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## Predicting *Aspergillus fumigatus* exposure from composting facilities using a dispersion model: A conditional calibration and validation



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### ABSTRACT

Bioaerosols are released in elevated quantities from composting facilities and are associated with negative health effects, although dose–response relationships are unclear. Exposure levels are difficult to quantify as established sampling methods are costly, time-consuming and current data provide limited temporal and spatial information. Confidence in dispersion model outputs in this context would be advantageous to provide a more detailed exposure assessment. We present the calibration and validation of a recognised atmospheric dispersion model (ADMS) for bioaerosol exposure assessments. The model was calibrated by a trial and error optimisation of observed *Aspergillus fumigatus* concentrations at different locations around a composting site. Validation was performed using a second dataset of measured concentrations for a different site. The best fit between modelled and measured data was achieved when emissions were represented as a single area source, with a temperature of 29 °C. Predicted bioaerosol concentrations were within an order of magnitude of measured values (1000–10,000 CFU/m<sup>3</sup>) at the validation site, once minor adjustments were made to reflect local differences between the sites ( $r^2 > 0.7$  at 150, 300, 500 and 600 m downwind of source). Results suggest that calibrated dispersion modelling can be applied to make reasonable predictions of bioaerosol exposures at multiple sites and may be used to inform site regulation and operational management.

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### 1. Introduction

Composting in Europe has seen significant growth in recent years, as the waste industry diverts waste from landfill. Key in driving change is the European Landfill Directive (1999/31/EC). Bioaerosols are aerosolised biological particles and include many forms of fungi, bacteria, pollen, fragments, by-products and constituents of cells (Douwes et al., 2003). Typically these are small particles (<10 µm) (Dowd and Maier, 2000; Galès et al., 2015; Tamer Vestlund et al., 2014), enabling them to penetrate deeply into the lung (Douwes et al., 2003; Ivens et al., 1999). They have been associated with adverse health effects, including allergic and non-allergic asthma, chronic bronchitis, rhinitis and aspergillosis, that give rise to associated public concern (Pearson et al., 2015; Searl 2008; Swan et al., 2003). Bioaerosols can be released in elevated quantities at composting facilities, particularly when the material is agitated (Taha et al., 2006). However, the exposure patterns and

**Abbreviations:** ADMS, atmospheric dispersion modelling system; CERC, Cambridge environmental research consultants; CFU, colony forming units; F, F-test; FB, fractional bias; LOD, limit of detection; MD, mean difference; ME, modelling efficiency; RMSE, root mean square error; VBNC, viable but not culturable; WIBS, wideband integrated bioaerosol sensors.

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dose-response relationships of bioaerosols from composting are not well understood and data are limited (Pearson et al., 2015). To some extent this is a result of current measurement techniques which rely on capturing and culturing bioaerosols. This is time consuming and expensive, and only provides a snapshot of exposure spatially and temporally (Douglas 2013; Williams et al., 2013). Dispersion modelling (local scale mathematical prediction of the dispersion and dilution of pollutants within the atmosphere) has the potential to overcome these limitations by predicting a continuous exposure surface but it has been little utilised, primarily due to a lack of data to establish input parameters and for model testing.

The aim of this study was to evaluate the ability of a calibrated dispersion model to predict bioaerosol dispersion from open windrow composting facilities.

A limited number of studies have modelled bioaerosol dispersion from composting facilities (e.g. ADAS and SWICEB, 2005; Douglas 2013; Drew et al., 2005, 2007a; Environment Agency, 2001; Shi and Hodson 2012; SNIFFER, 2007; Taha et al., 2005, 2006; Tamer Vestlund, 2009; Williams et al., 2013). Many do not fully report the input values used. In those that do, large variations exist in parameterisation, often with a lack of justification (Douglas, 2013). Meanwhile, inverse modelling of measured ambient bioaerosol concentrations have produced source term estimates spanning several orders of magnitude (Douglas, 2013; Shi and Hodson, 2012). In part, this reflects a limited knowledge of source characteristics and how best to represent them in dispersion models along with uncertainties about the interpretation of “snapshot” measurements of ambient bioaerosol concentrations. Whilst dispersion models have been validated for a variety of chemical and particulate emissions from well-quantified sources (Derwent et al., 2010), they have, to our knowledge, never been properly calibrated and validated for an open windrow composting scenario. Doing so would give greater confidence in predicted exposures and allow dispersion modelling to be employed as a cost effective way of estimating spatial and temporal patterns at local and national scales. This could aid future epidemiological studies, as recommended future research in a recent cross-sectional ecological study which analyses respiratory hospital admission risk near large-scale composting facilities (Douglas et al., 2016). Furthermore confidence in modelled output concentrations has the potential to inform site management strategies and the statutory permitting process.

## 2. Materials and methods

### 2.1. Dispersion model

The Atmospheric Dispersion Modelling System (ADMS), version 4.2 was employed. ADMS is a Gaussian-based dispersion model developed by Cambridge Environmental Research Consultants (CERC) in which the atmospheric boundary layer is characterised by the Monin-Obukhov length and boundary layer depth (CERC, 2015a). It can simulate plume rise and is capable of accounting for various plume dispersion phenomena including dry and wet deposition (CERC, 2015a). It has been extensively validated (CERC, 2015b) within its specified capabilities, covering a variety of sources, topography and gaseous pollutants and has been widely used, particularly in UK-based dispersion modelling studies. It was chosen here because it has been the most extensively used model in bioaerosols studies to date (Drew et al., 2007a; Shi and Hodson 2012; Taha et al., 2007; Williams et al., 2013).

### 2.2. *Aspergillus fumigatus* monitoring data

The fungi *Aspergillus fumigatus* was chosen as an indicator bioaerosol component because; (i) it is widely monitored (Pearson

et al., 2015); (ii) it has important potential health implications (Environment Agency 2010; Nadal et al., 2009; Pearson et al., 2015; Vilavert et al., 2012); (iii) it is known to be emitted in elevated quantities above background from composting processes; (iv) it is included in the English Environment Agency's position statement on acceptable bioaerosol levels from composting at a community scale (Environment Agency, 2010). Data described by Pankhurst et al. (2011) were used for calibration and validation. These include repeated and replicated sampling results taken over two years from two commercial open windrow composting facilities. The facilities represent typical open windrow sites in England. Site A (used for calibration) is located in a rural area, and is licensed to process 74,999 t of green waste per annum. Site B (used for validation) is located near to an industrial estate and is licensed to process 25,000 t of green waste per annum. Site A was used for calibration as the location is very typical of most composting facilities in the UK in terms of composting techniques and tonnages, as well as being located in a flat, rural area with limited other impacts on the local meteorology. Site B has a more complex local meteorology, and was therefore a good test of the calibration results when used for validation. Numerous samples (411 at site A and 389 at site B) were collected at various locations over 14 (Site B) and 15 (Site A) sampling days respectively. Sampling locations were spatially-referenced and included upwind, on-site and downwind areas. Downwind samples were taken at regular distances from the site boundary up to approximately 300 m (Site A) and 600 m (Site B). Exact locations for the downwind sampling changed depending on wind direction and site accessibility.

