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Can dispersion model predictions be improved by increasing the temporal and spatial resolution of the meteorological input data?

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Introduction

In the case of a major pollution incident, terrorist attack, or a radioactive event such as the Chernobyl disaster in 1986, dispersion models are used to predict the transport of pollution away from its source, so allowing potentially affected areas to be warned or even evacuated. Thus it is important for both economic and human health reasons that there is continued research in developing and evaluating dispersion models.

The UK Met Office has developed NAME III (Numerical Atmospheric-dispersion Modelling Environment) as its third-generation dispersion model. In addition to emergency response applications, NAME III can also be used for air-quality modelling and to source attribution problems (Jones, 2004). Some recent examples for which NAME III has been used include predicting the spread of the smoke plume caused by the Buncefield Oil Depot fire in December 2005 (Webster *et al.*, 2006) and for investigating the mechanisms for the farm-to-farm spread of foot and mouth disease (Gloster *et al.*, 2004).

So how does a dispersion model work? Particles of a pollutant released into the atmosphere form a 'plume' or 'cloud' which spreads out and gradually moves away from its source. To calculate the spread of a plume, dispersion models require data to be input to the model (Turner, 1994), which typically include:

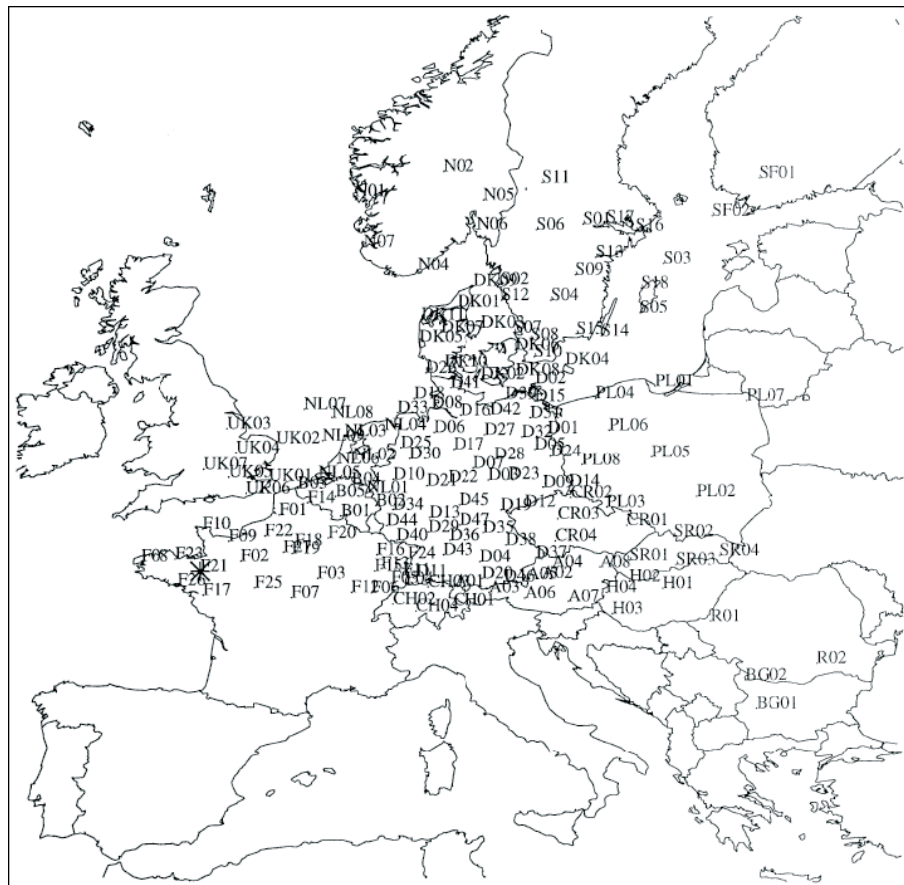
- Emissions parameters: source height and location, exit velocity and temperature and the mass flow rate of the pollutant.
- Meteorological data: wind speed and direction, temperature, stability of the air and the boundary layer height. More complex models (such as NAME III) use many additional meteorological fields to enhance the accuracy of their predictions.

- The topography of the surrounding area is used for long-range applications.
- Details of any obstructions to the flow, such as buildings, are important for shorter-range applications.

