

Modelling large concentrations of dispersing hazardous gases

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My areas of interest:

- The relationship between moments of concentration
- The probability density function (pdf) of concentration
- The distribution of large concentrations

The relationship between moments of concentration

- Péclet number $Pe = ul/\kappa$ usually large

u, l = velocity, length scales

κ = (molecular) diffusivity

- **Turbulent advection**: **fast**, stretches plume/cloud out into thin sheets/strands of relatively high concentration
- **Molecular diffusion**: **slow**, only mechanism for changing concentration of a piece of fluid

Concentration $\Gamma(\underline{x})$

Mean concentration $C = E\{\Gamma\}$ (on centreline $C = C_0$)

Central moments $\mu_n = E\{[\Gamma - C]^n\}$

Normalised moments $K_n = \frac{\mu_n}{\mu_2^{n/2}}$ for $n = 3, 4, \dots$

(skewness K_3 , kurtosis K_4)

Mole & Clarke (1995):

$$\begin{cases} K_4 = a_4 K_3^2 + b_4 \\ K_5 = a_5 K_3^3 + b_5 K_3, \end{cases}$$

Chatwin & Sullivan (1990); Sawford & Sullivan (1995):

$$\begin{cases} \frac{\mu_2}{(\alpha\beta C_0)^2} = \hat{C}(1 - \hat{C}) \\ \frac{\mu_3}{(\alpha\beta C_0)^3} = \hat{C}(\lambda_3^2 - 3\hat{C} + 2\hat{C}^2) \\ \frac{\mu_4}{(\alpha\beta C_0)^4} = \hat{C}(\lambda_4^3 - 4\lambda_3^2\hat{C} + 6\hat{C}^2 - 3\hat{C}^3) \end{cases}$$

$$\hat{C} = \frac{C}{\alpha C_0}$$

α , β , λ_n , a_n , b_n essentially constant across plume, vary slowly with downstream distance X

Mole, Schopflocher & Sullivan (2008):

$$\lambda_n^{n-1} \approx a_n \lambda_3^{2(n-2)}$$

$$a_6 = \frac{3a_4a_5^2}{5a_4^2 - 2a_5}$$

+ similar for a_7, a_8, \dots in terms of a_4, a_5

The distribution of large concentrations

- Short-range dispersion of toxic/flammable gases:
high concentrations important for hazard assessment
- Balance between advection/diffusion at small length scales where large concentrations are found: independent of large scale flow
⇒ **universal character for large concentrations**

- Statistical extreme value theory:

Above a high threshold θ_T , distribution of a random variable takes asymptotic form of **Generalised Pareto Distribution (GPD)**:

$$g(\theta) = \frac{1}{a} \left\{ 1 - \frac{k(\theta - \theta_T)}{a} \right\}^{1/k-1}, \quad a > 0, \quad \theta > \theta_T$$

Finite maximum possible concentration

$$\Rightarrow k > 0, \quad \theta \leq \theta_{\max}$$

$$\theta_{\max} = \theta_T + \frac{a}{k} < \text{largest source concentration}$$

Modelling large concentrations

- Direct methods
 - from experimental measurements (e.g. Mole, Anderson, Nadarajah & Wright 1995; Lewis & Chatwin 1995; Anderson, Mole & Nadarajah 1997; Munro, Chatwin & Mole 2001; Schopflocher 2001; Schopflocher & Sullivan 2002; Xie, Hayden, Robins & Voke 2007)
 - from DNS
 - from LES (e.g. Xie, Hayden, Robins & Voke 2007): an issue with whether small scales where one expects largest concentrations are adequately resolved

Maximum concentration θ_{\max} and GPD parameters have to be estimated: most usual method would be to consider all Γ larger than a high threshold and fit GPD by Maximum Likelihood

- Mole, Schopflocher & Sullivan (2008) proposed an indirect method:

Assume pdf can be written as

$$p(\theta) = (1 - \eta)f(\theta) + \eta g(\theta) \quad \eta > 0$$

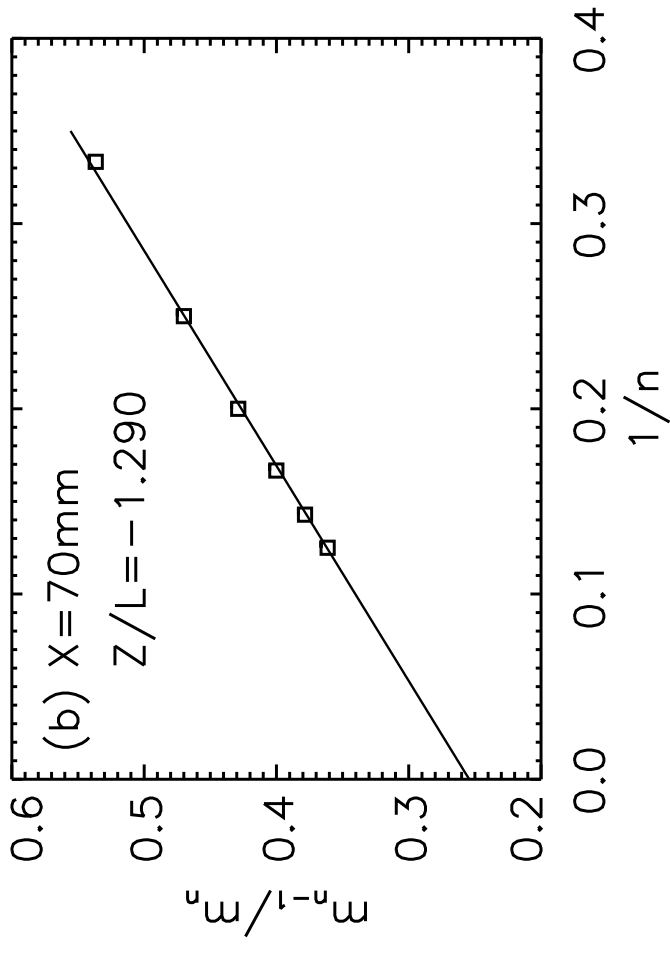
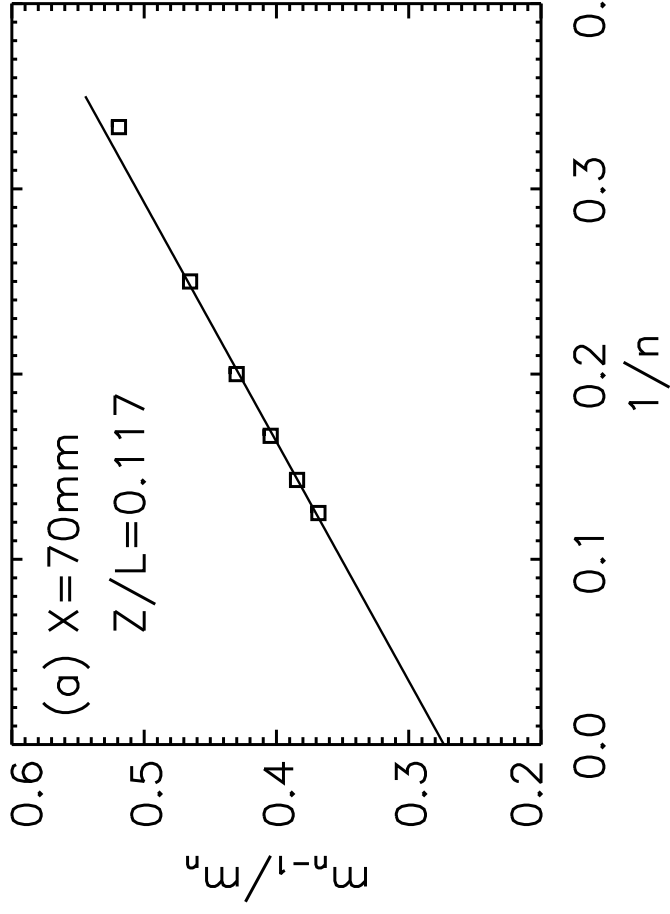
for some function f which is negligible for large θ , and taking $\theta_T = 0$.

Absolute moments $m_n = E\{I^n\}$

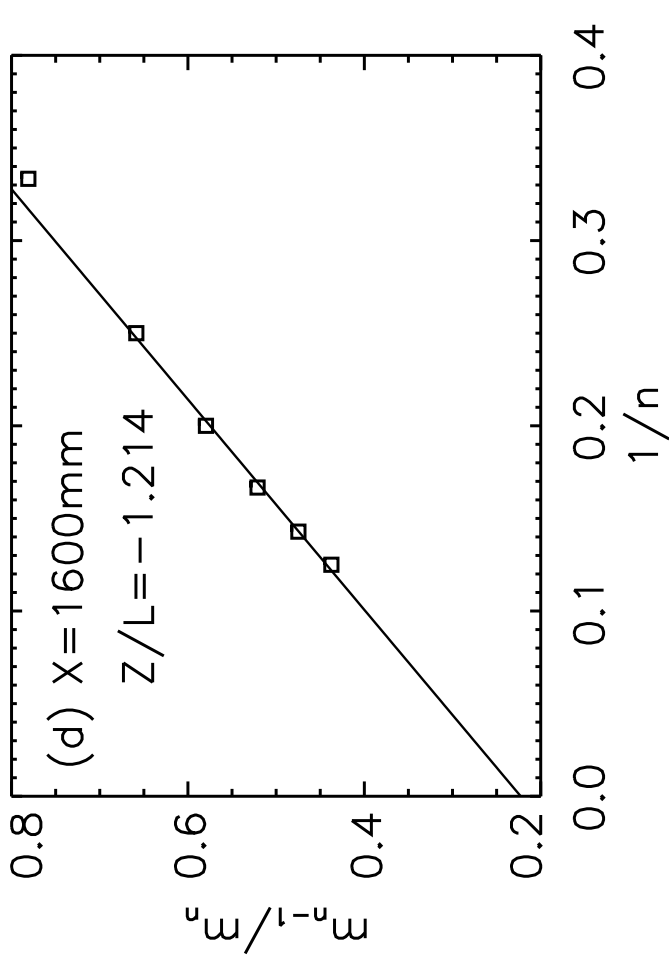
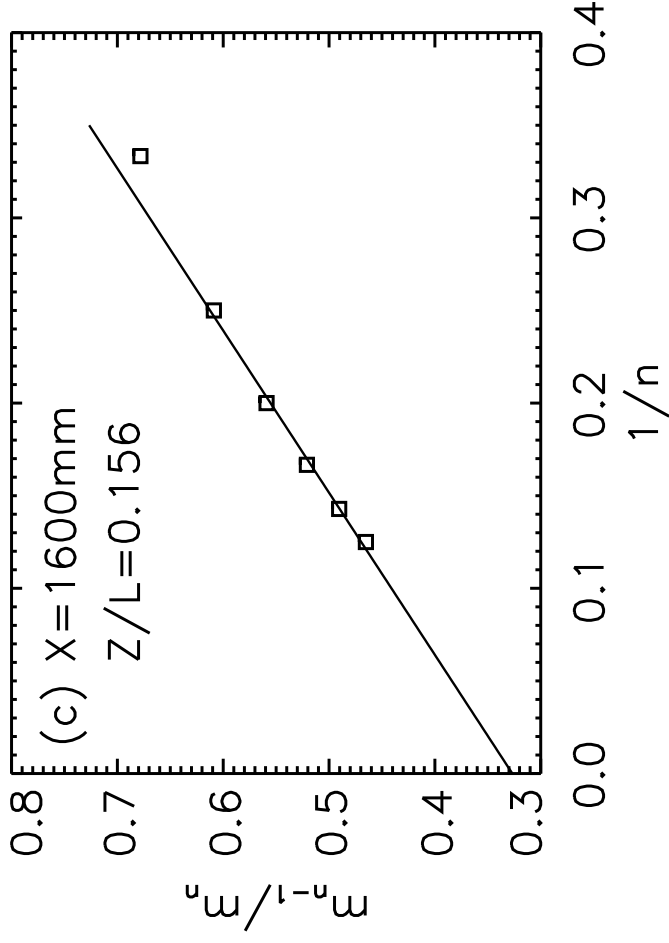
Large $n \Rightarrow m_n$ dominated by large concentrations