Filter samplers were used to collect all samples. These samplers have a high lower limit of detection (LOD) due to the low air flow rate ( $2.2 \text{ L min}^{-1}$ ) of 757 Colony Forming Units per cubic metre ( $\text{CFU/m}^3$ ), which generated multiple apparent ‘zero’ values (i.e. within the range of 0 to  $756 \text{ CFU/m}^3$ ). ‘Zero’ values were, therefore, recoded as 756 to represent the worst case scenario (LOD-1). Averages of sample replicates were used for comparison with model predictions. The data show a general decrease in bioaerosol concentration with dispersal distance, although a secondary concentration peak was apparent 100–150 m from the site boundary (Pankhurst et al., 2011), which was attributed to buoyancy effects.

### 2.3. Calibration and validation

Calibration was performed using an iterative trial and error procedure, modifying model input parameters one-at-a-time in order to minimise the discrepancy between predicted and measured bioaerosol concentrations. The procedure followed was originally developed for river flow forecasting (Nash and Sutcliffe, 1970). The goodness of fit was calculated after each modification via a series of statistical tests (2.4).

Initially, a basic model setup was adopted, excluding the use of advanced model options such as dry and wet deposition for which parameterisation would be difficult for bioaerosols from composting, given limited prior knowledge. A single meteorological scenario was used, and a single output concentration at each distance downwind was calculated in the first instance. This facilitated direct comparisons between the sampled data and modelled outputs. Input parameters were modified within ranges relevant to bioaerosol emissions from composting, constructed from the literature (ADAS and SWICEB, 2005; Danneberg et al., 1997; Douglas 2013; Dowd and Maier, 2000; Drew et al., 2007a; Environment Agency 2001; Millner et al., 1980; SNIFFER, 2007; Taha and Pollard 2004; Taha et al., 2006, 2007; Tamer Vestlund 2009; Williams et al., 2013) (Table 1). Optimisation was performed on the most sensitive model input parameters first (i.e. those for which small changes in the model input values result in large changes in the modelled outputs) generated via a sensitivity analysis (Douglas, 2013). The

**Table 1**

Model input values initially used in the calibration (based on results from Douglas, 2013 – Appendix A). Ranges of modifications were based on current literature. Model inputs which provided the best goodness of fit between the modelled and measured data are also shown. All model input values not stated below were kept at the model default values.

Model input parameter (units)	Initial input value	Range for modifications <sup>a</sup>	Optimal values
Source type	Area	–	Area
Specific heat capacity of the pollutant (J/°C/kg)	1519	800–2100	1519
Molecular mass of the pollutant (g)	25.324	15–45	28.966
Source Height (m)	2.65	0–5	2.65
Source geometry (m)	13.30 × 17.00	0.5–15	44.00 × 9.50 to represent a composting windrow, estimated used aerial maps (centred on the grid coordinates of the centroid of the site area)
Pollutant exit velocity (m/s)	2.90	0–25	2.95
Pollutant temperature (°C)	35.10	0–60	29.00
Pollutant emission rate (g/m <sup>2</sup> /s) <sup>b</sup>	1 × 10 <sup>5</sup>	1 × 10 <sup>6</sup> –9 × 10 <sup>10</sup>	9.00 × 10 <sup>6</sup>
Pollutant properties	New pollutant named 'AF' – kept at default values	–	New pollutant named 'AF' – kept at default values
Surface Roughness (m)	0.87	0.005–1.500	0.20
Meteorological data	See Appendix A	–	Hourly meteorological data collected from the nearest weather station was used (purchased from the UK meteorological office). Only the hours in which the samples were taken were extracted and used (calms option used)
Background pollutant levels <sup>c</sup>	Not used	756.00 g/m <sup>3</sup>	756.00 g/m <sup>3</sup>
Model output grid	See Appendix A	–	Specified points based on the GPS data of the actual sampling point were used to allow direct comparison between modelled and monitored data
Pollutant output averaging time	Short term 30 min	–	Short term 30 min

<sup>a</sup> Based on ADAS and SWICEB (2005), Danneberg et al. (1997), Douglas (2013), Dowd and Maier (2000), Drew et al. (2007a), Environment Agency (2001), Millner et al. (1980), SNIFFER (2007), Taha and Pollard (2004), Taha et al. (2006, 2007), Tamer Vestlund (2009), and Williams et al. (2013).

<sup>b</sup> Proxy for CFU/m<sup>2</sup>/s.

<sup>c</sup> Proxy for CFU/m<sup>3</sup>.

pollutant emission rate was altered at various stages of the calibration process (within specified uncertainty limits) to adjust the overall magnitude of predicted concentrations (rather than the spatial pattern) since predicted concentrations at all locations varied approximately linearly with emission rate (Johnson, 2011). Initial parameter values are summarised in Table 1.

Validation of the model for bioaerosol emissions from composting was performed using the optimal model input values obtained via calibration. Model predictions were compared to measured data collected at a second site (Site B) in order to evaluate model performance with an independent data set. It should be noted that ADMS does not have the option to estimate pollutant concentrations in CFU/m<sup>3</sup>. Therefore, g/m<sup>3</sup> were used as a proxy for CFU/m<sup>3</sup>. Differences in local conditions between site A and site B, such as meteorology and source geometry, were accounted for by using data from the nearest meteorological station and changing the typical windrow length, based on aerial images. All other parameters were left unchanged.

#### 2.4. Statistical analysis

Goodness of fit (including degree of association and coincidence) between the modelled and measured data were determined using the Root Mean Square Error (RMSE), Modelling Efficiency (ME), correlation coefficient (r), coefficient of determination (r<sup>2</sup>), F-Test (F), Mean Difference (MD) and Fractional Bias (FB) using MS Excel (Appendix B). These are recognised fit statistics and have been used in several other model calibration and validation studies (CERC 2015b; Chang et al., 2012; Hollis et al., 2011; Katerji et al., 2010; Ludwig et al., 2011).