A Lagrangian dispersion model, such as NAME III, then simulates the emission of the pollutant through the release of large numbers of particles into the atmosphere, with each particle representing a fixed mass of pollutant. Particles are transported due to advection (along the axis of the plume) and a turbulent component (leading to a cross-axial spread of the plume). The individual three-dimensional (3D) trajectories of the particles are followed through the atmosphere, with concentrations calculated by determining the total mass of the pollutant

within a set volume. Alternative types of dispersion model are available, such as Eulerian models, which calculate concentrations at set grid points and are based on a stationary 3D Cartesian grid.

To ensure the predictions from dispersion models are realistic, various model evaluation experiments have been performed. These experiments usually take the form of a known tracer being released from a source at an accurately recorded rate. The tracer is then tracked over a distance through the use of sampling stations which record the tracer concentration over a predetermined time interval. Some examples of long-range experiments include the Cross Appalachian Tracer Experiment (CAPTEX) in 1983 (Ferber *et al.*, 1986), the Across North America Tracer Experiment



(ANATEX) in 1987 (Draxler *et al.*, 1991) and most recently, the European Tracer Experiment (ETEX) (van Dop *et al.*, 1998).

ETEX observations

ETEX took place across Europe in autumn 1994. This experiment consisted of two 12-hour releases of perfluorocarbons (an inert and environmentally safe tracer) from Monterfil in northwest France. The concentrations of these tracers were sampled and recorded as three-hour averages, over three days following each release, by 168 sampling stations scattered across northern Europe (Figure 1). The releases were simulated in real time under emergency response conditions by 28 long-range dispersion models. The first release was well simulated by the models, but the model predictions from the second release were poor.

The major difference between the two releases was the meteorological conditions during the tracer release. In particular, towards the end of the second 12-hour release (beginning at 1500 UTC on 14 November), a cold front passed over the source location, as shown in Figure 2. The passage of the cold front led to an abrupt change in the surface wind conditions, from strong southwesterly winds prior to its passing, to weaker westerly winds at the release site afterwards (Gryning *et al.*, 1998).

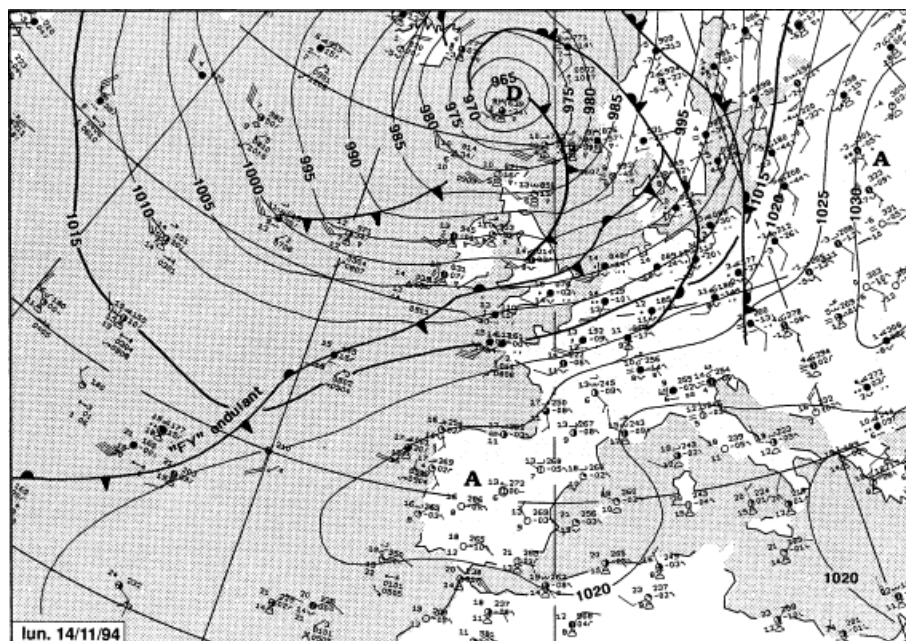
This study examines the second tracer release. The aim was to determine if a better representation of the front, achieved by increasing the temporal and/or spatial resolution of the meteorological input to the model, would have resulted in improvements in its predictions.