Large concentrations GPD

$$\Rightarrow \frac{m_{n-1}}{m_n} \approx \frac{1}{a} \left(\frac{1}{n} \right) + \frac{k}{a}$$



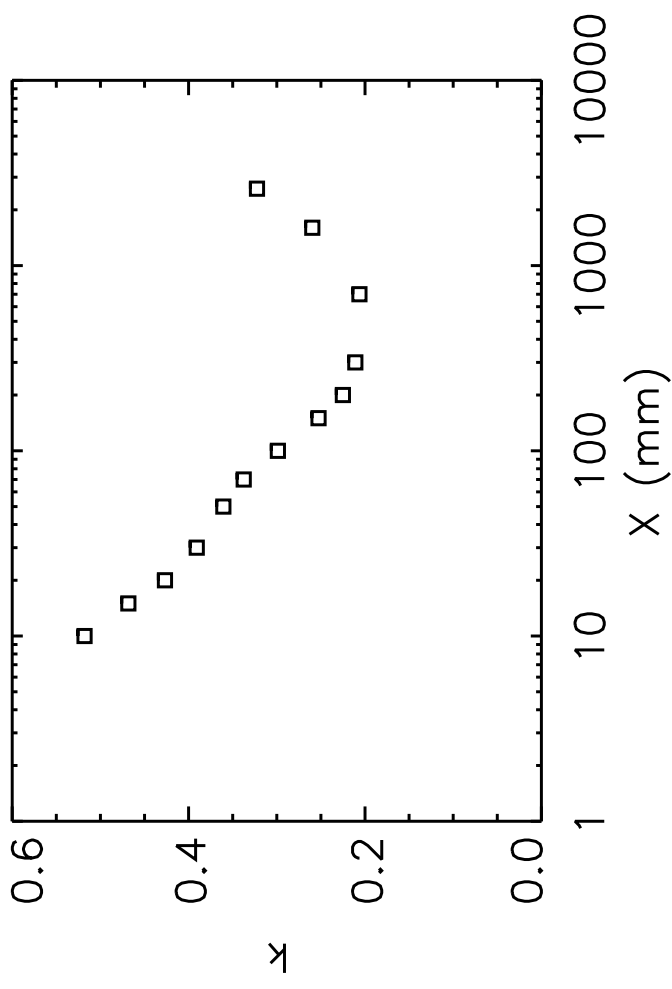
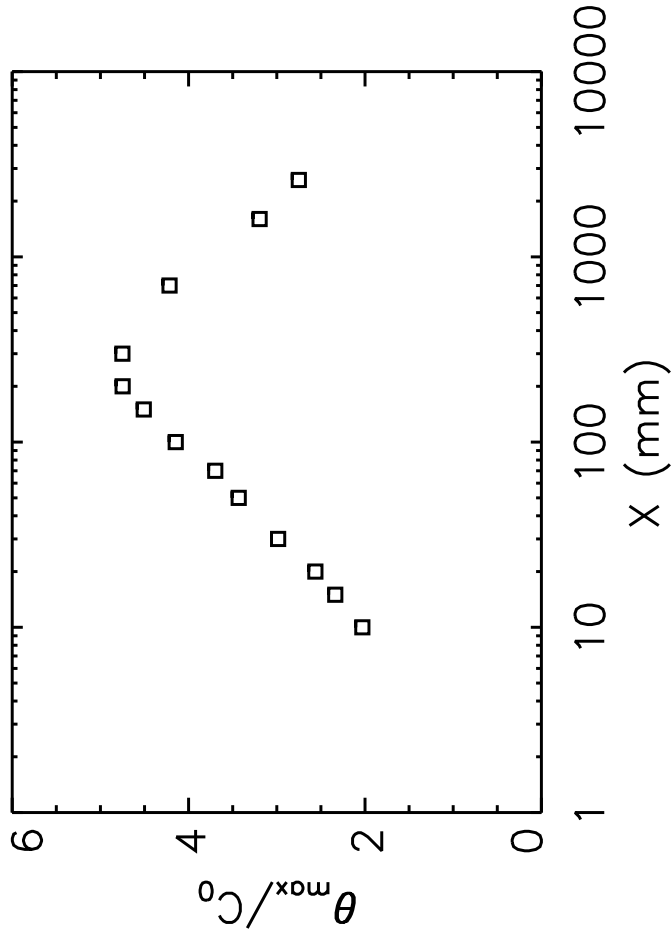
Linear fits to the moment ratios from line source, grid turbulence experiments of [Sawford & Tivendale \(1992\)](#)