The criteria used to evaluate the quality of each goodness of fit statistic (Appendix C) were based on acceptance values reported in other model validation studies (CERC 2015b; Chang et al., 2012; Hollis et al., 2011; Katerji et al., 2010; Ludwig et al., 2011). Values reported in these studies were broad ranging. For clarity, we used

a categorisation and colour-coding system based on these studies where statistical values which were considered to be a good fit in all studies were colour coded dark grey and classified as having a 'very good fit'. If criteria values were considered a good fit based on some criteria but not on others then these were classified as having a 'reasonable fit' and colour coded light grey (Appendix C). The calibration process was stopped when input value modifications resulted in marginal or no change in the statistical tests. Statistics were calculated to allow comparison with samples grouped by the specific distances downwind measured at 50, 80, 100, 150, 180, 250, 280 and 300 m.

### 3. Results

#### 3.1. Calibration

36 adjustments were made to the initial model inputs, summarised in Fig. 1 (full details in Appendix D) to obtain a best fit between predicted and monitored bioaerosol concentration data. The parameter set which resulted in the best fit between the modelled and monitored data is presented in Table 1.

Goodness of fit statistics are presented in Table 2a and illustrated graphically in Fig. 2a. It was not possible to calculate some statistics, due to division by zero errors (e.g. when the sum of the modelled minus the mean modelled values equal zero: Appendix B). Table 2a and Fig. 2a also show comparisons between measured concentrations and initial model predictions prior to calibration. The uncalibrated model clearly underestimates the measured concentrations resulting in a poor model fit (Table 2a). This bias appeared to be corrected by the calibration procedure. The calibrated model was able to predict downwind concentrations reasonably well (Fig. 2a), even capturing the 'secondary peak' of bioaerosol concentration observed at 100–150 m downwind (Pankhurst et al., 2011). Values for RMSE (which measures the degree of coincidence) and

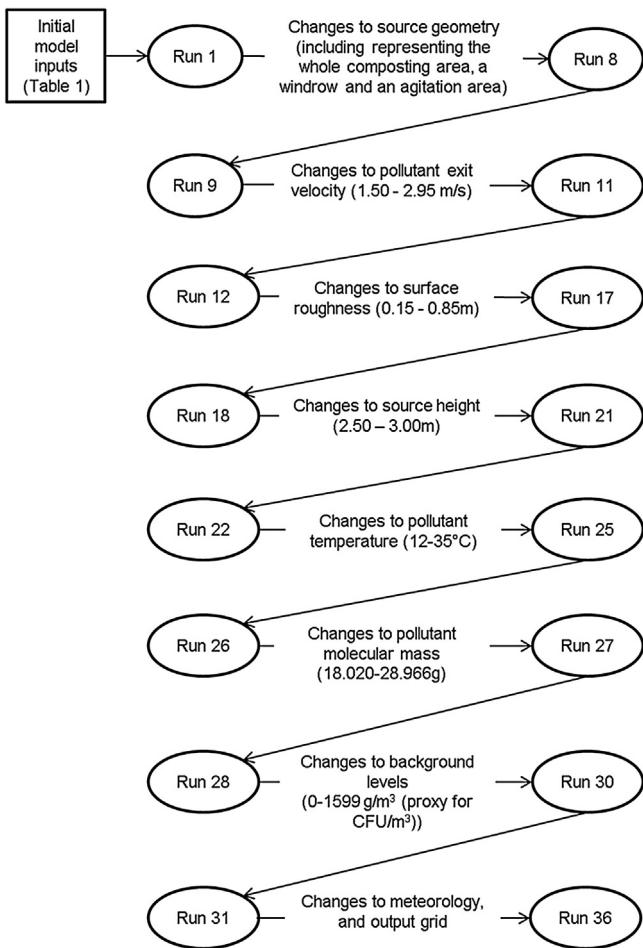
**Table 2**  
Statistical test results for a) model calibration and b) model validation. Shaded cells indicate the quality of the fit statistic against the criteria shown in Appendix C and rounded to 1DP. 'NP' denotes that it was not possible to calculate the statistic.

a) Comparison between the initial and final model calibration runs

Statistical test	Initial model run									Final model run						
	50	80	100	150	180	250	280	300	50	80	100	150	180	250	280	300
RMSE	153.8	69.2	233.1	144.5	90.9	131.2	89.9	90.7	47.9	0.0	242.0	339.7	27.2	57.3	3.8	113.1
ME	-0.6	-25.8	-0.2	-0.8	-25.3	-1.2	NP	-1116.1	0.9	NP	-0.3	-7.0	0.2	0.7	NP	-1.0
r	NP	NP	NP	NP	NP	NP	NP	NP	1.0	NP	-0.2	0.2	0.9	1.0	NP	1.0
r <sup>2</sup>	NP	NP	NP	NP	NP	NP	NP	NP	1.0	NP	0.1	0.0	0.8	1.0	NP	1.0
F	NP	NP	NP	NP	NP	NP	NP	NP	92.2	NP	0.2	0.1	6.5	2027.3	NP	NP
MD	7967.4	556.4	1755.4	3573.8	899.3	2793.7	679.4	704.5	-761.7	-0.1	1038.6	-3524.3	-93.7	-845.3	-14.4	-336.2
FB	1.8	1.0	2.0	1.9	1.6	1.9	1.6	1.7	-0.1	0.0	0.8	-0.7	-0.1	-0.3	-0.0	-0.6