Some common problems were seen with all the model predictions for the poorly simulated second tracer release (Ryall and Maryon, 1998; van Dop *et al.*, 1998; Potemski *et al.*, 2008) including:

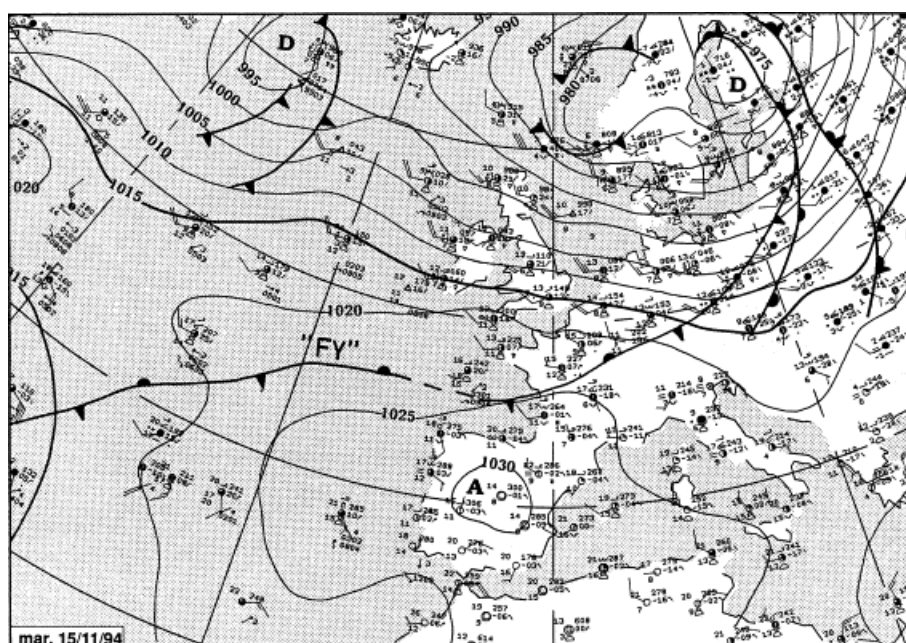
- The over-prediction of surface concentrations.
- The failure to simulate the correct direction and speed of the plume for tracer released behind the cold front.

Several hypotheses for the causes of these poor predictions have been suggested:

- Over-prediction of surface concentrations may be due to insufficient horizontal or vertical diffusion or transport. Frontal ascent linked to the passage of the cold front could have removed some of the tracer from the boundary layer, which, if not modelled correctly, would lead to higher predicted concentrations at the ground than observed (Gryning *et al.*, 1998; Ryall and Maryon, 1998; van Dop *et al.*, 1998).
- The failure to capture rapid changes in the meteorology, in particular the changes in wind speed and direction



(a) 1200 UTC on 14 November 1994



(b) 1200 UTC on 15 November 1994

Figure 2. Surface weather maps for 1200 UTC on 14 and 15 November 1994 (Gryning *et al.*, 1998).

associated with the cold front. Initially the released tracer was advected strongly eastwards. However, the tracer released behind the front was carried at a slower rate to the eastsoutheast, as illustrated in Figure 3 (left). The meteorological input into the models (using a three-hourly temporal resolution and a 50 kilometre spatial resolution) did not pick up this abrupt change in wind conditions and the subsequent reorientation of the plume, resulting in the tracer cloud moving as one, instead of the two distinct areas seen in the observations (Ryall and Maryon, 1998).

As highlighted in these hypotheses, it is believed that a major issue that led to poor tracer concentration predictions for the second tracer release in all the models was the poor representation of a cold front that passed over the source location near the end of the tracer release period. If the wind fields associated with this front are not sufficiently resolved by the model through the meteorological data input, then poor dispersion results are to be expected. Thus, by increasing the temporal and spatial resolution of the meteorological data input to the dispersion model, it is hypothesized that improvements in the predictions would be seen.

