
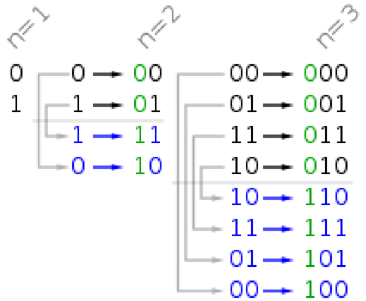


# YOU REAP WHAT YOU SOW

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# Complex Systems

| | |
|---|---|
| Sampling | • Representative.<br>• Variance. |
| Experiment design | • Baseline, signal, calibration, drift, interference.<br>• Data preprocessing and processing. |
| Factor analysis | • Variable reduction, temperature…<br>• Controlled, uncontrolled, masquerading. |

# Exposure Identification

Compliance to:

EU Directive 98/24/EC

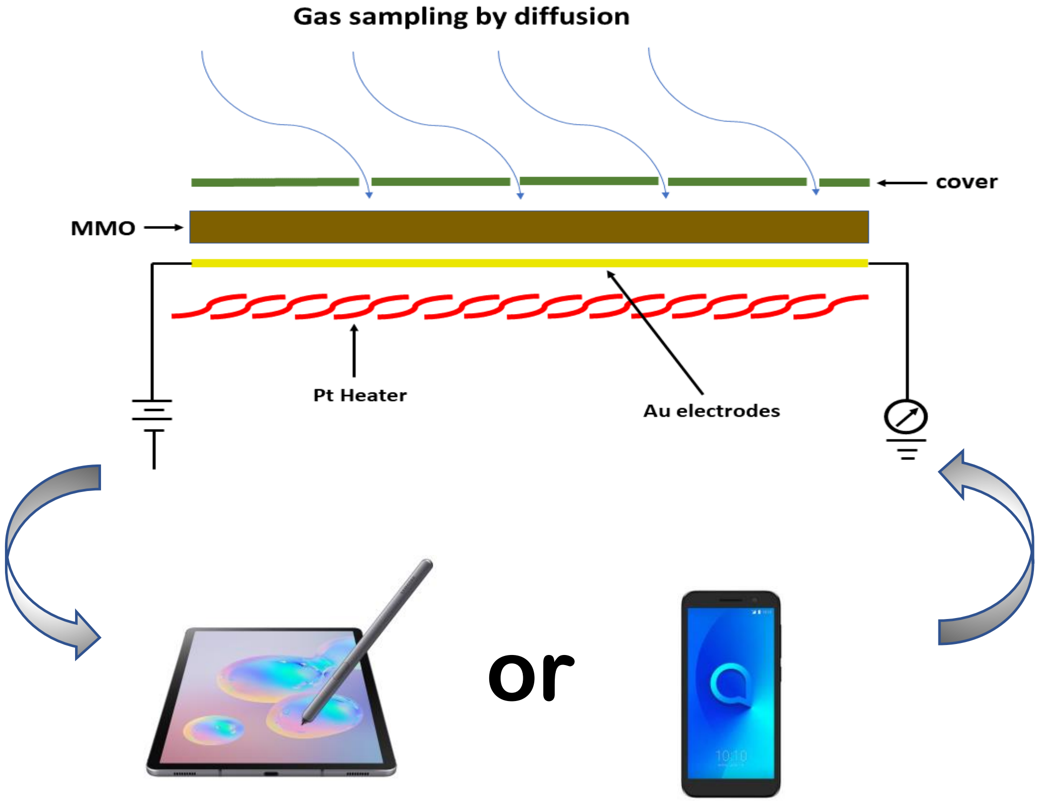
US OSHA 29 CRF 1910

Time Weighted Averages (TWA) of exposure monitoring – EH40

$$\frac{\Sigma c_i(t_i)}{\Sigma t_i} = \frac{c_1(t_1) + c_2(t_2) + \ldots\ldots\ldots + c_n(t_n)}{t(total)}$$

*$c_i$ = the exposure concentration mg $m^{-3}$*
*$t_i$ = associated exposure time in hours*

