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

  $\kappa =$ (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 $C = \mathsf{E}\{\Gamma\}$ (on centreline $C = C_0$)

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

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

(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):

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

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

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

Mole, Schopflocher & Sullivan (2008):

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

$$a_6 = \frac{3a_4a_5^2}{5a_4^2 - 2a_5} \qquad + \text{ similar for } a_7, a_8, \ldots \text{ in terms of } a_4, a_5$$

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 $\Rightarrow$ 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):

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

  Finite maximum possible concentration

$$\Rightarrow k > 0, \qquad \theta \leqslant \theta_{\text{max}}$$

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

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

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

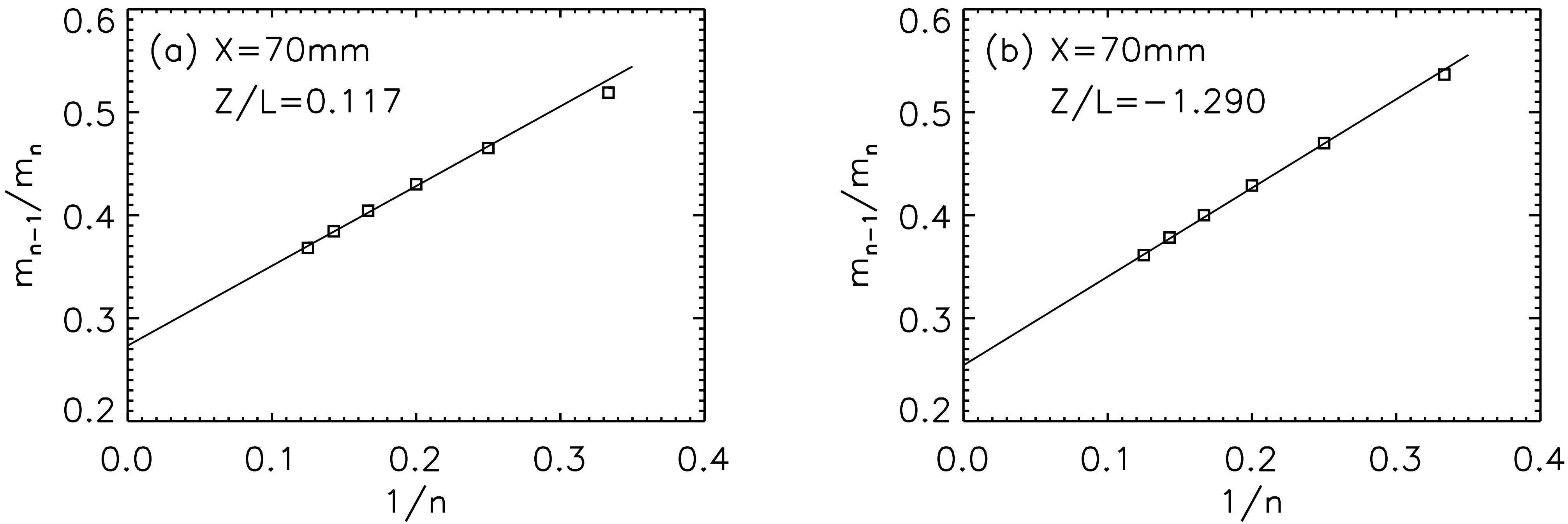
  for some function f which is negligible for large θ, and taking $\theta_T = 0$.

  Absolute moments $\quad m_n = \mathrm{E}\{\Gamma^n\}$

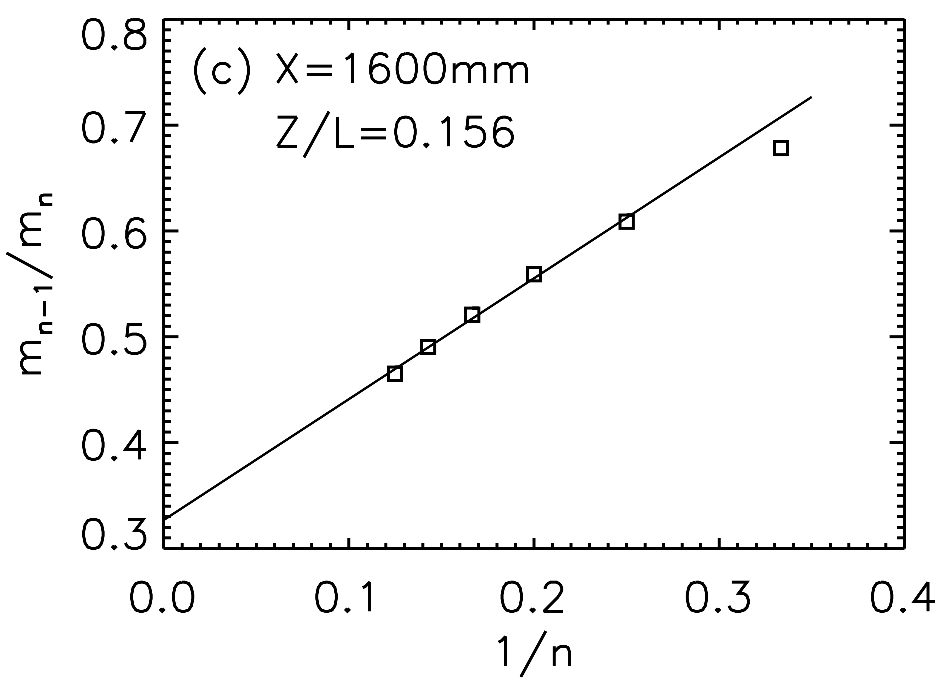
  Large $n \quad \Rightarrow \quad m_n$ dominated by large concentrations