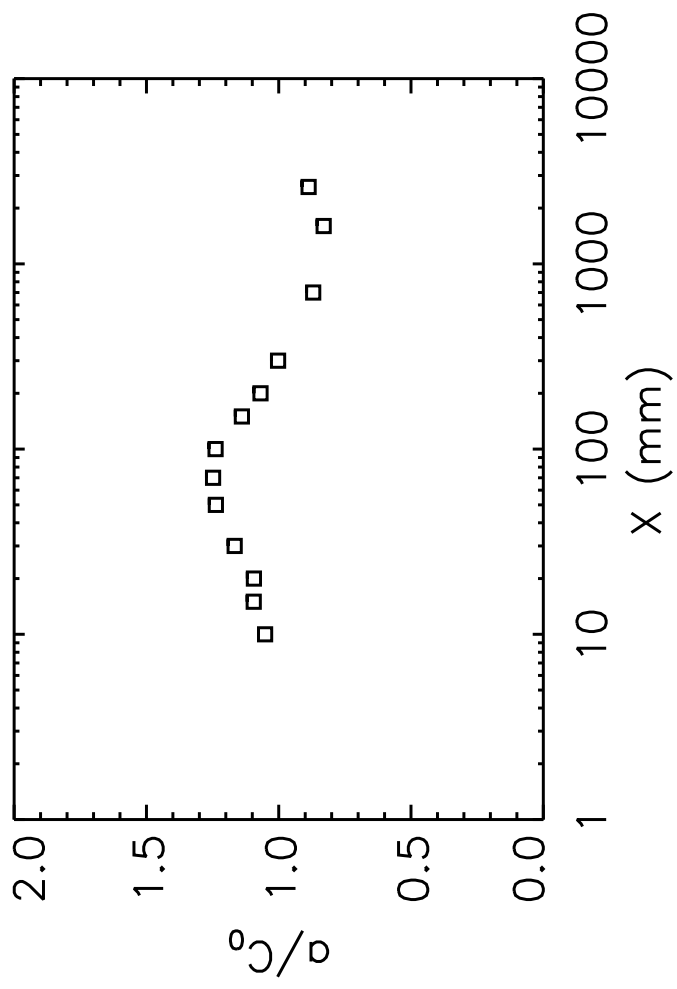
Practical issues with fitting – need to strike a balance:

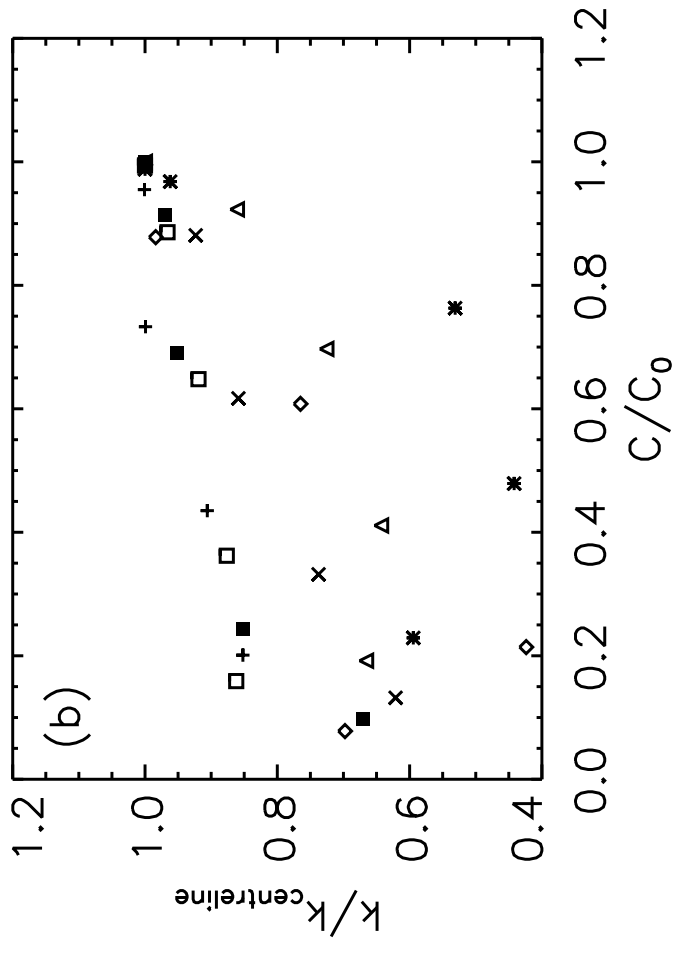
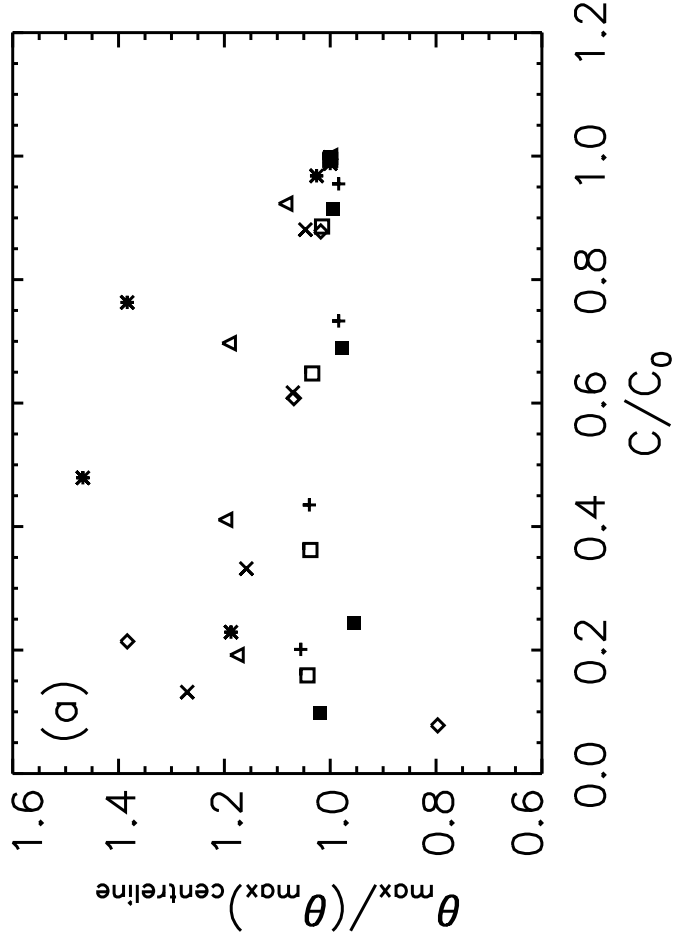
- n too small: asymptotic result does not apply
- n too large: for finite dataset this will just estimate maximum possible concentration by maximum measured concentration

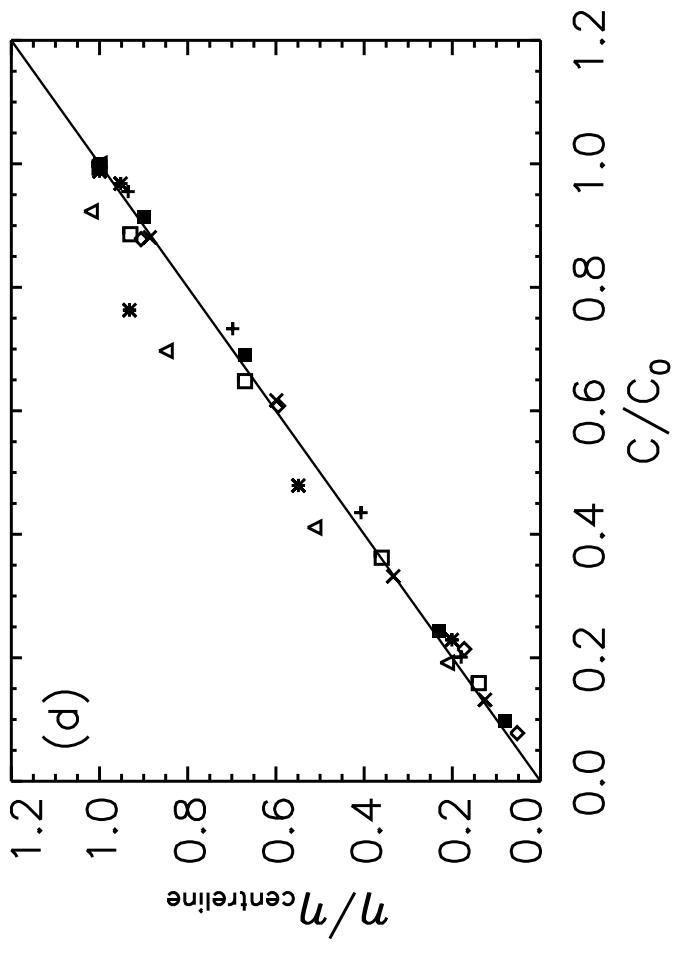
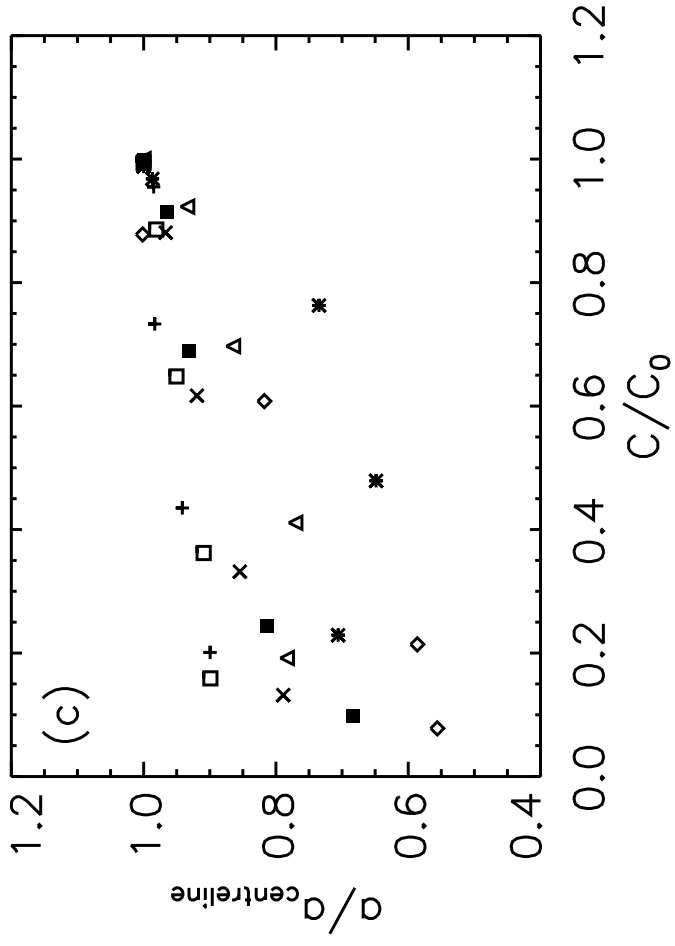
Centreline:



□ Least squares fit to $n = 4, \dots, 8$







Mole, Schopflocher & Sullivan (2008): for the moment results quoted earlier

$$\frac{\theta_{\max}}{C_0} \approx \frac{\alpha\beta\lambda_3^2 a_4 a_5}{5a_4^2 - 4a_5} + (1 - \beta)\frac{C}{C_0}$$

5 parameters: α , β , λ_3 , a_4 , a_5

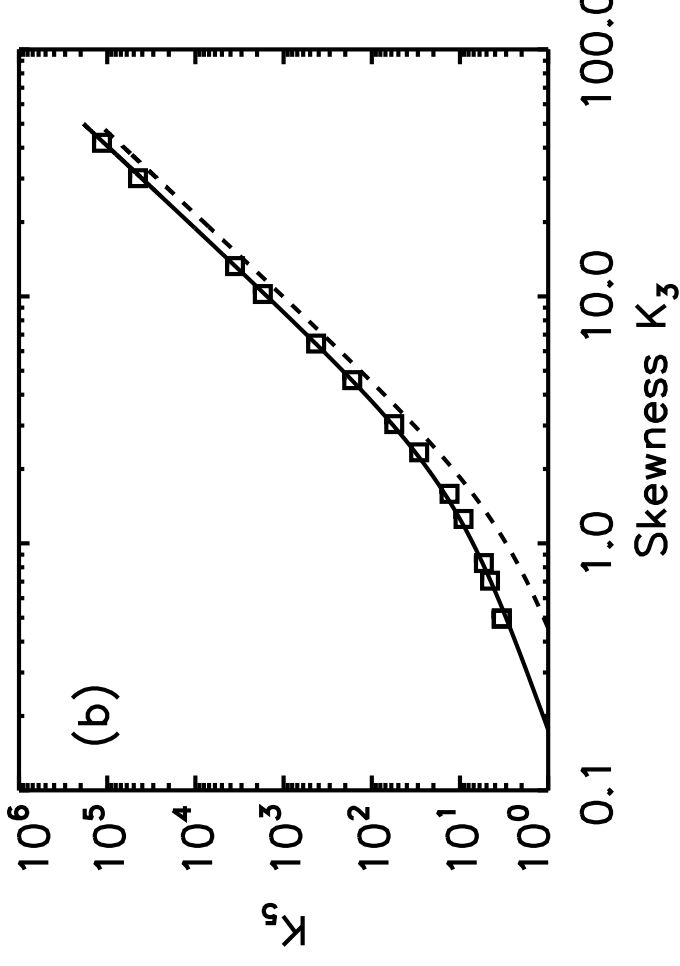
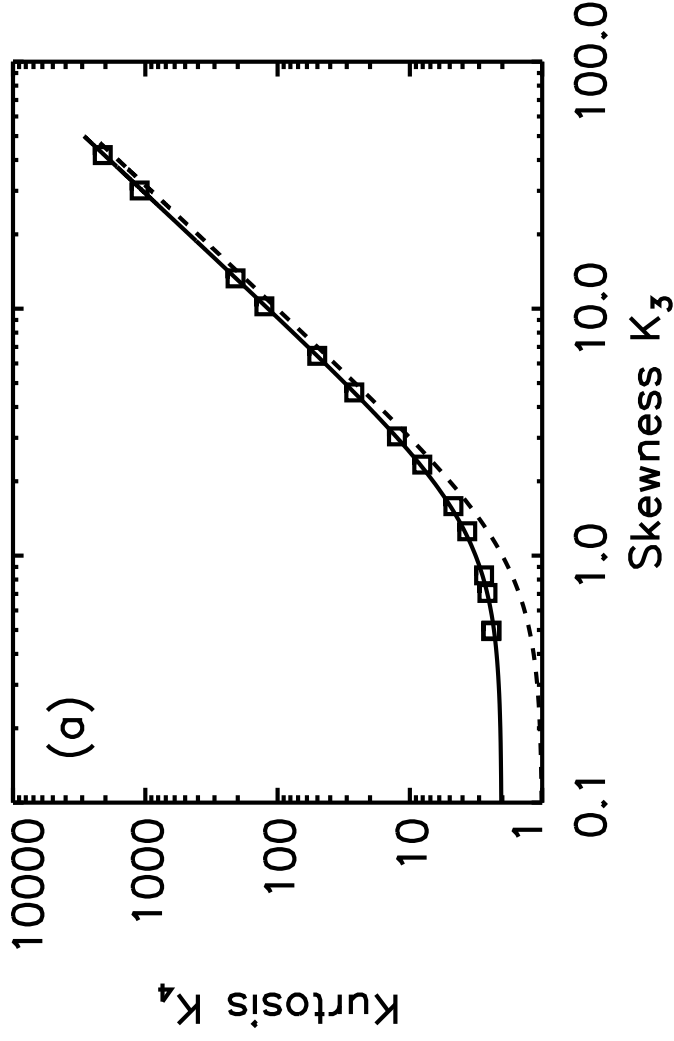
Weak dependence on C/C_0