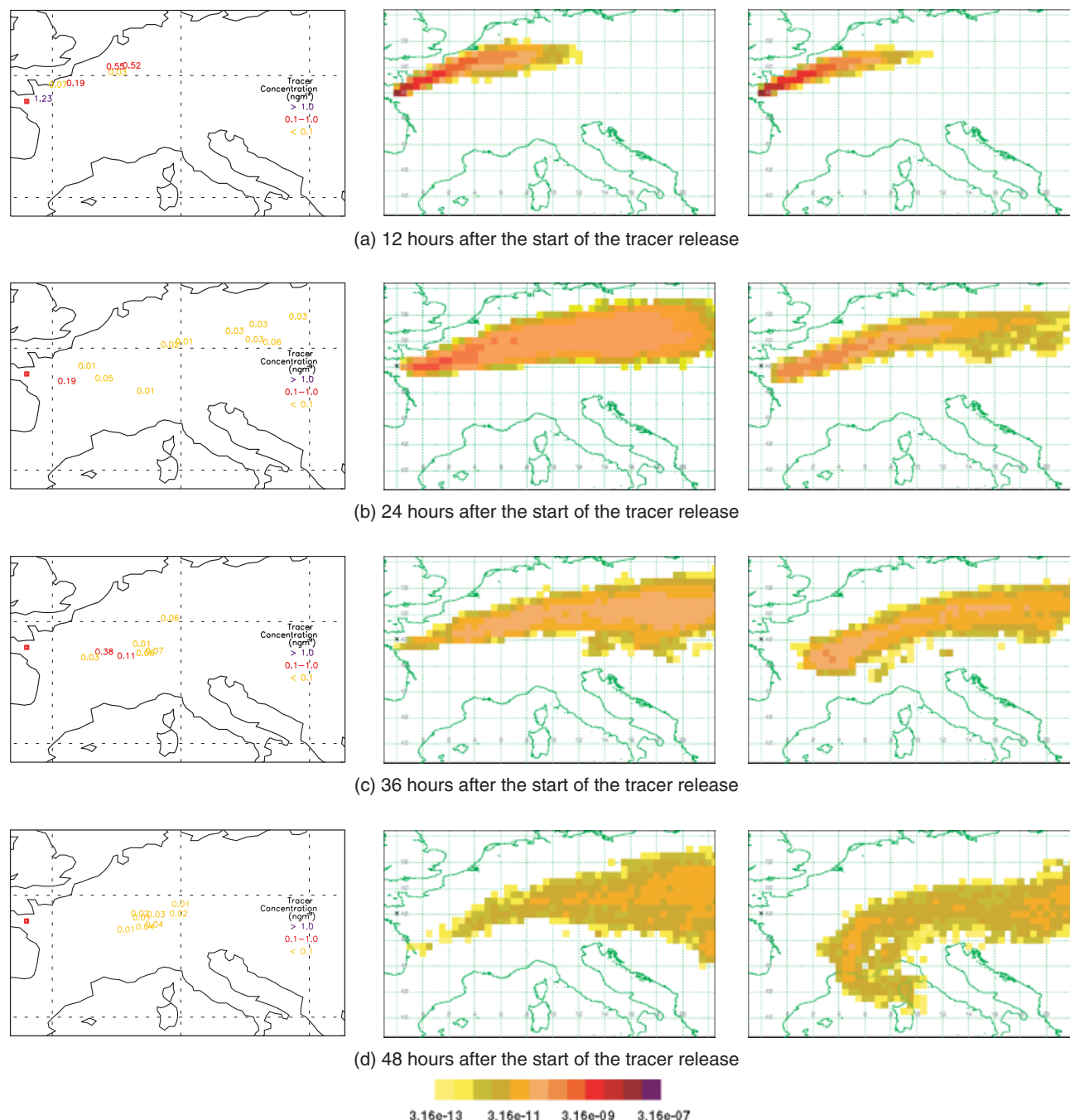


Figure 3. Surface tracer concentrations 12, 24, 36 and 48 hours after the start of the tracer release. Left: Observed surface concentrations (ngm^{-3}). The release site is indicated by the red dot. The tracer cloud was observed to initially move rapidly eastwards (a, b). Tracer released after the passing of the cold front can be seen to be carried more slowly to the eastsoutheast (b, c, d). Note that due to the sparsity of the observations, plotting these results as contours would be misleading due to the high potential for interpolation errors. Centre: Model output of surface concentrations (ngm^{-3}) using a 0.442° spatial resolution. Right: Model output of surface concentrations (ngm^{-3}) using a 0.110° spatial resolution. Both model outputs use a 30-minute temporal resolution and are plotted on a 0.5° resolution grid for comparison.

NAME model simulation results

Predicted concentrations were modelled using NAME III as this model had recently been made available for use at Reading University and is suitable for use in long-range experiments such as ETEX. To investigate the impact of changing the temporal and spatial resolution of the meteorological data input, NAME III was run using temporal resolutions from three-hourly input to 15-minute input and spatial resolutions of 0.442° latitude (approximately 50 kilometres) \times 0.442° longitude and

the higher 0.110° latitude (approximately 12 kilometres) \times 0.110° longitude.

The meteorological data used were produced from a Met Office NWP global analysis, which has a spatial resolution of $0.5625^\circ \times 0.375^\circ$. This was run from 0000 UTC on 14 November 1994 for a period of four days, to produce boundary conditions for a limited area model (LAM) for a region covering the North Atlantic and western Europe. This LAM was then run for the same days, with a spatial resolution of $0.442^\circ \times 0.442^\circ$. This domain size and resolution were chosen to replicate the meteorological input into

NAME II that was used in Ryall and Maryon (1998). Similarly, the North Atlantic LAM was used to produce boundary conditions for a smaller LAM domain over Europe. A forecast was then produced using a European LAM with a spatial resolution of $0.110^\circ \times 0.110^\circ$.