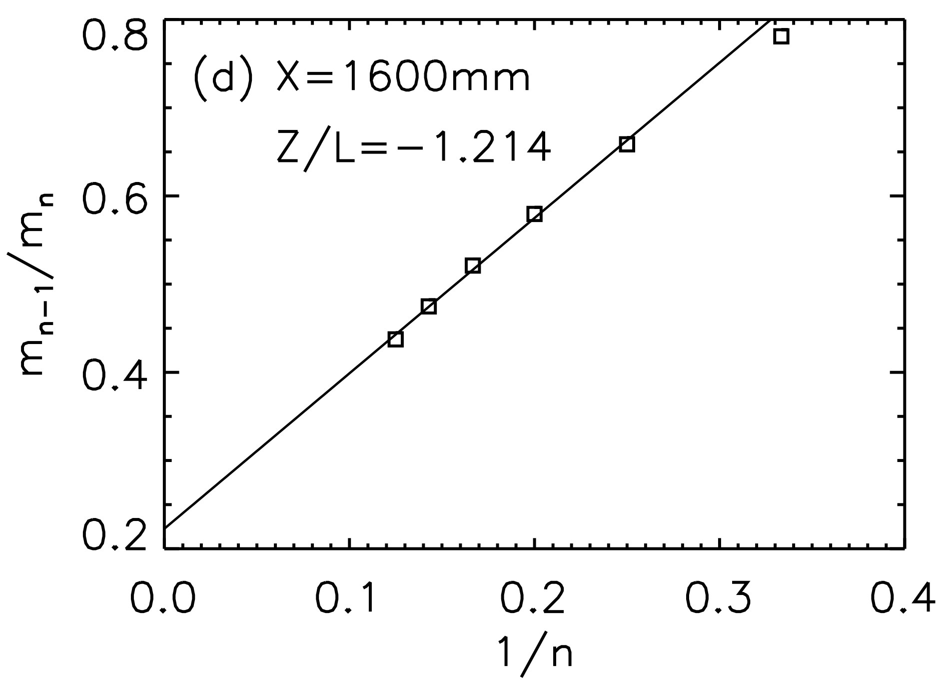
  Large concentrations GPD

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



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



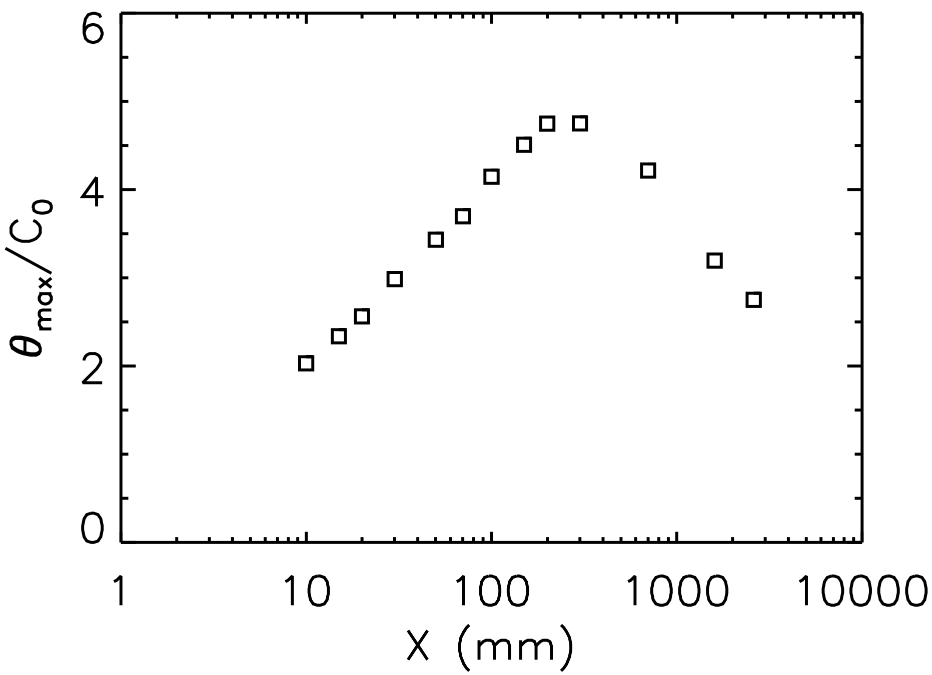


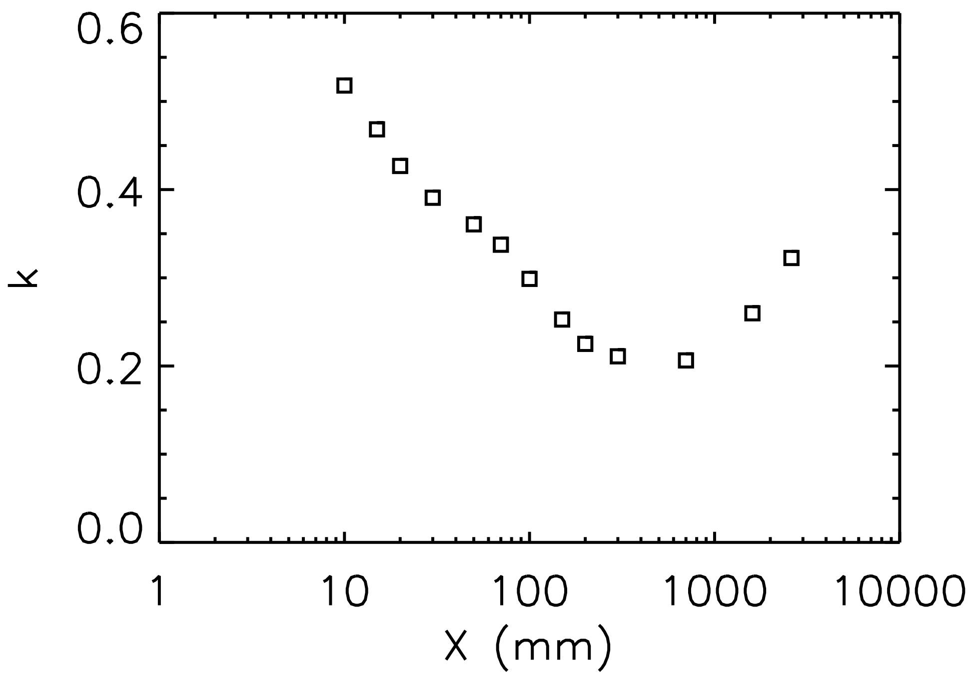
