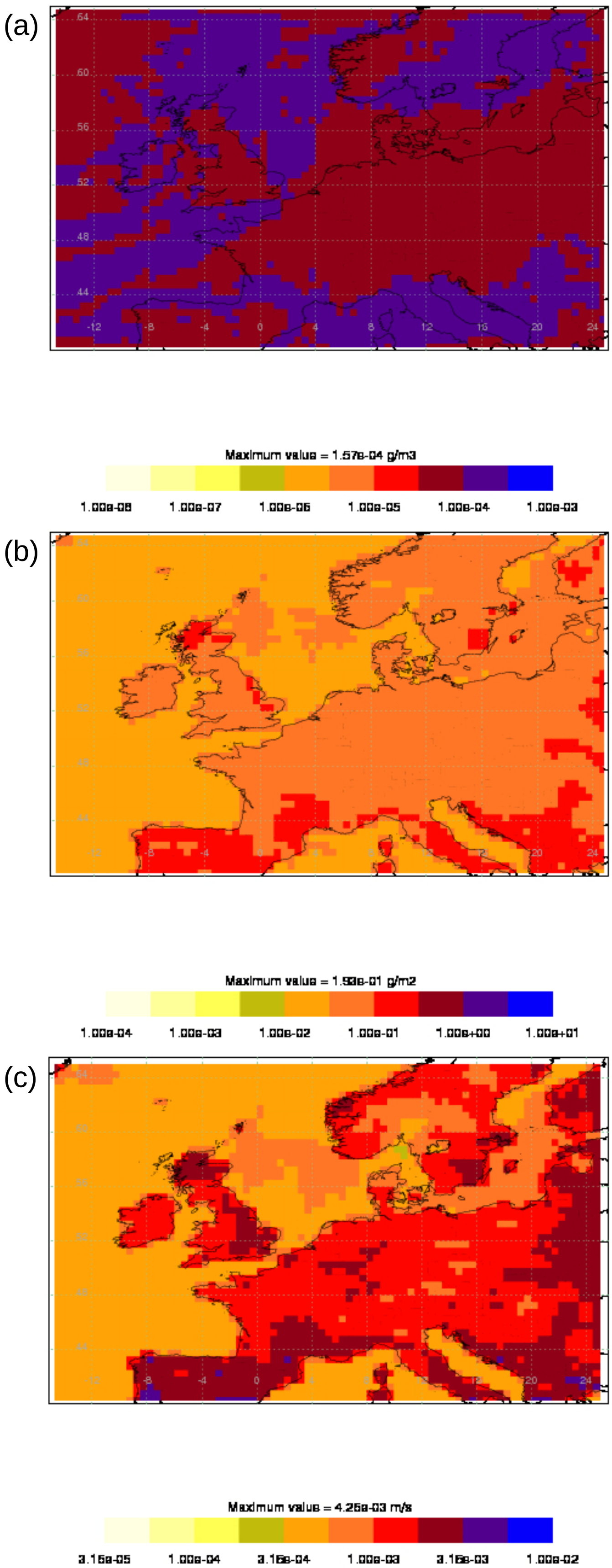

Figure 3: (a) NAME predicted boundary layer average air concentrations, (b) NAME predicted total dry deposition, and (c) NAME predicted average dry deposition velocity of ozone over 6 days using the land use dry deposition scheme.