Qualitatively, there is little difference when varying the temporal resolution, although there is a tendency for the peak concentrations to be reduced as the temporal resolution is increased from three hours to 15 minutes (not shown). However, when the spatial resolution is increased, there are considerable differences. The predicted

concentrations and their evolution over time, using a 30-minute temporal resolution, are shown in Figure 3 (centre and right) for the two different spatial resolutions. Throughout the simulation the plume is narrower when using the higher (12 kilometres) spatial resolution meteorological data. The surface plume also does not extend as far to the east.

Another major change caused by increasing the spatial resolution, is the extension of the westward half of the tracer cloud further south later in the simulation (Figures 3(c) and 3(d)). Ahead of the front, the meteorological conditions were such that the tracer was rapidly advected eastwards; however the abrupt change in wind conditions caused by the passing of the front meant that the tracer released behind it was carried at a slower rate towards the east-southeast (Ryall and Maryon, 1998). The southern extension of the predicted plume may therefore be caused by the release of some of the tracer behind the cold front. Increasing the spatial resolution has enabled the change in wind speed and direction associated with the front to be better resolved by the model. This suggests a quantitative improvement in predictions through this increase in resolution. Note, however, the apparent 'curl' of the tracer cloud for the 0.110° spatial resolution in Figure 3(d) cannot be verified against the observations due to a lack of sampling stations in southern Europe (Figure 1).

Overall, when comparing individual stations, the spatial distribution of the surface tracer plume appears to agree better with the observations for the simulation which uses the higher spatial resolution meteorological data.

Statistical analysis of the NAME simulation

To quantify the changes in the predicted plumes caused by changing the temporal and spatial resolutions, statistical analysis was performed. Two of the statistics that were used are now described. Note that although many reports on model validation are available with statistics for the first ETEX tracer release, there are no corresponding results for the second release. While some papers – for example Stohl *et al.* (1998) and Potempski *et al.* (2008) – give some of the statistics used in this study, their preprocessing of the data, the time span used for the calculation, or their definition of the statistic itself, is different, so their values are not comparable and hence not given here.

The first statistic is the Pearson's correlation coefficient (r), calculated by following the methodology of Mosca *et al.* (1998). Statistics at each sampling time are based on around 20 sampling stations (Figure 4). This determines how well the modelled and observed tracer concentrations agree

spatially. The Pearson's correlation coefficient can be positive or negative, with values ranging from -1 to $+1$. Complete positive correlation, given by a value of $+1$, indicates that high predicted concentrations occur at the same time and location as the high observed concentrations. A correlation close to zero or negative suggests no skill in the model prediction. Confidence intervals for the Pearson's correlation coefficient are calculated using Fisher's z -transform (Wilks, 1995).

Figure 5 shows Pearson's correlation coefficient (r) for changes in temporal and spatial resolution. For the first 24 hours after the start of the tracer release, the variation in r with time is very similar for both the low spatial resolution (Figure 5(a)) and the high spatial resolution (Figure 5(b)). In addition, varying the temporal resolution of the meteorological input does not appear to change the value of r for either simulation. During the first 24 hours, r is either close to zero, no correlation, or close to 1, high correlation. A likely explanation is that initially, when the plume is narrow, two neighbouring observation sites may record very different tracer concentrations as the plume passes over one but not the other. Hence small errors in the model wind direction early in the simulation can lead to large errors in r . The sparse sampling network relative to the plume width enhances this problem.

In the later period of 24–48 hours after the start of the tracer release, although increasing the temporal resolution still does not affect the correlation coefficient, increasing the spatial resolution does result in a significant increase in the correlation for the majority of the time period. This is indicated by the confidence intervals in Figure 5(b) lying significantly above zero and not overlapping with the confidence intervals shown in Figure 5(a). By increasing the spatial resolution, the wind fields associated with the cold front are better resolved. This leads

to the model now being able to represent the tracer released behind the front and its slower advection to the east-southeast. The effects of this are more apparent later in the simulation once the tracer has moved along a significantly different course than if the front had not been as well resolved. Hence the increased spatial resolution leads to a significant improvement in the correlation for the second half of the simulation.