# Sensors and their Data  for Prediction and Protection

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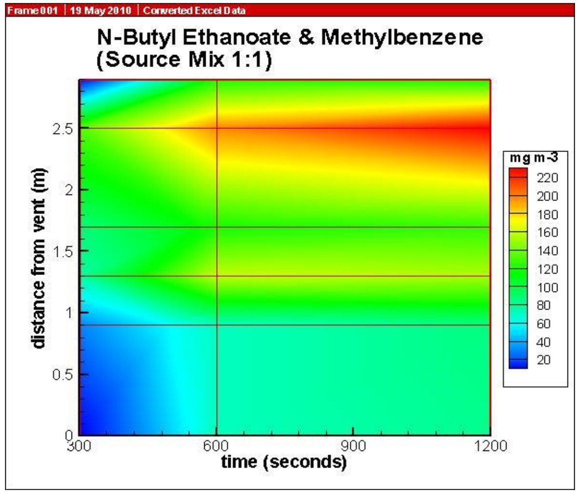


# MMOS Sensor Calibration

**Table 1** MMOS Specifications with ***New Heater Control Circuit.***

| **Sensor Application** | **Solid State (semiconductor)** |
|---|---|
| Response frequency | 1 Hz (average of 30 secs) |
| Limits of VOC Detection | ≥ 1 ppm (VOC dependent) |
| Ambient Operating Temperature | 253 – 333 K |
| Baseline<br>In Clean Air at 294 K and 50% RH | 100 KΩ ± 5 KΩ (when measuring VOCs < 50 ppm),<br>100 KΩ ± 5 KΩ (when measuring VOCs > 50 ppm and <500 ppm) |
| Typical Response<br>n-butyl ethanoate | ≤420 KΩ ± 5 KΩ (VOCs < 50 ppm),<br>300 - 870 KΩ ± 5 KΩ (VOCs> 50 ppm and <500 ppm) |
| Typical Response<br>methylbenzene | ≤300 KΩ ± 5 KΩ (VOCs < 50 ppm),<br>240 - 800 KΩ ± 5 KΩ (VOC's> 50 ppm and <500 ppm) |
| Typical Response<br>n-butyl ethanoate : Methylbenzene; 1 : 1 | ≤350 KΩ ± 5 KΩ (VOCs < 50 ppm),<br>267 - 800 KΩ ± 5 KΩ (VOCs >50 ppm and <500 ppm) |

# Performance characteristics

- Linear range – no, calibrate over < 50, 50 – 100 and 80 - 500 ppm ranges.
- Sensitivity (LOQ) good – defined by the heater control electronics.
- Selectivity poor – improved a little by heater control electronics.
- Bias – drift (relatively slow response but reproducible).
- Precision – levels are repeatable and reproducible.
- **Ruggedness** – sensor or experiment.
  - Sensor: robust against airflow, ambient temperatures, humidity ✓
  - Experiment: introduction of factors and variables.

# MMOS Sensor Calibration – controlled (complete mixing) in 1 $m^3$

12 sensors (6 x 2), 6 repeats 50 ppm n-butyl ethanoate (NBE)

| VOC type (mg $m^{-3}$) | Precision (repeatability and reproducibility) | CV | Calibration $R^2$ (10, 20, 30, 50, 80 ppm) |
|---|---|---|---|
| n Butyl Ethanoate | ± 1.6 mg $m^{-3}$ (50 ppm, 237 mg $m^{-3}$)* | 0.7 | 0.904 – 0.999 (average 0.99) |
| Methylbenzene | ± 2 mg $m^{-3}$ (50 ppm, 188 mg $m^{-3}$)* | 1.1 | 0.992 – 0.999 (average 0.98) |
| 1:1 Mix Supply of n butyl ethanoate and methylbenzene | ± 4 mg $m^{-3}$ (80 ppm, 340 mg $m^{-3}$)* | 0.9 | 0.899 – 0.999 (average 0.99) |