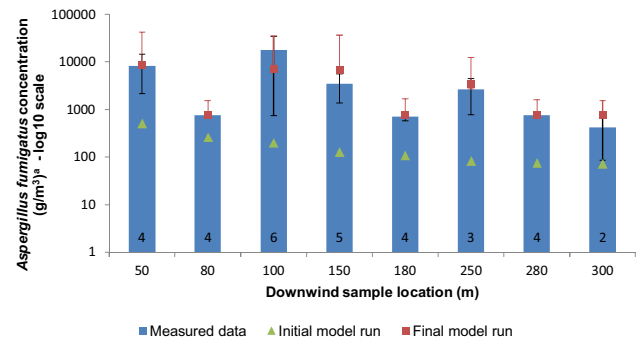
b) Model validation

	50	100	150	200	300	400	500	600
RMSE	739.1	1558.2	2082.1	610.0	1585.3	933.8	618.0	293.0
ME	-105.2	-32.9	-1492.6	-62.1	-1549.8	NP	-36.0	-6.9
r	0.1	0.4	1.0	0.6	0.8	NP	1.0	1.0
r <sup>2</sup>	0.0	0.2	1.0	0.4	0.7	NP	1.0	1.0
F	0.0	5.2	NP	9.4	23.9	NP	547.4	2216.6
MD	-15303.2	-35332.8	-24160.9	-7794.3	-6530.9	-3563.6	-6328.8	-5005.8
FB	-1.4	-1.6	-1.8	-1.1	1.6	-1.4	-1.3	-0.9

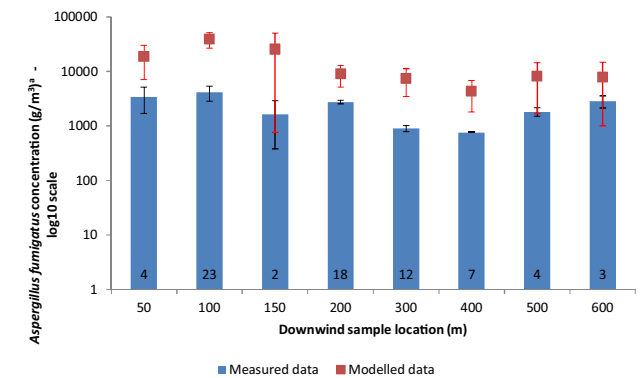


**Fig. 1.** Summary of the alterations made to the model inputs in the model calibration process (full details in Appendix D).

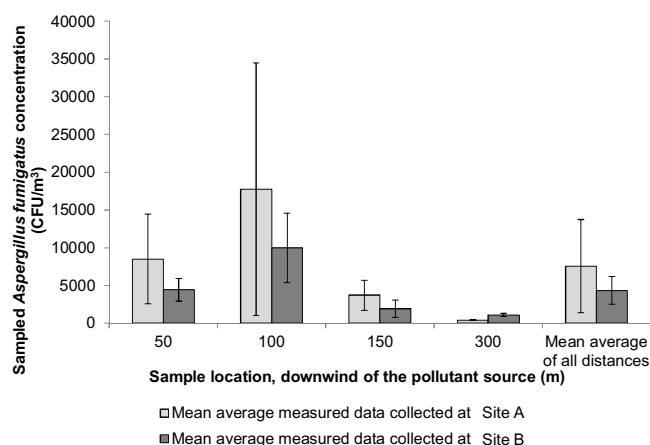
a) Comparison between the initial and final calibration model runs



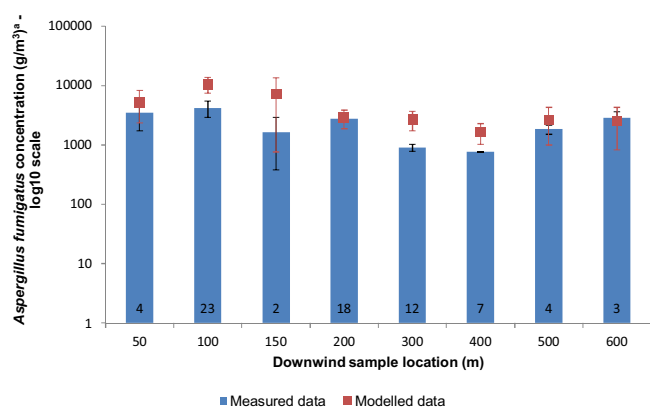
b) Model validation



**Fig. 2.** Modelled and measured concentrations of *A.fumigatus* for (a) model calibration and (b) model validation. Graph A shows the modelled data at the start of the calibration process (initial model run) and at the end of the process (final model run). The measured data presented represent the arithmetic mean of the measured data at that particular downwind location. Error bars on the modelled (red) and measured (black) data denote minima and maxima. The numbers at the base of the measured data bars indicate the number of samples taken at that distance. 1 - Proxy for CFU/m<sup>3</sup>.



**Fig. 3.** Comparison of the sampled data collected at Site A and Site B, at coherent downwind locations (50, 100, 150 and 300m). Error bars denote the standard error of the arithmetic mean.



**Fig. 4.** Modelled and measured concentrations of *A. fumigatus* for the model validation after changes to the emission rate. Error bars denote minima and maxima for modelled (red) and measured (black) data. The numbers at the base of the measured data bars indicate the number of samples taken at that distance. 1 – Proxy for CFU/m<sup>3</sup>.

$r$  and  $r^2$  (which measure the degree of association) between the modelled and measured data, all indicated a good fit.

### 3.2. Validation

Performance of the optimised model in the validation process is summarised in Fig. 2b and Table 2b. Similarly to the calibration, it was not possible to calculate some goodness of fit statistics due to division by zero errors.

Fig. 2b indicates that predicted concentrations tend to overestimate measured concentrations in the validation, although the spatial trend is captured quite well (high  $r$  and  $r^2$  values: Table 2b). This suggests that the emission rate used may have been too high. This explanation is corroborated in Fig. 3 which shows the measured concentration data from Sites A and B at downwind locations of 50, 100, 150 and 300 m.

Measured *A. fumigatus* concentrations at Site B were significantly lower (by an average of 75%) than those in comparable samples collected at Site A. The emission rate was, therefore, reduced by 75% from  $9 \times 10^6$  g/m<sup>2</sup>/s to  $2 \times 10^6$  g/m<sup>2</sup>/s (proxy for CFU/m<sup>2</sup>/s). Results are presented in Table 3 and Fig. 4, respectively.

Fig. 4 indicates that the new emission rate resulted in better agreement between the model outputs and the measured data (predicted bioaerosol concentrations within an order of magnitude of measured values: 1000–10,000 CFU/m<sup>3</sup>), although the predictions

remain consistently higher than the observations. The statistical results (Table 3) show a reduction in RMSE (from 293 to 2082 to 21–469) and FB values closer to zero (from  $-1.8$ – $1.6$  to  $-1.2$ – $0.1$ ). The degree of association resulting from the adjusted emission rate remains the same. Overall, the results from the emission-adjustment indicated a reasonable fit.