The second statistic considered is the fractional bias (FB) which is as defined and used by Stohl *et al.* (1998). The FB can be positive or negative, which indicates over- or under-prediction respectively of the model concentrations in comparison to the observations. The possible values for FB can vary from $+2$, extreme over-prediction, to -2 , extreme under-prediction. A value of ± 0.67 indicates that the observations and predictions agree to within a factor of 2, which is considered to be a good prediction. FB does not give any information about the quantity of occurrences of over- and under-predictions. Hence, although a 'perfect' model would have an FB of zero, if the model does have a value of zero this does not necessarily mean that all the predictions agree with the observations. It may be instead that half the results are over-predictions, while the other half are under-predicting the concentrations. Spatial analysis of results can help determine if this is the case. Confidence intervals for the FB are calculated using the jackknife method (Martinez and Martinez, 2002).

Figure 6 shows the FB for changes in spatial and temporal resolution. For the first 24 hours the FB is strongly positive (over-prediction) for both spatial resolutions and there is no significant difference due to increasing the temporal resolution of the meteorological input. Spatial analysis of the results (not shown here) supports this, with the model over-predicting concentrations at nearly all stations during this

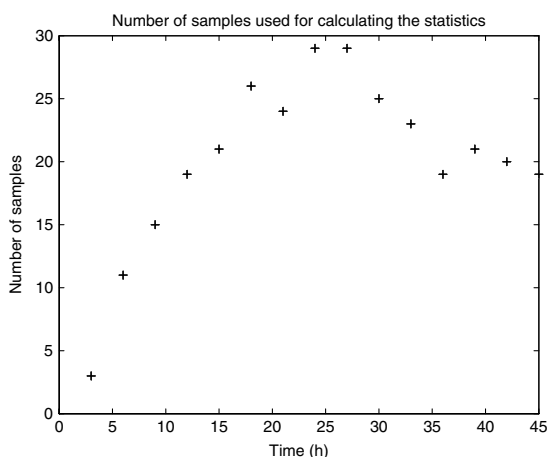


Figure 4. Number of samples used for calculating the statistics at each time interval. Time is given as hours after the start of the tracer release. Near the start of the release, due to the small plume size only covering a limited area, few sampling stations can be seen to record any tracer. The results of the statistics are therefore more likely to be reliable after the first few hours. Note that although 168 sampling stations were set up for the experiment, very few in comparison actually recorded the tracer.