Reference	Surface	Deposition velocity (m/s)	Notes
Hill and Chamberlain (1971)	Vegetation	1.67×10^{-2}	
Rich et al. (1970)	Bean leaves	6.0×10^{-3}	
Thorne and Hanson (1972)	Petunia	2.3×10^{-3}	Herbaceous
Thorne and Hanson (1972)	Osteosperium	2.1×10^{-3}	Herbaceous
Thorne and Hanson (1972)	Chrysanthemium	1.6×10^{-3}	Herbaceous
Thorne and Hanson (1972)	Camelia (young)	7.3×10^{-4}	Woody
Thorne and Hanson (1972)	Bougainvillia	5.0×10^{-4}	Woody
Thorne and Hanson (1972)	Ginkgo	3.3×10^{-4}	Woody
Thorne and Hanson (1972)	Quercus	3.2×10^{-4}	Woody
Thorne and Hanson (1972)	Camelia (mature)	2.5×10^{-4}	Woody
Garland (1977)	Soil	1.8×10^{-2}	4% water content
Garland (1977)	Sand	8.4×10^{-3}	27% water content
Garland (1977)	Peat	1.4×10^{-2}	43% water content
Garland (1977)	Peat	4.6×10^{-3}	74% water content
Garland (1977)	Grass	5.5×10^{-3}	In presence of SO_2
Garland (1977)	Grass	7.4×10^{-3}	In presence of SO_2
Regener (1957)		3.5×10^{-3}	Diabatic condition
Regener (1957)		7.0×10^{-3}	Neutral condition
Kroening and Ney (1962)	Ground surface	2.0×10^{-3}	
Galbally (1968)		4.0×10^{-3}	
Galbally (1968)		1.4×10^{-2}	Diabatic condition
Kelly and McTaggart-Cowan (1968)		1.4×10^{-2}	Neutral condition
Aldaz (1969)	Juniper bush	2.0×10^{-2}	Assume ozone density of 40 µg m^{-3}
Aldaz (1969)	Sand or dry grass	6.0×10^{-3}	Assume ozone density of 40 µg m^{-3}
Aldaz (1969)	Snow	1.6×10^{-3}	Assume ozone density of 40 µg m^{-3}
Aldaz (1969)	Fresh water	7.0×10^{-4}	Assume ozone density of 40 µg m^{-3}
Aldaz (1969)	Ocean	4×10^{-4}	Assume ozone density of 40 µg m^{-3}
Aldaz (1969)	Distilled water	2×10^{-4}	Assume ozone density of 40 µg m^{-3}
Galbally (1969)		9.5×10^{-3}	Diabatic condition
Galbally (1969)		1.0×10^{-3}	Unstable condition
Galbally (1971)		1.2×10^{-2}	Neutral condition
Galbally (1971)		2.0×10^{-3}	Diabatic condition
Turner et al. (1973)	Bare fine sandy loam	5×10^{-3}	Reference height 0.025m
Wilbrandt (1975)		1.1×10^{-2}	Unstable
Van Dop et al. (1977)	Dry grass	1.3×10^{-3}	Reference height > 5m, z/L=-0.3

Table 1: Field and laboratory measurements of ozone dry deposition velocities as collated by McMahon and Denison (1979)