## 4. Discussion

To our knowledge, this is the first time that a dispersion model has been calibrated and validated for *A. fumigatus* emissions from composting facilities. Validation was based on multiple sampling points taken over a period of two years. The results provide generic and specific insights into how to improve model representation of bioaerosol emission and dispersion. This is likely to lead to improved confidence in temporal and spatial exposure predictions which can provide more cost effective bases for bioaerosol risk assessment. Further model applications have the potential to aid policy formulation, influence the design of epidemiological studies, guide site management strategies and inform the permitting process and its conditions.

The agreement between modelled outputs and measured data was best achieved when:

- Emissions are represented as a single area source with a geometry relating to the size of a typical windrow;
- An initial emission temperature of 29°C [within the range of observed values obtained from thermal imaging employed to quantify emission temperatures by Douglas (2013)] and an exit velocity of 2.95 m/s [rather high, but this has never been quantified before in the composting context] are employed;
- Background concentrations are set to the LOD-1 for the sampling method;
- Meteorological data collected from the nearest weather station are used;
- A short term averaging time of 30 min is used [consistent with the typical duration of bioaerosol measurements, although even shorter averaging times may help better-capture peak concentrations (Drew et al., 2007b)];
- Emission rate is adjusted in proportion to the measured data.

Previous studies have used a range of emission rates when modelling bioaerosol emissions from composting facilities. ADAS and SWICEB adopted a low emission rate of  $4.0 \times 10^{-7}$  g/m<sup>2</sup>/s as they converted CFU/m<sup>3</sup> into mg/m<sup>3</sup>. Other modelling studies did not convert emissions rates, resulting in values ranging from  $2.0 \times 10^1$ – $8.9 \times 10^8$  CFU/s (point sources: SNIFFER, 2007; Taha et al., 2006) and  $9.4 \times 10^1$ – $3.6 \times 10^5$  CFU/m<sup>2</sup>/s (area sources: Drew et al., 2007a; SNIFFER, 2007) which are in-line with the emission rate ( $2 \times 10^6$  g/m<sup>2</sup>/s) used in this study.

There have been a few previous attempts to compare modelled bioaerosol emissions from composting facilities with measured data (e.g. Drew et al., 2007a; SNIFFER, 2007; Tamer Vestlund, 2009; ADAS and SWICEB, 2005). However, formal (quantitative) comparisons between model outputs and measured concentrations were often not made in these studies, which makes goodness of fit difficult to assess. Furthermore, most previous comparisons have used a low number of sampling points (typically 2–3) and, in general, appear to have underestimated measured bioaerosol concentrations by up to three orders of magnitude. The exception is the study by ADAS and SWICEB (2005) in which ADMS predictions (also employing an area source) appear to be reasonable compared to measured concentrations, albeit at only three locations (47, 97, and 147 m downwind of the emission source). In contrast, Drew et al. (2007a) have reported that current risk

**Table 3**  
Statistical test results for the validation run after changes to the emission rate. Shaded cells indicate the quality of the fit statistic against the criteria shown in Appendix C and rounded to 1DP. 'NP' denotes that it was not possible to calculate the statistic.

Statistical test	50	100	150	200	300	400	500	600
RMSE	170.4	369.0	468.7	120.0	386.6	235.7	69.2	21.4
ME	-4.6	-0.9	-74.7	-1.4	-91.2	NP	0.5	1.0
R	0.1	0.4	1.0	0.6	0.8	NP	1.0	1.0
r <sup>2</sup>	0.0	0.2	1.0	0.4	0.7	NP	1.0	1.0
F	0.0	5.2	NP	9.4	19.2	NP	547.4	2216.6
MD	-1860.8	-6389.9	-5439.0	-1579.2	-1805.0	-899.1	-794.9	310.0
FB	-0.4	-0.9	-1.2	-0.0	-1.0	-0.7	-0.4	0.1

assessment methods recommended by regulators in Europe tend to over-estimate bioaerosol exposure to receptors. In the most recent modelling study (Williams et al., 2013), visual comparisons of ADMS-predicted concentration patterns of *A. fumigatus* and total bacteria, with data collected at four different sites over a period of a year were generally poor.

#### 4.1. Strengths, limitations and future work

Although the datasets used in this study were collected over short time scales (i.e. sampling periods of 2–3 weeks per site in a two year period), they are well replicated and provide insight into temporal and spatial variations of bioaerosol exposure. Uncertainties were minimised by always employing the same sampling team, using the same sampling equipment and enumerating bioaerosols in the same laboratory. Approximately eight 30-min samples were collected per day (Pankhurst et al., 2011) at each location. The data from Site A were collected at locations up to 300 m downwind of the source, whereas data from Site B were collected up to 600 m downwind of source. Fewer samples were taken at Site A compared to Site B due to access difficulties. The presence of buildings north of Site B may have affected pollutant dispersal but these effects were not modelled. The reasonable association between modelled and measured concentration data suggests that they were not a major influence on dispersal or deposition. However, this influence should be considered in the design of future modelling studies (there is a feature in ADMS to account for buildings but this cannot currently be used when the source is represented by an area).

Although the measured data used in this study provides useful insights into how *A. fumigatus* concentrations vary along downwind transects, they offer limited information on plume variation or temporal stability. The sampling method employed is time consuming, expensive and provides only a 'snapshot' of exposure in space and time. Moreover, it relies on culturing samples and hence captures only viable, culturable bioaerosol fractions. Although non-viable, or viable but not culturable (VBNC), fractions may have been present (and could have the potential to contribute to ill health: Pearson et al., 2015; Searl, 2008) they would not be recorded in the samples using this method. Exposure to potentially harmful bioaerosol components could, therefore, be underestimated, particularly if large variations occur outside the sampling period. In addition, the method used had a high LOD. Samples with concentrations < LOD were assumed to have concentrations equal to LOD-1, representing a 'worst case' scenario. Other values could have been chosen (e.g. zero or half the LOD), although it is unlikely that this would have affected the calibration process. Further investigation of low-level background concentrations of bioaerosols is required, as highlighted by Pearson et al. (2015).

Some of the challenges which arose in calibration and validation can be attributed to the fact that the measured data were not collected explicitly for this purpose. Bioaerosols data can be collected for various reasons (e.g. for risk assessment or simply to help

understand dispersal and deposition dynamics) which may not be fully compatible with evaluating dispersion models. Further validation is required by applying the optimal parameter combination to other sites and comparing predicted concentrations to independent observations. It would be advantageous if modelled outputs could be compared to more spatially and temporally rich measured data for a more robust validation. Continuous sampling methods such as Wideband Integrated Bioaerosol Sensors (WIBS) (O'Conner et al., 2015), are still being developed, but have the potential to collect high frequency data, in a variety of weather conditions, and to include non-viable and VBNC fractions.