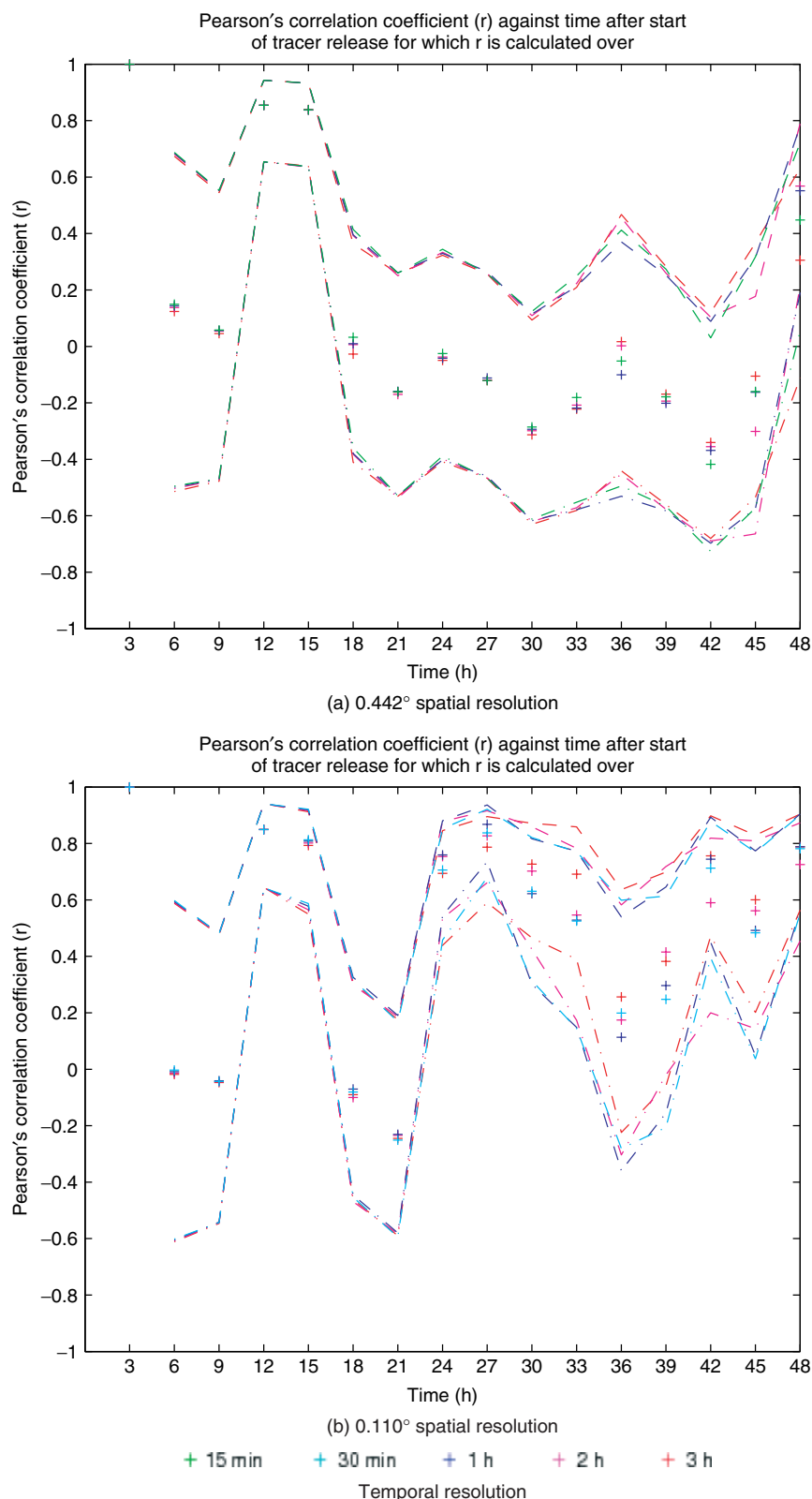


Figure 5. Pearson's correlation coefficient calculated for each sampling time (three-hourly), for each of the temporal resolutions and for (a) 0.442° spatial resolution and (b) 0.110° spatial resolution. Time is given as h after the start of the tracer release. Confidence intervals for each temporal resolution are shown as dashed lines.

period. Note that the highest concentrations occur in the first 24 hours as after this the tracer plume spreads out further, leading to the dilution of the tracer and hence lower concentrations. Initially high concentrations, coupled with small errors in the angle of the plume axis can cause a high

predicted concentration to coincide with a low measured concentration, resulting in the large over-prediction of the concentration and hence a high FB. Following this initial period, the FB is observed to decline significantly as the tracer concentrations are better predicted.

For the lower spatial resolution it can be observed (Figure 3) that the plume is more spread out and hence peak concentrations are lower than for the higher spatial resolution simulation. This results in an artificially lower FB, particularly when using the lower temporal resolutions such as 3-hourly meteorological input. However, increasing the temporal resolution can be seen (Figure 6(b)) to significantly reduce the FB for the higher (0.110°) spatial resolution. The reasons for this were considered by examining the vertical structure of the tracer cloud (not shown). This indicated that increasing the temporal resolution, at the high spatial resolution, leads to increased vertical lifting of the plume due to frontal ascent. This enhanced lifting leaves less tracer to advect at ground level, hence causing lower surface concentrations and a consequent reduction in the FB. Notice there is no significant difference in the FB if the meteorological input is increased beyond one hour.

Conclusions

This study has simulated the second tracer release from the ETEX experiment, using the Met Office's dispersion model NAME III. The aim was to determine if improving the representation of the front that passed over the source location during the release, through increasing the temporal and spatial resolution of the meteorological input to NAME III, would lead to improvements in the model predictions of the plume location and concentrations.

It is concluded that increasing the spatial and temporal resolution of the meteorological input data, does lead to improvements in the simulation, particularly in the period 24–48 hours after the start of the release.

Increasing the spatial resolution from 0.442° latitude \times 0.442° longitude to 0.110° latitude \times 0.110° longitude leads to significant improvements in the spatial location of the tracer cloud. In particular, tracer released behind the passing cold front is observed to be more accurately simulated due to the better representation of the wind fields associated with this front.

Increased temporal resolution leads to some improvements in the magnitude of surface concentrations. However, these improvements are seen to be important only for the highest spatial resolution. An increase in both the spatial resolution and the temporal resolution to a one-hourly input of meteorological data gives the best results, with improvements observed in both the location of the tracer cloud and in the predicted concentrations.