*** At standard ambient temperature and pressure, homogeneity was checked and confirmed.**

# Gaussian (normal) distribution – precision.

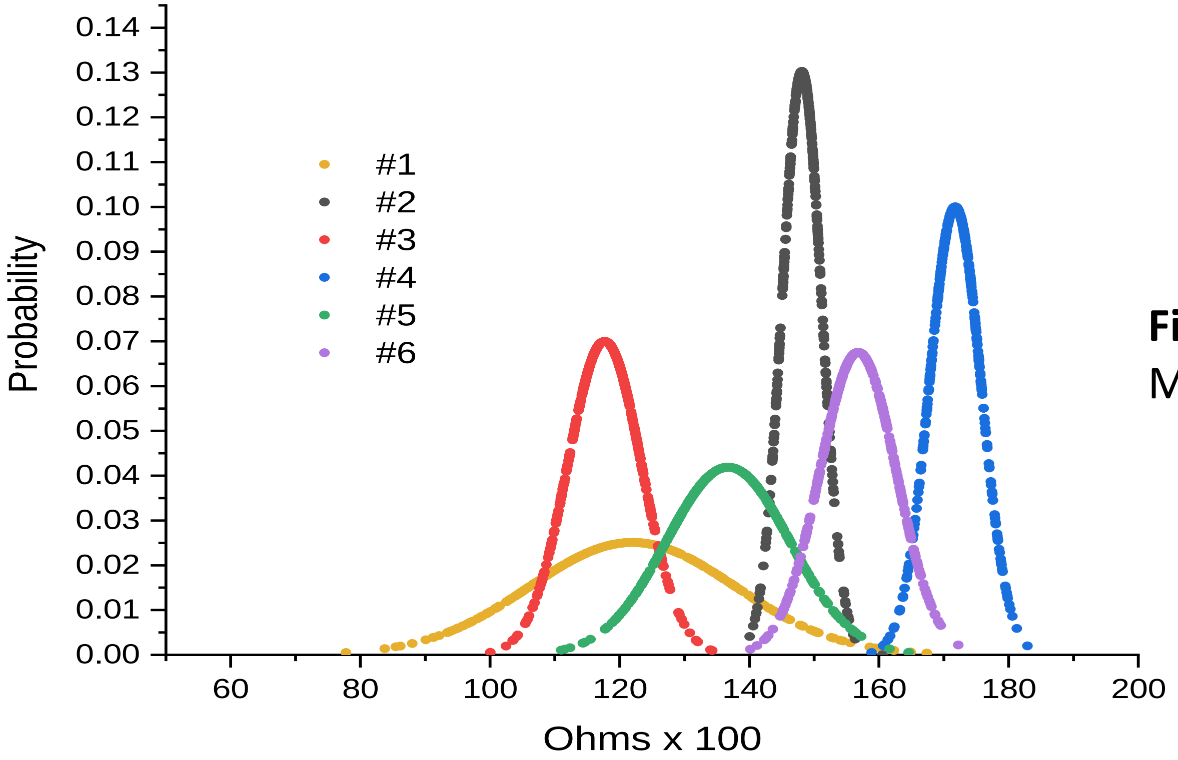
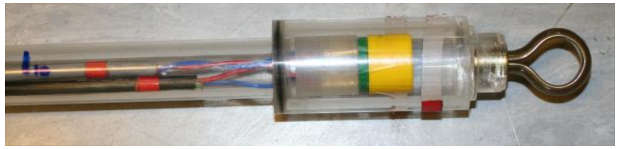