The measured concentration data used here for calibration and validation are well within the range of bioaerosol concentrations reported in other exposure studies (Appendix E, taken from Pearson et al., 2015). This suggests that the parameters obtained could be applicable to other sites. The secondary peak observed between 100 and 150 m downwind, has not been reported, elsewhere. It is reasonable to attribute this to buoyancy effects on the pollutant plume but this should be confirmed with additional studies. The downwind transect sampling approach adopted may not have collected samples close to the centre of the pollutant plume due to varying wind directions. This could also result in false secondary peaks.

Only the most commonly enumerated bioaerosol component (*A. fumigatus*) was included in this study, despite other bioaerosol components being measured. Future studies should explore other bioaerosol components, once richer datasets become available with priority given to fractions such as endotoxin, which are known to cause inflammatory responses (Pearson et al., 2015).

We recognise that modelling emissions as a single area source is a simplification of the actual nature of emissions from composting facilities, which can be complex. This assumption allows simple and practical model set-up and has been shown to generate tolerable predictions. It represents a reasonable first step towards a phased modelling approach (i.e. using initial screening to determine whether more detailed investigation is required or not), similar to SCAIL-Agriculture, a screening tool for agricultural emissions (SCAIL, 2016). In a regulatory and facilities management context, complex model set-ups require more time, data and modelling expertise which are often not available. Refinements of the calibration process may be warranted in future studies where more detailed modelling is required (i.e. by describing the source characteristics in more detail). However, there is no guarantee that this will improve the goodness of fit. In any case, dispersion modelling is a simplification of a complex set of atmospheric processes and will, therefore, always contain a degree of uncertainty.

Predicted exposure is directly proportional to the assumed emission rate which can be used to scale the absolute magnitude of model outputs. In the validation process, emission rate was adjusted on the basis of the discrepancy between the average sampled concentrations at different downwind distances at Sites A and B. This essentially represents an additional calibration step

but serves to highlight the importance of getting a good estimate of site-specific emission for this type of modelling. Independent quantification of source strength in this field has not yet been successful, and has been identified as a major limitation in previous dispersion modelling exercises (Douglas 2013; Drew et al., 2007a; Taha et al., 2006; Williams et al., 2013). Difficulties include the uncontrolled and open nature of the release and the practical difficulties of taking measurements in close proximity to dangerous heavy machinery (Douglas, 2013). Further work is required to quantify independently a source term, for future use in dispersion modelling.

It is recommended that future studies further-test the applicability of the optimised parameter set reported in this study, by using it in modelling of other composting sites where bioaerosol concentrations have been measured. This will underpin generic confidence in this type of dispersion modelling as a tool for managing exposure and public health risks and will allow temporal and spatial patterns to be predicted. This information would be useful for researchers, site managers and regulatory bodies and has potential to influence the permitting process, predicting when and where regulatory limits may be exceeded and how best to mitigate the risks. In contexts where dispersion models can be used to provide accurate exposure assessments of bioaerosol emissions, this could aid our understanding bioaerosol risks, as highlighted in a recent small-area ecological study (Douglas et al., 2016). Finally, additional calibration and validation tests need to be completed for enclosed and in-vessel process sites, as our understanding of how to represent these site types needs improvement. Emission criteria for buildings and stacks are more readily defined than dispersed area or volume sources.

## 5. Conclusions

The calibration and validation of an existing numerical dispersion model applied to the emission of *A. fumigatus* from composting facilities is presented in this paper. The results suggest that good correlations and coincidence between predicted concentrations and measured data after validation as suggested by the goodness of fit statistics ( $r^2 > 0.7$  at 150, 300, 500 and 600 m downwind of source). The application of properly calibrated models could have huge benefits for facilities management, regulation and assessing public health risks. Optimal results were obtained by assuming (i) emission at a single area source; (ii) a pollutant temperature of 29 °C; (iii) an exit velocity of 2.95 m/s; (iv) a background concentration set to the LOD of the sampling method employed and (v) a short term averaging time of 30 min. Modelling in this field is challenged by limited knowledge regarding the properties of the bioaerosol source characteristics and the dispersion properties of bioaerosol particles from composting facilities and emissions are often complex, highly variable, uncontrolled and uncontained. Further work is required to confirm whether the parameterisation of the model described here can be applied more generally to other sites, bioaerosol fractions and weather conditions.

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## Appendix A

Modelled output concentrations from a sensitivity analysis (SA), as described in Douglas (2013), were compared to sampled *Aspergillus fumigatus* from site A as measured and described by Pankhurst et al. (2011). The concentrations were compared via a means with error plot using Statistica 11 (© StatSoft, Inc. 1984–2012) at 10, 100 and 250 m downwind of the source (these distances are present in both the SA modelled output data, and in the measured data). A means with error plot of the sampled data was produced for each distance downwind, with a 95% confidence interval and the modelled output data was overlaid via a scatter plot for each of the source types to indicate which modelled outputs corresponded to the measured data (Fig. A1).

Fig. A1 shows that the modelled outputs when modelling with an area source type are within the confidence interval of the mean sampled data. Line source outputs were clustered below the lower limit of the confidence interval, but were in the same order of magnitude as the sampled data (data not visible) and point source outputs were found three orders of magnitude above the upper confidence interval of the sampled data (data not visible). The plots produced at 100 m and 250 m showed similar results (not presented). The median input values of any model outputs that fell within a 95% confidence interval of the mean of the measured data were used as initial model input values for the model calibration (Table A1).