Work in progress

- Comparing this moment-based method with others (including Maximum Likelihood applied to values above high threshold)
 - Bias and confidence intervals using simulated datasets
 - Comparison of results for experimental data

General message

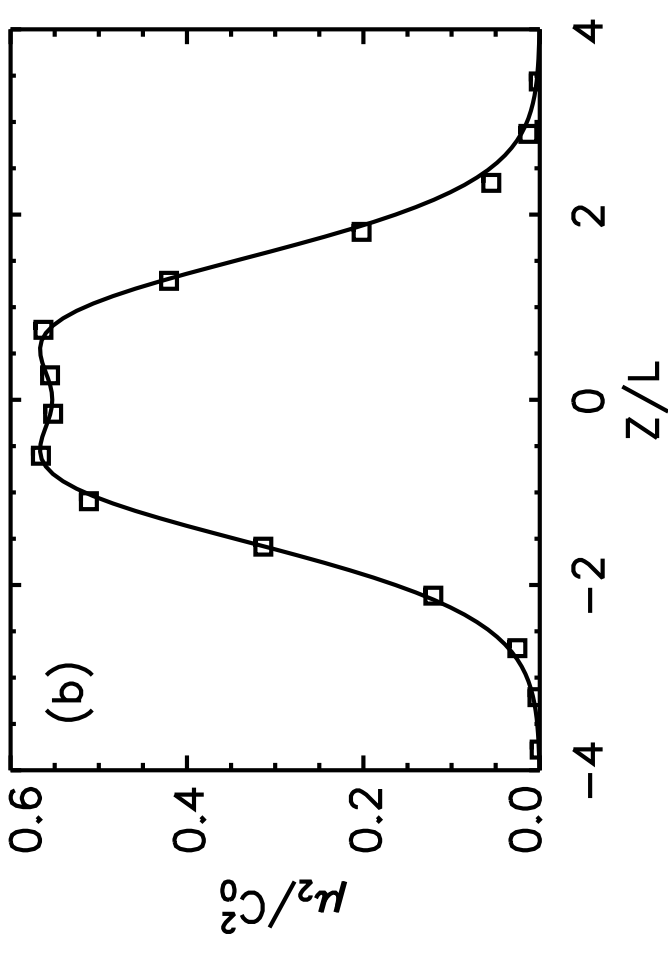
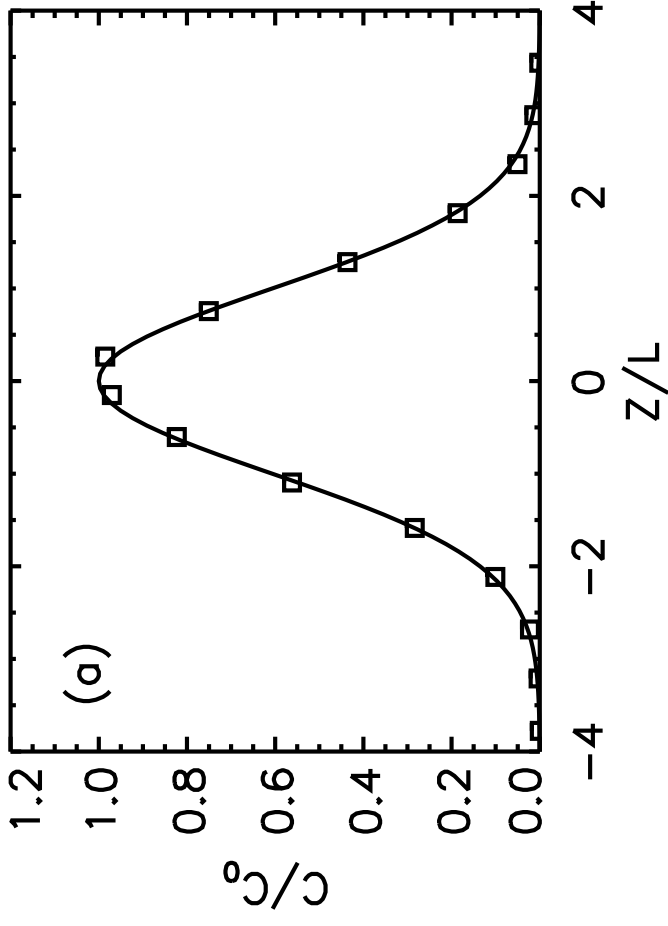
- Large concentrations deserving of more research effort