**Figure 1.** Measurement precision of six MMOS sensors – controlled **50 ppm NBE** in 1 $m^3$

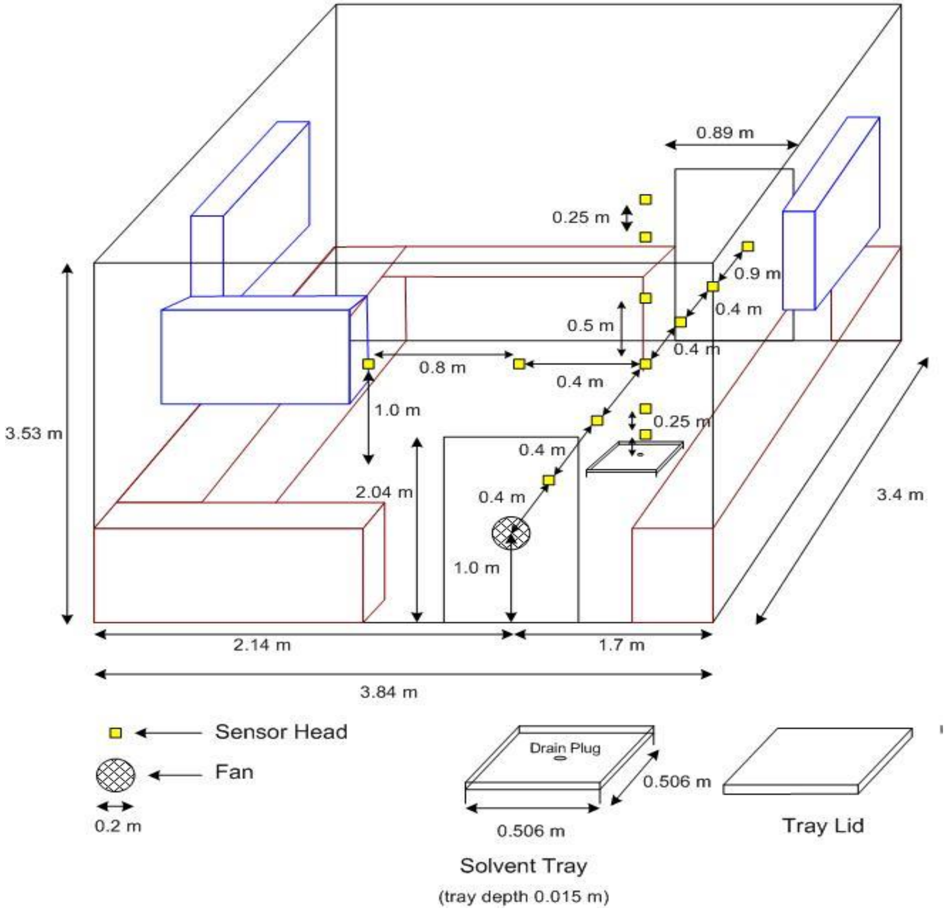
# VOC Measurement – under natural and mechanical ventilation

Omni directional hot sphere anemometer

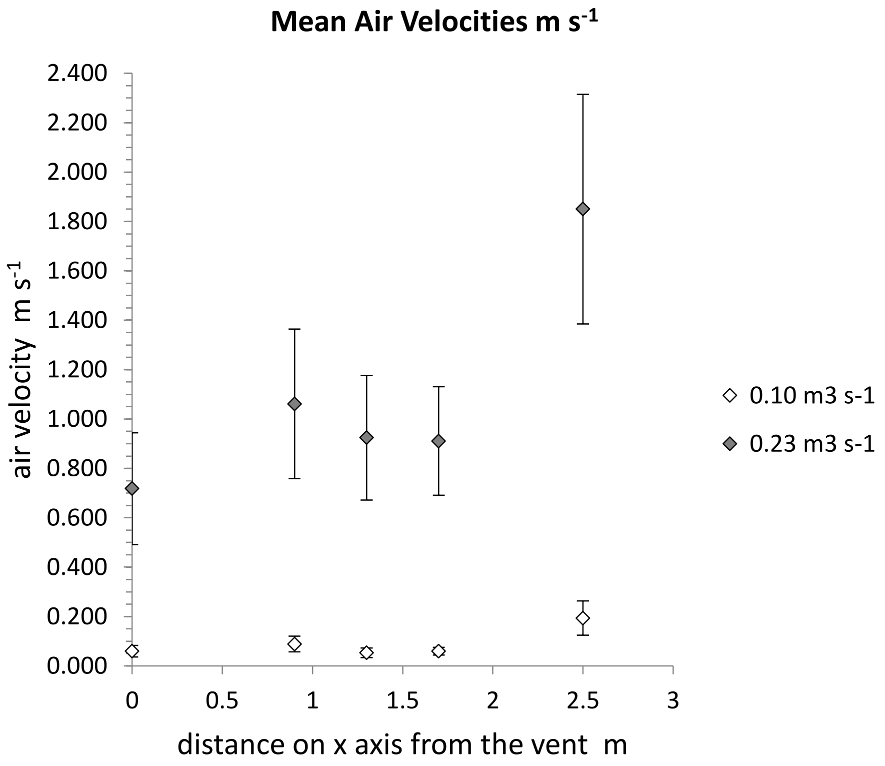
| Supply $m^3 s^{-1}$ (outlet $m s^{-1}$) | VOC surface air velocity $m s^{-1}$ | Bulk air velocities $m s^{-1}$ |
|---|---|---|
| 7.3 (3.5) | 0.09 | 0.02 – 0.2 |
| 10.4 (5.0) | 0.08 | 0.03 – 0.3 |
| 16.7 (8.0) | 1.0 | 0.2 – 2.0 |