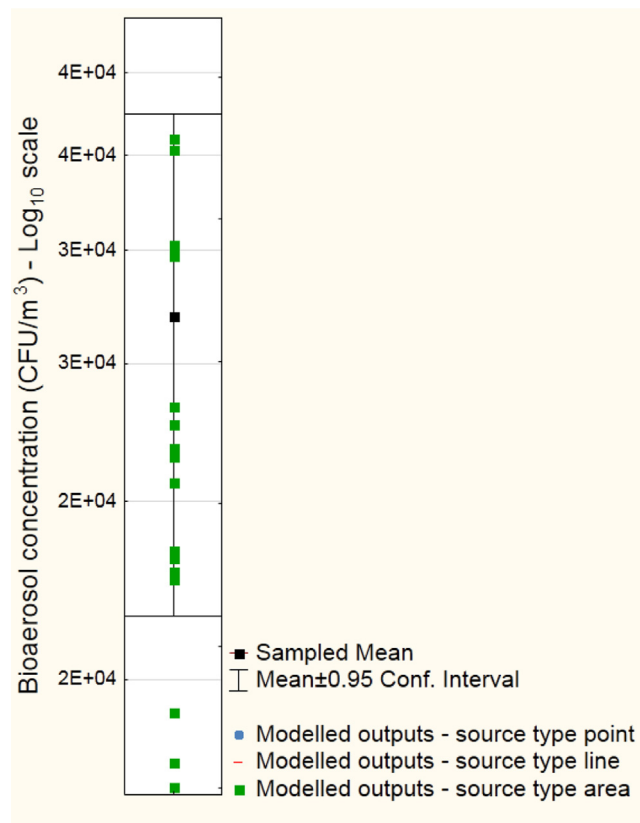


Fig. A1. Measured arithmetic mean (with a confidence interval of 95% from the sampled mean) and modelled output data generated from the SA at 10 m downwind.

**Table A1**

The range and median of the modelled input values used that resulted in modelled outputs that were within a 95% confidence interval of the mean measured data.

Model input parameter (units)	Range	Median value
Source type	Area	Area
Specific heat capacity of the pollutant (J/°C/kg)	1017–2021	1519
Molecular mass of the pollutant (g)	19.945–30.703	25.324
Source height (m)	0.66–4.64	2.65
Pollutant exit velocity (m/s)	0.93–4.87	2.90
Pollutant temperature (°C)	17.4–52.7	35.1
Surface Roughness (m)	0.42–1.32	0.87
Minimum value of the Monin-Obukhov length at the dispersion site (m)	128–189	159
Source geometry (horizontal) (m)	12.06–21.52	17.00
Source geometry (vertical) (m)	12.47–14.13	13.30

The meteorological data used in the SA was based on historical UK meteorological data (Douglas, 2013). The median of the meteorological data was used in the initial model run as an arbitrary value in the initial model adjustments. As this presented a constant wind direction, the grid used to specify where the modelled outputs should be calculated was a transect based on the distances of the measured data downwind of the site. The pollutant emission rate is not presented in Table A.1 as this parameter was not included in the SA as the sensitivity is already known. Therefore an initial emission rate of  $1 \times 10^5$  (g/m<sup>2</sup>/s – as a proxy for CFU/m<sup>2</sup>/s) will be used, based on previous emission rates used

to model the composting scenario literature (ADAS and SWICEB, 2005; Douglas, 2013; Danneberg et al., 1997; Dowd and Maier, 2000; Drew et al., 2007a; Environment Agency, 2001; Millner et al., 1980; SNIFFER, 2007; Taha and Pollard, 2004; Taha et al., 2006, 2007; Tamer Vestlund, 2009; Williams et al., 2013), and was altered intermittently throughout the calibration process.

## Appendix B

See Table B1.

**Table B1**

Summary of the statistical tests used throughout the model calibration, where  $o_i$  are the measured values,  $p_i$  are the modelled values,  $\bar{o}$  is the average of the measured data,  $\bar{p}$  is the average of the modelled data and  $n$  is the number of samples.

Statistical test (Units)	Equation	Explanation of what the statistical calculation tests	Possible ranges
RMSE (%)	$= \frac{100}{\bar{o}} \sqrt{\sum_{i=1}^n (p_i - o_i)^2 / n}$	RMSE provides a percentage term for the total difference between modelled and measured values, proportioned against the measured mean (Loague and Green, 1991; Smith et al., 1996).	The lower and upper limits of the RMSE are 0 and $\infty$ respectively. A value of 0 denotes a perfect fit between model outs and sampled data (Loague and Green, 1991; Smith et al., 1996)
ME	$= \frac{(\sum_{i=1}^n (o_i - \bar{o})^2) - (\sum_{i=1}^n (p_i - o_i)^2)}{\sum_{i=1}^n (o_i - \bar{o})^2}$	ME assesses the accuracy of the modelled data by comparing the variance of the model outputs from the sampled values to the variance of the sampled values from the mean of the sampled data. In other words, this is a comparison of the efficiency of the ADMS model outputs to the mean of the sampled data	Values can be positive or negative with a maximum value of 1. Positive values indicate that the modelled values describe the trend of the sampled data better than simply taking the mean average of the sampled data. A negative value indicates that the mean average of the sampled data describes the sampled data better than the modelled values, and that the model is not performing sufficiently (Loague and Green, 1991; Smith et al., 1996, 1997)
r	$= \frac{\sum_{i=1}^n (o_i - \bar{o})(p_i - \bar{p})}{\left(\sum_{i=1}^n (o_i - \bar{o})^2\right)^{\frac{1}{2}} \left(\sum_{i=1}^n (p_i - \bar{p})^2\right)^{\frac{1}{2}}}$	Measures the linear relationship between the modelled and the sampled data (Chang and Hanna, 2004). It measures the degree of association between the modelled and the sampled data, but not necessarily the coincidence, (Addiscott and Whitmore, 1987).	Values of r can lie between –1 and +1. If r equals –1 or +1 then there is perfect negative or positive correlation between the sampled and modelled data respectively. If r is equal to 0 then this indicates that there is not any correlation between the modelled and the sampled data, but this could be because the values are not linearly related, (Smith et al., 1996) as non-linear relationships are not revealed by r, (Chang and Hanna, 2004).
r <sup>2</sup>	= rxr	r <sup>2</sup> is a development of r, as it measures how well the modelled values can be used to predict future outcomes as well as measuring how well the modelled data fits the sampled data, (Everitt, 2006)	Values can range between 0 and 1, indicating a bad and good fit respectively between the modelled outputs and the sampled data, (Smith et al., 1996)
F	$= \frac{(r^2/1)}{(1 - r^2)/(n - 2)}$	Measures the statistical significance of r (Smith et al., 1996)	Large values of F suggest that there is a good fit between the model outputs and the sampled data, (Snedecor and Cochran, 1989)



Table B1 (Continued)

Statistical test (Units)	Equation	Explanation of what the statistical calculation tests	Possible ranges
MD (CFU/m <sup>3</sup> )	$= \sum_{i=1}^n (o_i - p_i) / n$	M gives an indication of consistent errors or bias in the model, (Addiscott and Whitmore, 1987; Smith et al., 1996)	M can be positive or negative; if the modelled and sampled values are the same, then M will equal 0, (Smith et al., 1996)
FB	$= \frac{(\bar{o} - \bar{p})}{0.5(\bar{o} + \bar{p})}$	FB measures systematic bias in the model, (Chang and Hanna, 2004).	Values for FB range between –2 and +2 corresponding to extreme under- or over-prediction respectively, (Radonjic and Garisto, 2012). A perfect relationship between the modelled and the sampled values would result in FB equaling 0. It should be noted that it can be possible for FB to equal 0 even if the modelled data doesn't match the sampled data due to cancelling errors, (Chang and Hanna, 2004).