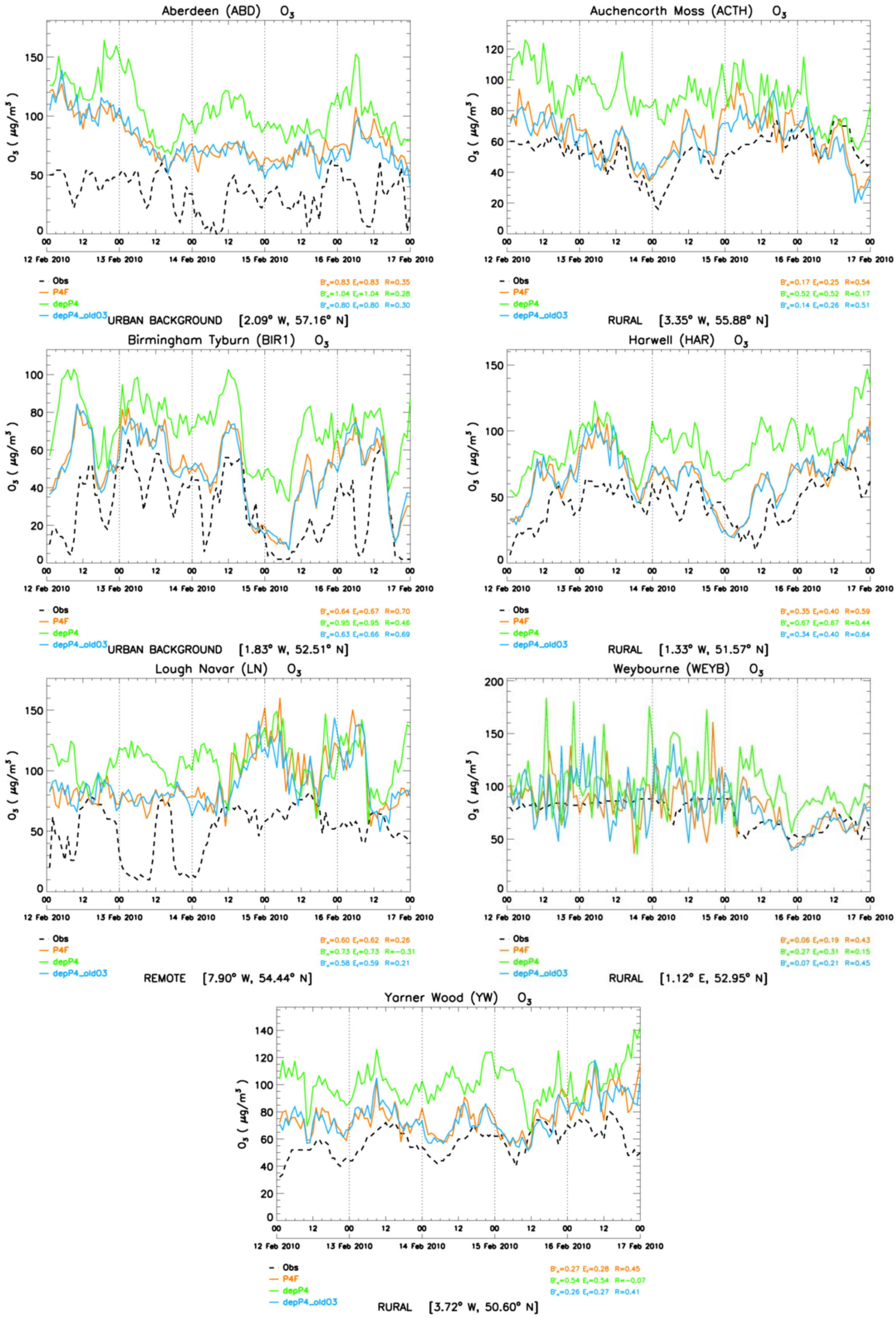

Figure 4: A comparison of observed ozone concentrations (black dashed line) and NAME predicted ozone concentrations from the high resolution modelling run using the original dry deposition scheme (orange line), the land use dry deposition scheme (green line) and the land use dry deposition scheme with the original scheme for ozone (blue line).

Other investigations

The aerodynamic resistances are well understood and hence provide an upper bound on the dry deposition velocity. Assuming that the surface provides no resistance to uptake of ozone (i.e., assuming R_c=0), the upper bound for the ozone dry deposition velocity is given by

$$v_d = \frac{1}{R_a + R_b},$$

where R_a is the aerodynamic resistance and R_b is the laminar layer resistance. It is interesting to see the effect of this upper bound on predicted ozone concentrations. Figure 5 shows a comparison at different UK sites of hourly observed ozone concentrations (black dashed line) with NAME predicted ozone concentrations from the course modelling runs using the original dry deposition scheme (orange line), using the land use dependent dry deposition scheme (green line), and using the upper bound dry deposition velocity (blue line). Predicted ozone concentrations using the upper bound for the dry deposition velocity are significantly lower than the predicted ozone concentrations obtained using the land use dry deposition scheme. This indicates that the surface resistance to ozone is, in general, significant and cannot be ignored. Overall there is still a tendency for NAME to over-predict ozone concentrations even when no resistance to uptake of ozone by the surface is assumed. This suggests that the ozone over-prediction cannot be attributed in its entirety to the dry deposition scheme and that some other process is in play (for example, an over-production of ozone in the model or too little depletion of ozone by other mechanisms). Occasionally the predicted ozone concentrations obtained using the original dry deposition scheme are lower than those obtained using the upper bound dry deposition velocity. There must, therefore, be occasions when the fixed dry deposition velocity in the original scheme is larger than the upper bound dry deposition velocity.