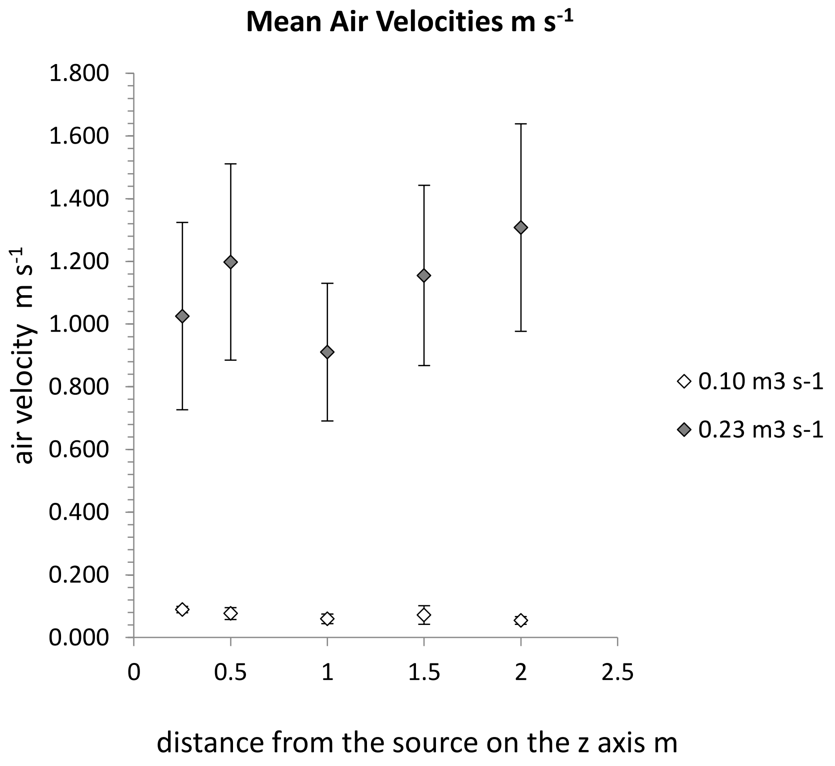


MMOS and housing



# Uncertainties in air velocities.



# Sampling Uncertainties (errors)?

- Fundamental – what was being measured ie homogeneity.
- Grouping and segregation – vapour densities?
- Long- range heterogeneity – pulsed and continuous sources explored.
- Periodic heterogeneity – was being measured ie. fluctuation – eddy diffusion.
- Incremental delimitation – wrong sensors, sampling locations.
- Incremental extraction – poor resolution, position interference.
- Preparation – contamination, deposition, sensor failure.

# VOC Measurement – under mechanical ventilation

12 sensors, 6 repeats

| VOC type (mg m$^{-3}$) | Precision, $s_{total}$ * ($s^2_{total} = s^2_{sam} + s^2_{evap} + s^2_{meas}$) | |
|---|---|---|
| n Butyl Ethanoate | ± 4 – 6 mg m$^{-3}$ (<24 - 450 mg m$^{-3}$) | Maximum measurement error: (from range) ±13% of the mean value (from range).<br><br>This includes variation due to sensor orientation in space (minimal contribution) and repeat measurements in situ. |
| Methylbenzene | ± 2 – 6 mg m$^{-3}$ (<20 – 690 mg m$^{-3}$) | |
| 1:1 Mix Supply of n butyl ethanoate and methylbenzene | ± 2 – 10 mg m$^{-3}$ (<20 - 398 mg m$^{-3}$) | |

*** Determined at ambient temperature and pressure at the time of measurement**

# Predictive Modelling – validation.

- Modified Neuman dispersion model, Neuman S.P. 1981.
- 1D on each Cartesian axis $x, y, z$.
- Convection, diffusion and their strength ratio.