Practical issues with fitting – need to strike a balance:

- n too small: asymptotic result does not apply

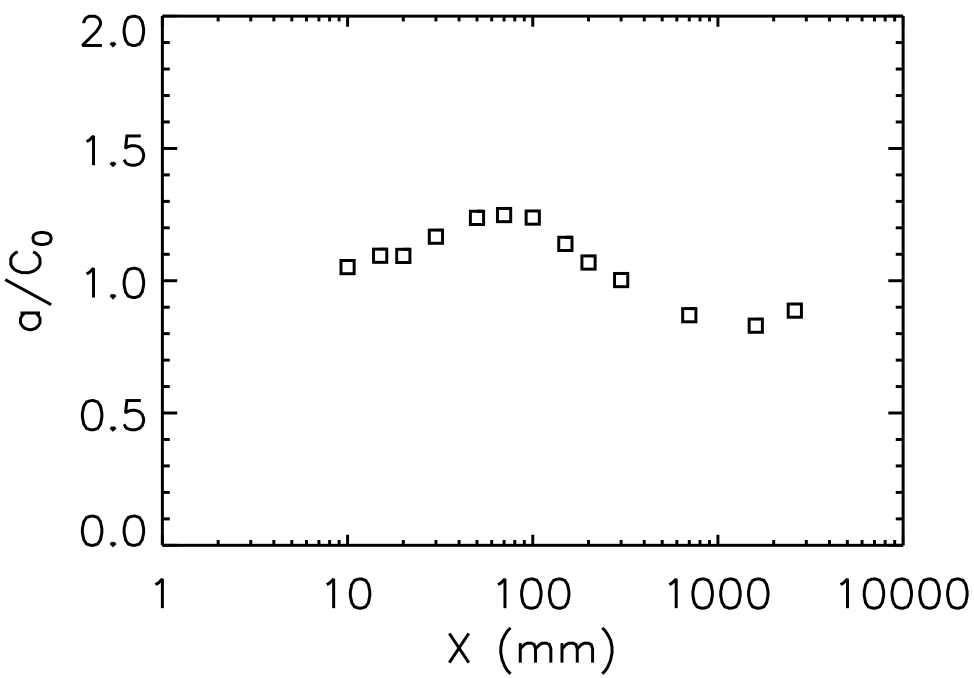
- n too large: for finite dataset this will just estimate maximum possible concentration by maximum measured concentration