Free tropospheric turbulence is known to be intermittent and patchy. Within NAME, a fixed low level of turbulence is applied throughout the free troposphere. We test here the effect on predicted ozone concentrations of reducing the free tropospheric turbulence. A further run using the land use dependent dry deposition scheme and reduced free tropospheric turbulence values (velocity variances (both horizontal and vertical) reduced by a factor of 100) was conducted. The effect of reduced free tropopsheric turbulence values on NAME predicted ozone concentrations can be large with either an increase or a decrease in predicted ozone concentrations possible. Lower levels of free tropospheric turbulence reduces the transport of (potentially ozone rich) air from the boundary layer into the free troposphere. Contrary to this, lower levels of free tropospheric turbulence reduces the mixing of free tropospheric ozone down to the boundary layer.

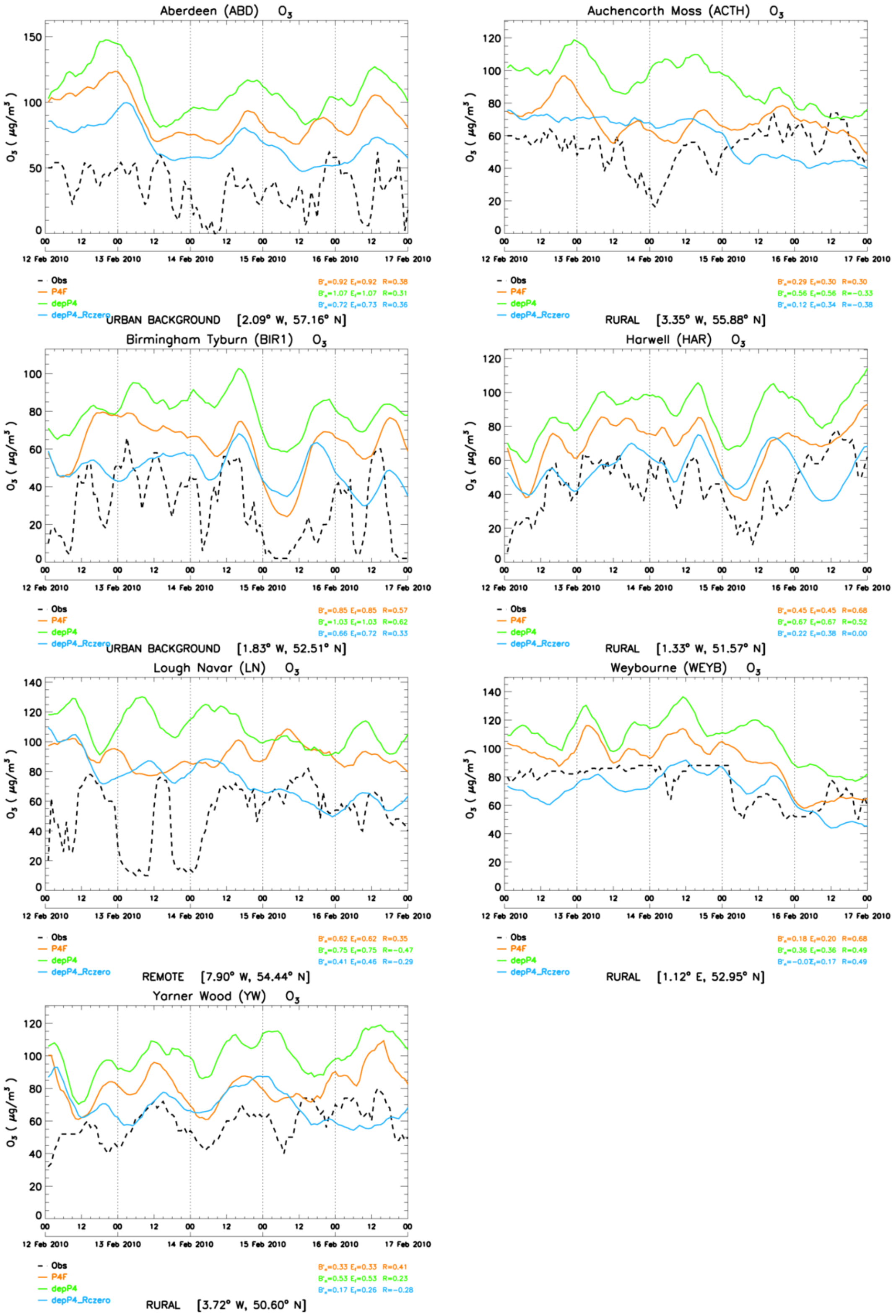

Figure 5: A comparison of observed ozone concentrations (black dashed line) and NAME predicted ozone concentrations from the course modelling run using the original dry deposition scheme (orange line), the land use dependent dry deposition scheme (green line) and the upper bound dry deposition velocity (blue line).