For use in practical applications, such as in emergency response scenarios where it is important to rapidly predict a pollutant's movement and its potential concentration, it should be recognized that a balance

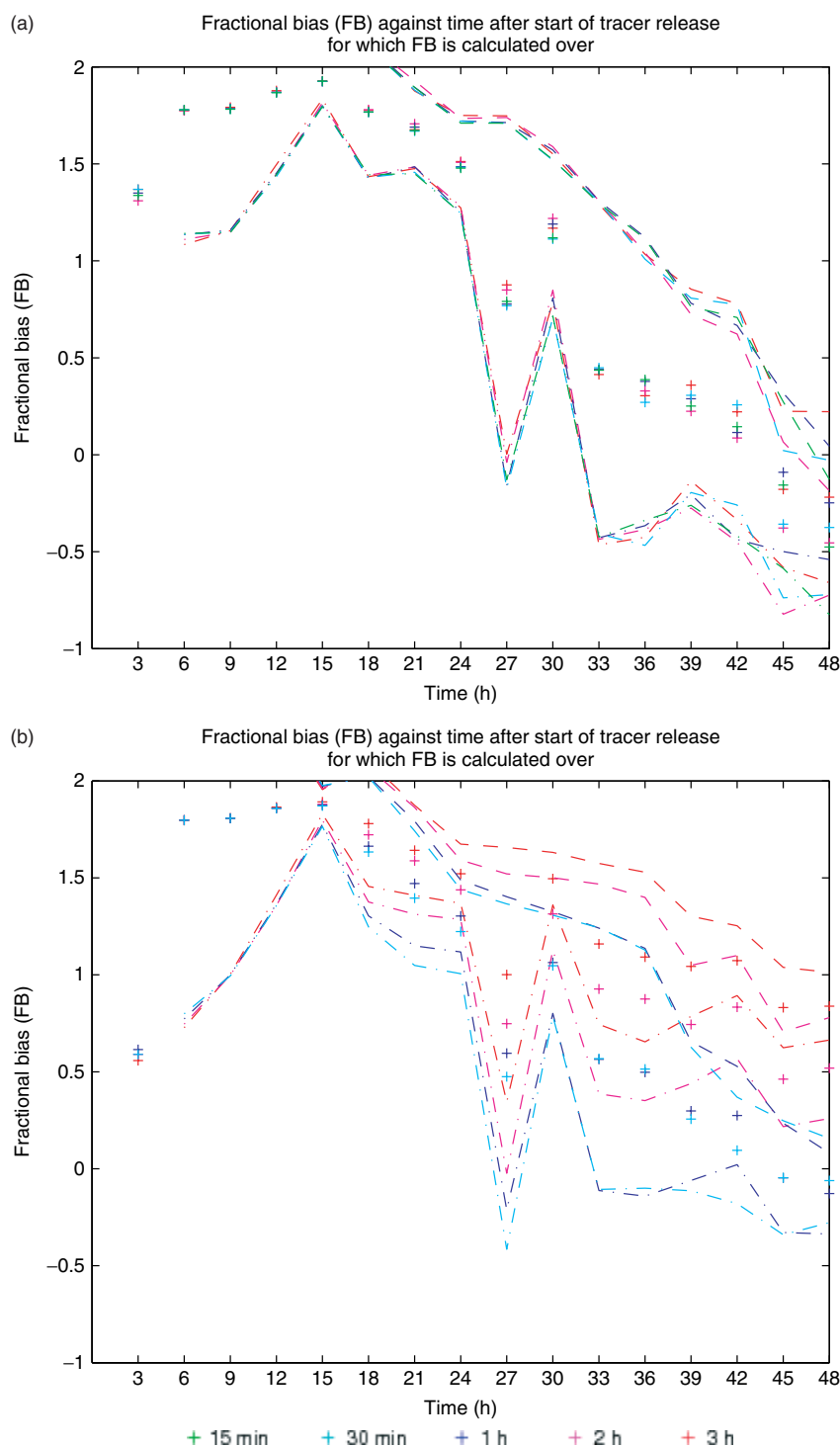


Figure 6. FB calculated for each sampling time (three-hourly), for each of the temporal resolutions and for (a) 0.442° spatial resolution and (b) 0.110° spatial resolution. Time is given as h after the start of the tracer release. Confidence intervals for each temporal resolution are shown as dashed lines.

needs to be reached between the value of increasing the spatial and temporal resolution of the meteorology, compared to the longer computational time needed to gain these significant improvements.

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