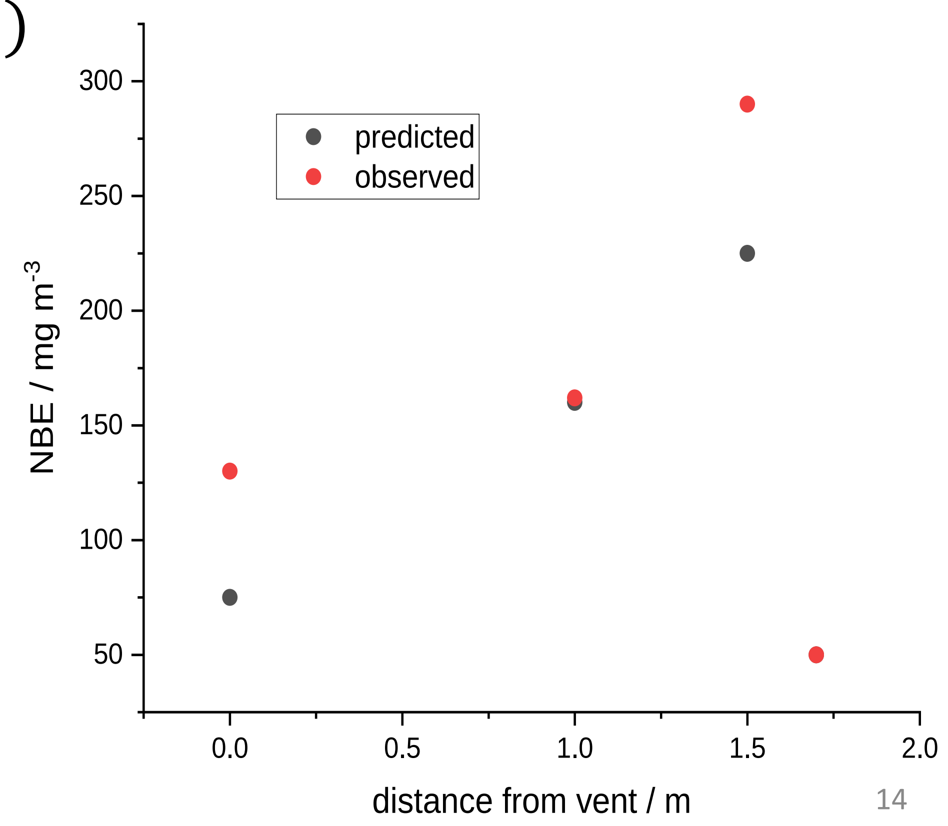
$$C(x_i, t_j) = \frac{1}{2} C_0 \left\{ erfc \left( \frac{dx_i - u_{xi} t_j}{2\sqrt{Kx_{i-1} t_j}} \right) + \frac{1}{2} \exp(-Sh)\ erf\ c \left( \frac{dx_i + u_{xi} t_j}{2\sqrt{Kx_{i-1} t_j}} \right) \right\}$$

# Fixed model parameters.

Using median effective diffusivities from MC simulation:

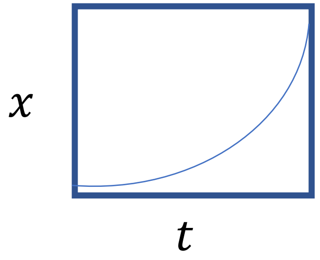
$$Cx\ (y,z),t\ (predicted)\ \leq\ Cx\ (y,z),t\ (observed)$$

Uncertainty in prediction: ranged from 10% through to 150% of the median observed concentration:



# Hypothesis

Each division in space and time presents a new average gradient of transport across that division.