Sawford & Tivendale (2008) line source, grid turbulence, $X = 50$ mm

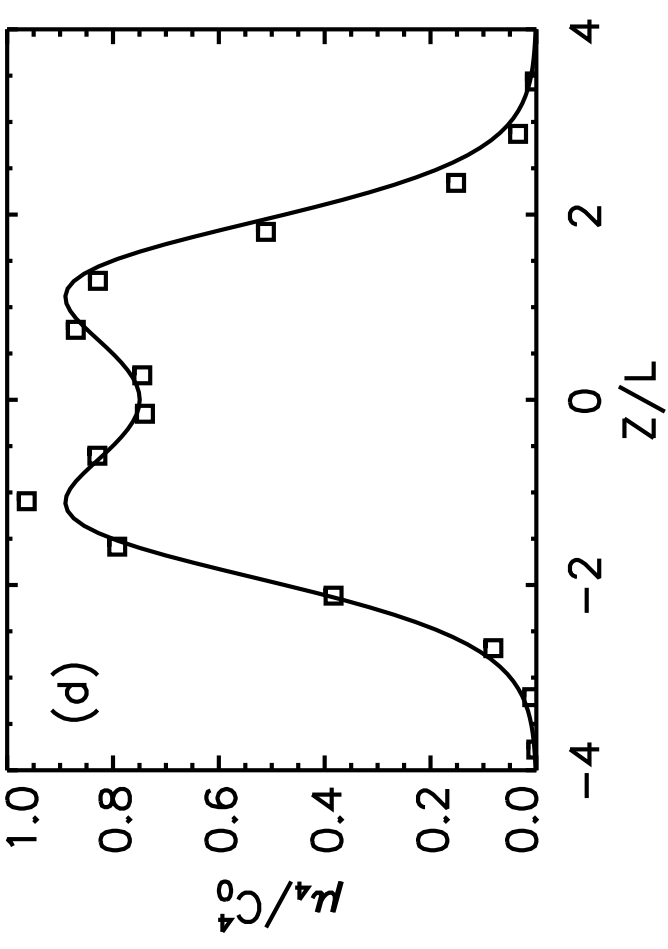
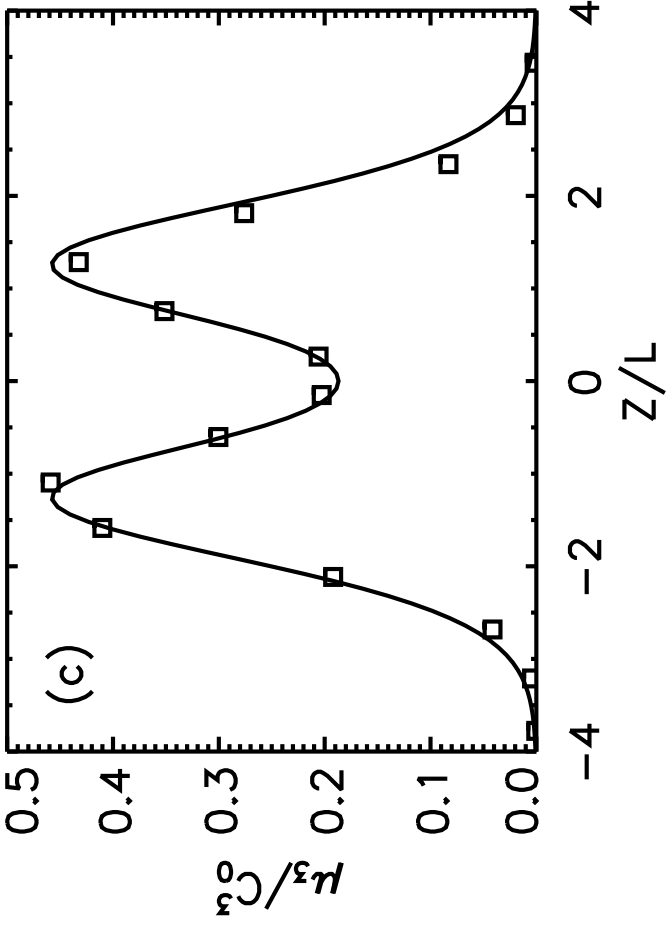
Solid curves: Mole & Clarke (1995) $a_4 = 1.161$, $b_4 = 2.025$, $a_5 = 1.485$, $b_5 = 5.647$

Dashed curves: $a_4 = b_4 = a_5 = 1$, $b_5 = 2$



Sawford & Tivendale (2008) line source, grid turbulence, $X = 50$ mm

$$\alpha = 1.729, \beta = 0.871, \lambda_3^3 = 1.161, \lambda_4^3 = 1.511$$



Sawford & Tivendale (2008) line source, grid turbulence, $X = 50$ mm