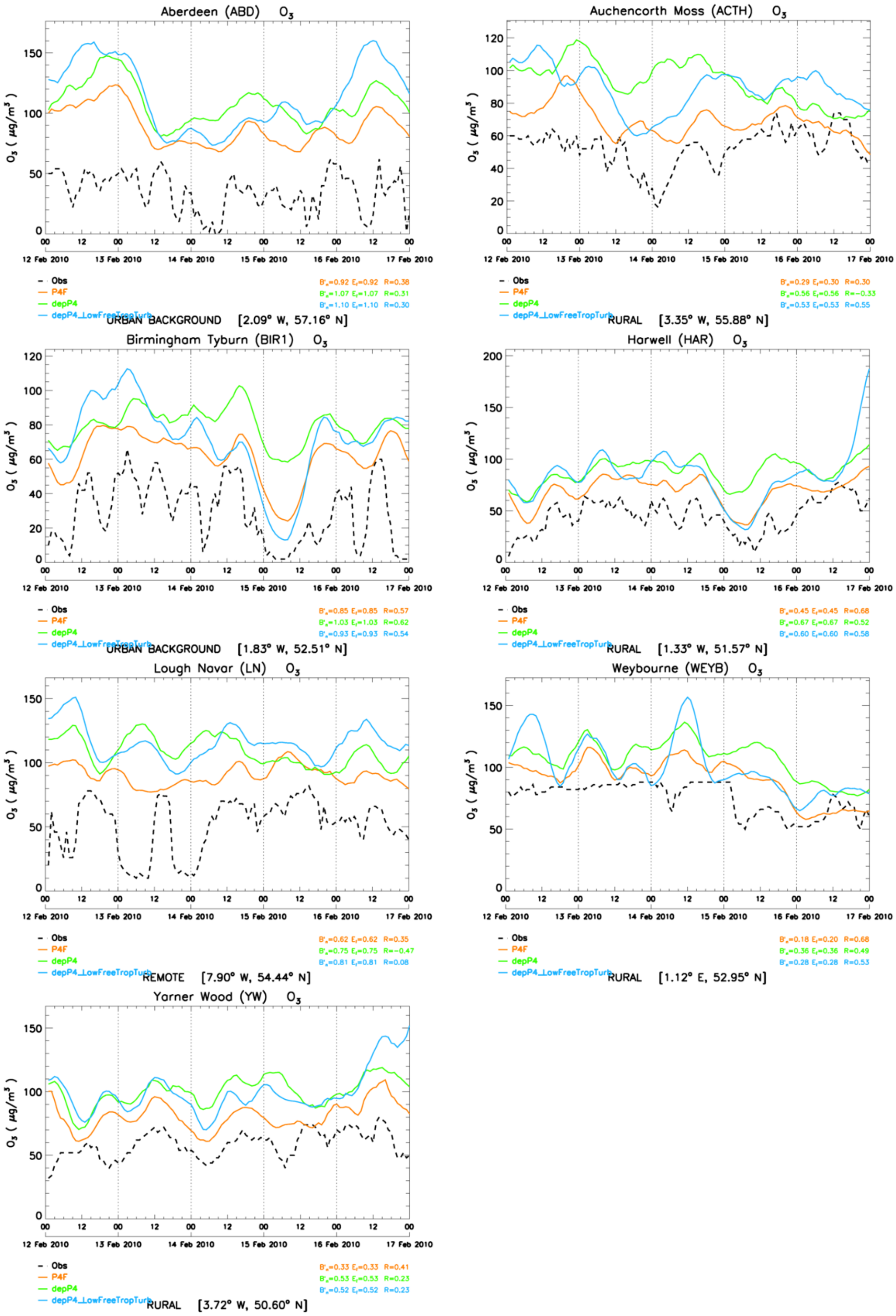

Figure 6: A comparison of observed ozone concentrations (black dashed line) and NAME predicted ozone concentrations from the course modelling run using the original dry deposition scheme (orange line), the land use dependent dry deposition scheme (green line) and the land use dependent dry deposition scheme with reduced free tropospheric turbulence values (blue line).

A summer study

A similar air quality run for a 6 day summer period (20th - 26th June 2010) was also conducted to compare results during a period when the vegetation is growing and in full leaf. The weather during this chosen summer period was dominated by a high pressure system. However, apart from this chosen selection criteria, the summer study period was randomly chosen and, unlike the February study period, it was not a period for which issues with NAME predicted ozone concentrations had been identified. Figure 7 compares hourly observed ozone concentrations (black dashed line) with NAME predicted ozone concentrations obtained from the course run using the original dry deposition scheme (shown in orange) and the land use dependent dry deposition scheme (shown in green). The surface resistance in the land use dependent dry deposition scheme is strongly dependent on the vegetation growth and hence is seasonally dependent. In general, NAME over-predicts ozone concentrations (although there are occasions and locations where ozone predictions are not over-predicted) and the degree of over-prediction is larger when the land use dependent dry deposition scheme is used. This suggests, as before, that the deposition velocities calculated by the land use dependent dry deposition scheme are smaller than the fixed deposition velocities over land and sea used in the original scheme.

Conclusions

This study suggests that ozone concentrations are generally over-predicted by NAME. Model runs using an upper bound for the dry deposition velocity suggest this over-prediction cannot be totally explained in terms of the dry deposition velocity for ozone and there must be some other process in play such as over-production of ozone or under-depletion of ozone by other mechanisms. The land use dependent dry deposition scheme generally results in higher NAME predicted ozone concentrations than the original dry deposition scheme, which used a fixed dry deposition velocity over land and over sea. These higher ozone concentrations have been shown to be due to lower overall dry deposition velocities for ozone from the land use dependent dry deposition scheme. The ozone dry deposition velocities given by the land use dependent dry deposition scheme are, however, within the range of field and laboratory measurements given in the literature. NAME predicted ozone concentrations can be strongly sensitive to free tropospheric turbulence levels although, in changing free tropospheric turbulence levels, ground level ozone concentrations do not necessarily change accordingly. Hence it is unlikely that NAME predictions of ozone concentration could be improved by changes to free tropospheric turbulence levels. It is useful for the user to be aware of the likely effects of invoking the different dry deposition schemes in NAME. However, this study has been inconclusive in identifying the particular errors in or corrections required to ozone concentration forecasting.