### Appendix C

A set of criteria were developed to determine whether a suitable goodness of fit had been achieved between the modelled and sampled data, and whether model modifications should be accepted or rejected. The criteria were based on statistical values reported within existing successful model calibration and validation studies (CERC, 2015b; Katerji et al., 2010; Hollis et al., 2011; Ludwig et al., 2011; and Chang et al., 2012). The criteria are presented in Table C1 below.

Table C1

Ranges used to classify the quality of goodness of fit statistics in calibration and validation (based on the thresholds presented in CERC, 2015c; Chang et al., 2012; Hollis et al., 2011; Katerji et al., 2010; Ludwig et al., 2011).

Statistical test	'Very good fit' (Dark grey category ranges)	'Reasonable fit' (Light grey category ranges)
RMSE	0 – 20	21 – 60
ME	0.75 – 1	0 – 0.74
r	0.6 – 1	0.15 – 0.59
r <sup>2</sup>	-1 - -0.6	-0.59 – -0.15
MD	0.6 - 1	0.4 – 0.59
FB	-10 – 10	11 - 100
	-0.5 – 0.5	-100 - -11
		0.51 – 1
		-0.51 - -1

### Appendix D

See Table D1.

**Table D1**

Alterations made to model input values during the calibration. The emission rate was altered intermittently (summarised at the bottom of the table).

Parameter changed (units)	Run no.	Value changed to	Reason for change	Run no resulting in best fit
Initial model run (Table 1)	1	Initial model run (Table 1)		
Source geometry (m)	2	155.0 × 44.0	Represent site area (estimated from aerial maps)	4 – same geometry as run 3, but altered emission rate (see below)
	3	44.00 × 9.5	Represent a windrow (estimated from aerial maps)	
	5	3.0 × 4.0	Represent an agitation area	
Pollutant exit velocity (m/s)	9	1.5	Arbitrary values based on observations of steam and dust clouds	4 – same pollutant exit velocity as the initial model run but altered emission rate (see below)
	10	2.2		
	12	0.20		
Surface roughness (m)	13	0.30	Represent agricultural areas and grassland	17
	15	0.25		
	16	0.15		
	17	0.20		
	18	3.00		
Source height (m)	19	2.50	Based on observations of compost pile height	17
	20	2.75		
	21	2.80		
	22	12		
Pollutant temperature (°C)	23	22	The average ambient temperate on sampling days	25
	25	29		
	26	28.966		
Pollutant molecular mass (g)	27	18.020	Based on initial thermal images of dust clouds (Douglas, 2013)	26
	28	1220	Model default	
Background levels (g/m <sup>3</sup> ) <sup>a</sup>	29	1599	Mean average measured upwind concentration	30
	30	756	Maximum measured upwind concentration	
	31	Included meteorology for the sampling time period collected from the nearest weather station. Grids changed based on GPS of the sampling locations	1-limit of detection of the sampling equipment	
Meteorological data and output grid	35	Used the calms option – user defined values		36
	36	Used the calms option – default values		
Emission rate (g/m <sup>2</sup> /s) <sup>b</sup>	4	5.00 × 10 <sup>5</sup>	Adjusted when the modelled outputs were over or under estimating the measured data as the emission rate is directly proportionate to output concentrations	See above
	6	5.00 × 10 <sup>6</sup>		
	7	3.75 × 10 <sup>6</sup>		
	8	3.00 × 10 <sup>6</sup>		
	11	1.00 × 10 <sup>6</sup>		
	14	8.00 × 10 <sup>6</sup>		
	24	9.00 × 10 <sup>5</sup>		
	32	8.00 × 10 <sup>6</sup>		
	33	4.95 × 10 <sup>6</sup>		
	34	9.00 × 10 <sup>6</sup>		

<sup>a</sup> Proxy for CFU/m<sup>3</sup>.<sup>b</sup> Proxy for CFU/m<sup>2</sup>/s.

## Appendix E

See Fig. E1.

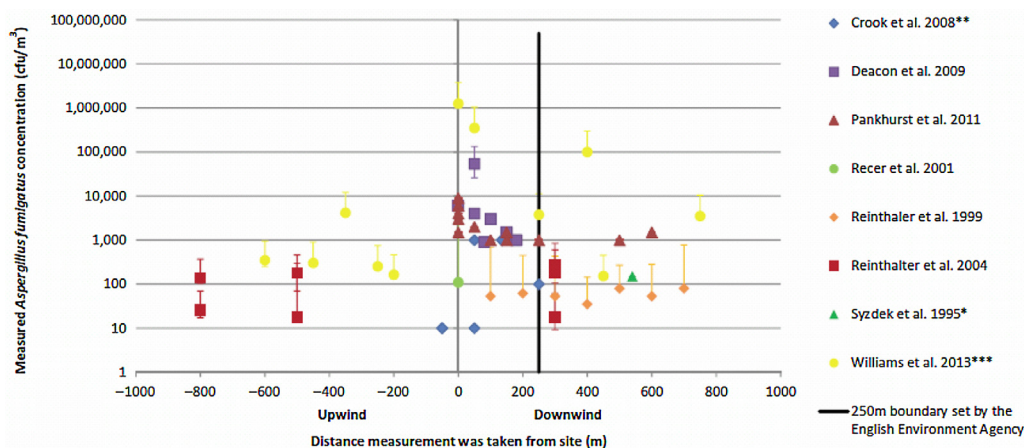


Fig. E1. Mean/median airborne *Aspergillus fumigatus* concentrations in communities near composting facilities. Taken from Pearson et al. (2015).

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# Predicting *Aspergillus fumigatus* exposure from composting facilities using a dispersion model: a conditional calibration and validation

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