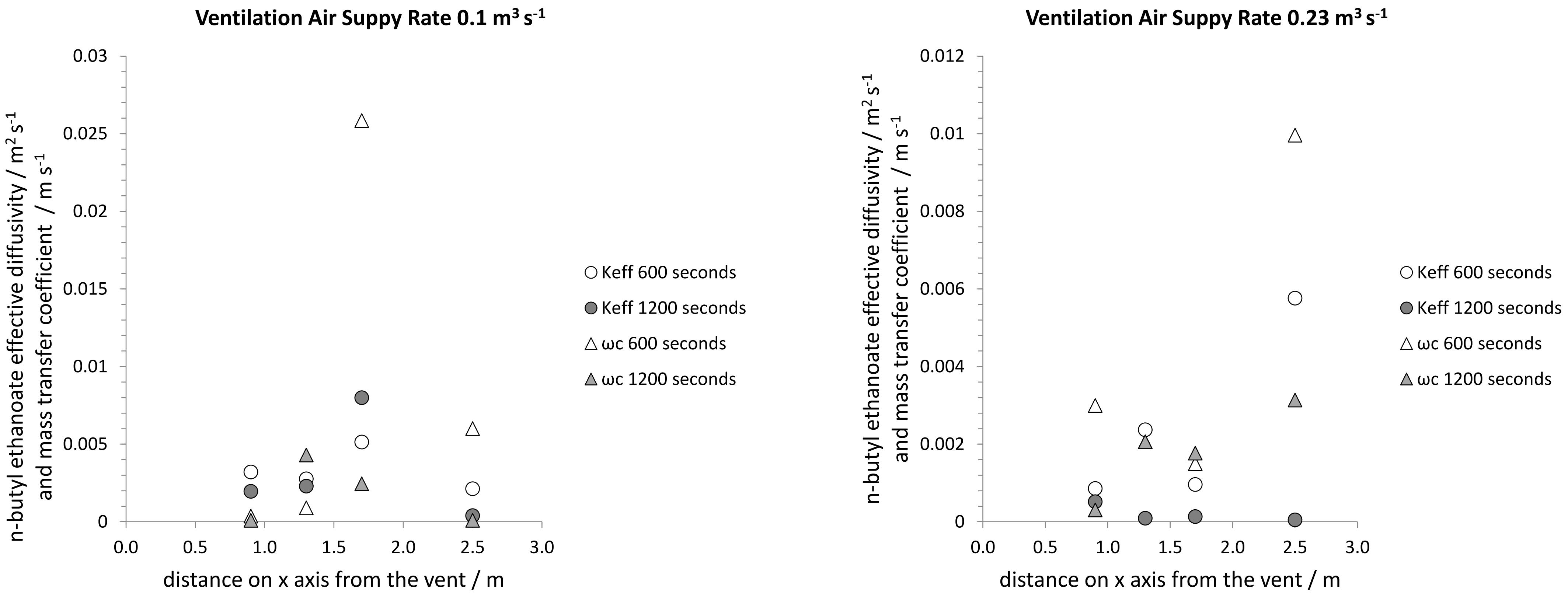



**ASSUMPTIONS**

- Within each division in time the airflow and vapour concentration dispersion is at steady state.

- The VOC vapour moves away from the source.