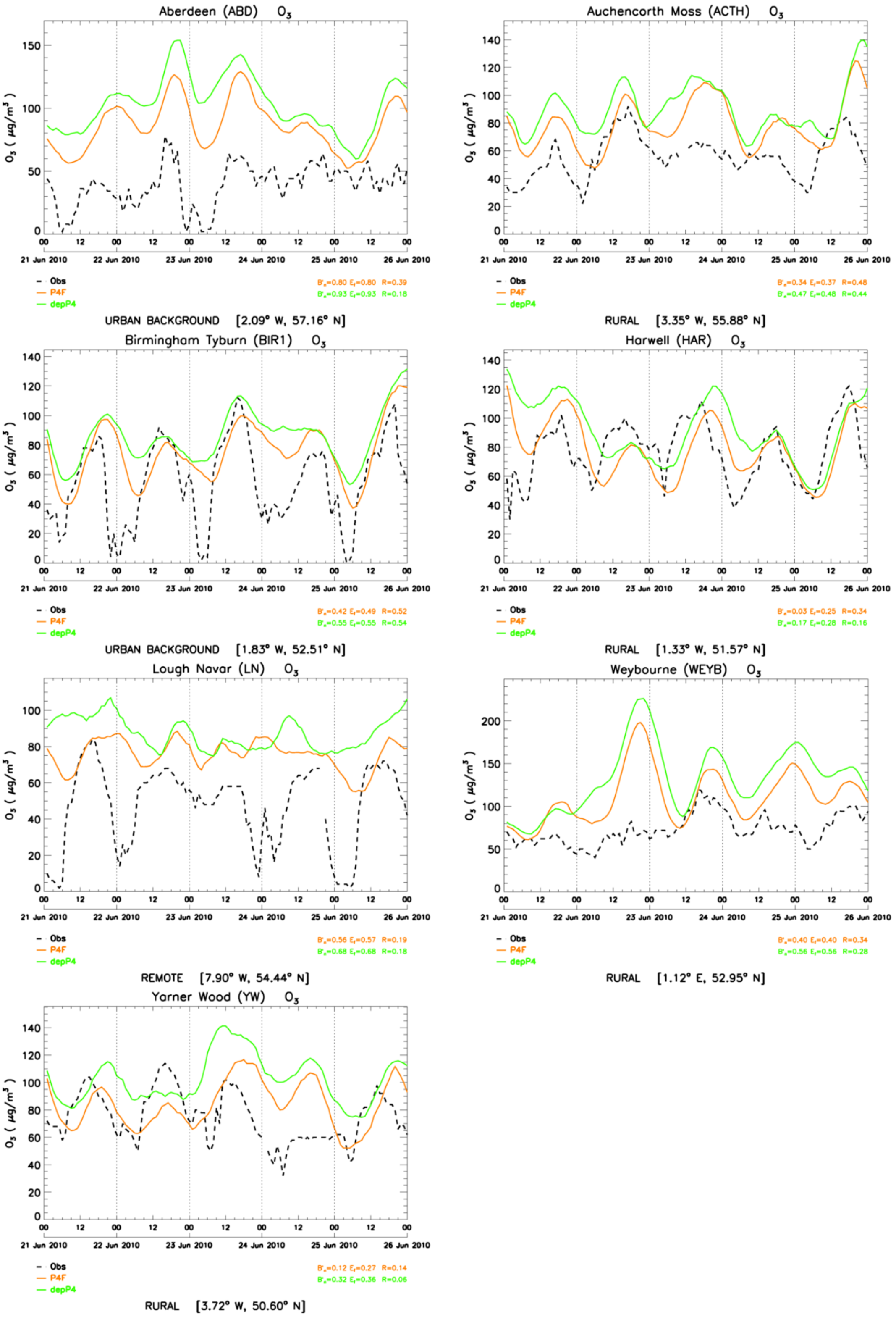

Figure 7: A comparison of observed ozone concentrations (black dashed line) and NAME predicted ozone concentrations from the course modelling run using the original dry deposition scheme (orange line) and the land use dependent dry deposition scheme (green line) during a summer period.

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