# Variable model parameters.



# Bayesian Monte Carlo updating of dispersion parameters

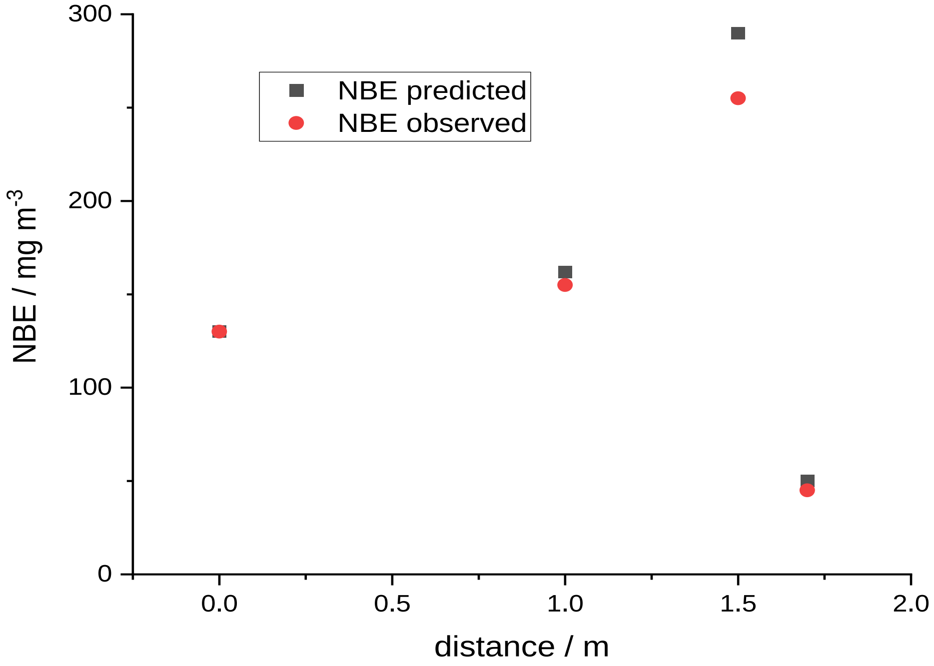
- Hypothesis: $P(C_{pred}\ \xi_{i\,j}/\ C_{obs}\ \xi_{i\,j}, K_{eff}\ \xi_{i-1\,j}, Sh\ \xi_{i-1\,j}, u\ \xi_{i\,j}, C_0)$
- Marginal posterior probability density functions of effective diffusivity ($K_{eff}$) values were then estimated.

$$P(K_{eff}\xi_{i-1\,j}/Cobs\xi_{i\,j}) = \frac{P(Cobs\xi_{i\,j}/Cpred\xi_{i\,j})P(Cpred\xi_{i\,j}) + P(Cobs\xi_{i\,j}/\overline{C}pred\xi_{i\,j})P(\bar{C}pred\xi_{ij})}{P(Cobs\xi_{ij}/Cpred\xi_{ij})P(Co)P(Sh/\xi_{i-1j})P(u_i)}$$

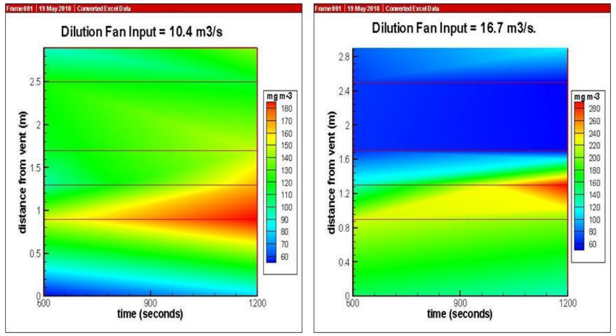
- β PERT distribution parameters were assigned and developed by MC simulation.

# Improved prediction - Using the marginal posterior ‘most likely’ $K_{eff}$

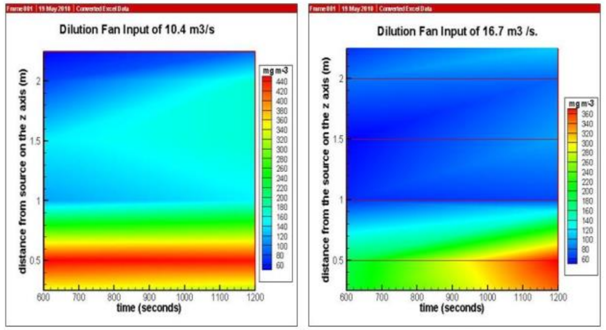
Uncertainty in prediction results: β PERT distribution ranged from ±10% through to ±50% of the ‘most likely’ parameter.




X Axis Comparison of NBE Vapour over time at two Dilution ventilation fan inlet rates:
10.4 m$^3$ s$^{-1}$ (4.83 m s$^{-1}$) & 16.7 m$^3$ s$^{-1}$ (7.0 m s$^{-1}$)




Z Axis Comparison of NBE Vapour over time at two Dilution ventilation fan inlet rates:
10.4 m$^3$ s$^{-1}$ (4.83 m s$^{-1}$) & 16.7 m$^3$ s$^{-1}$ (7.0 m s$^{-1}$)




(a)

# Gas sampling by diffusion