Centreline:

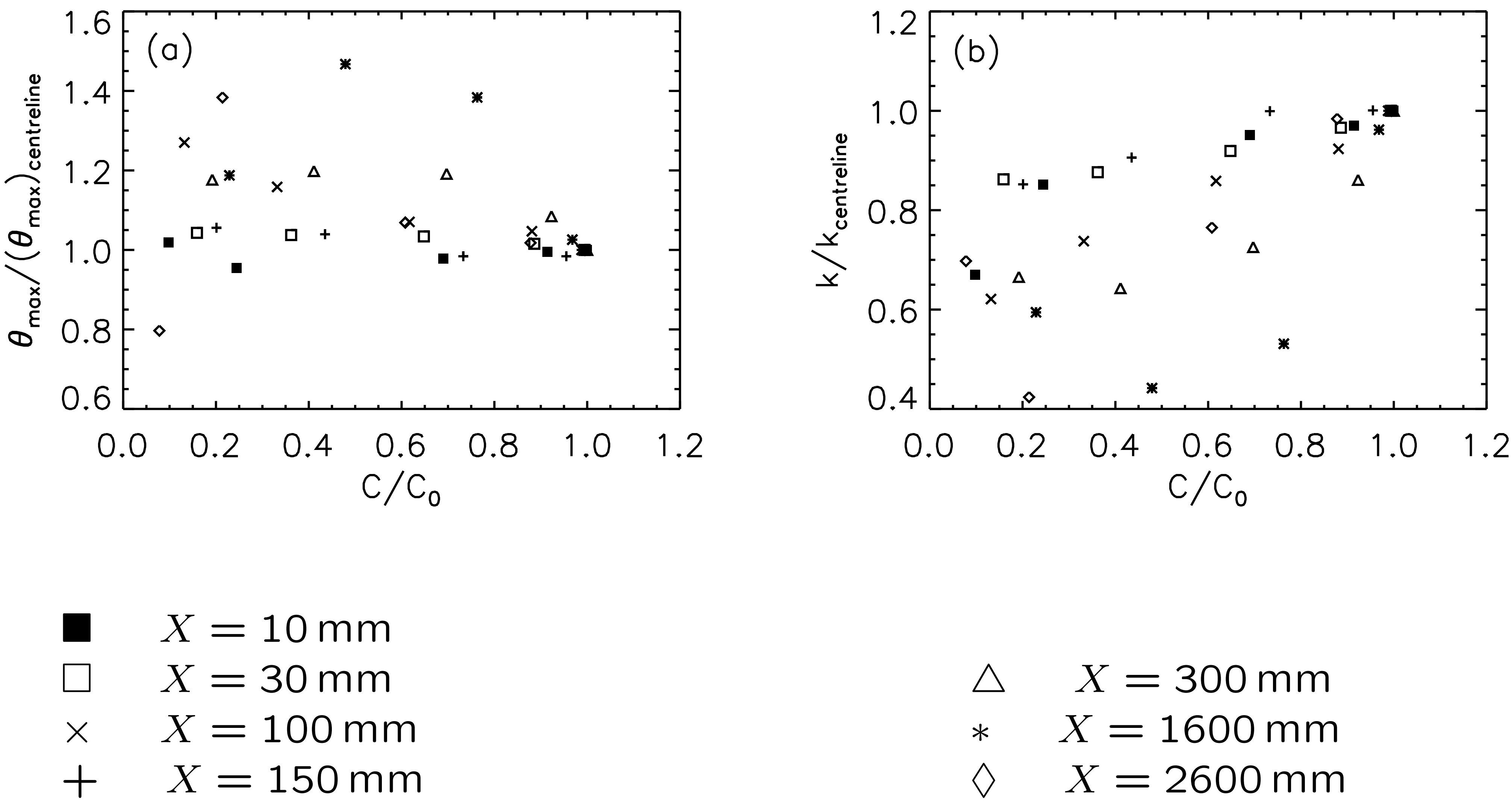




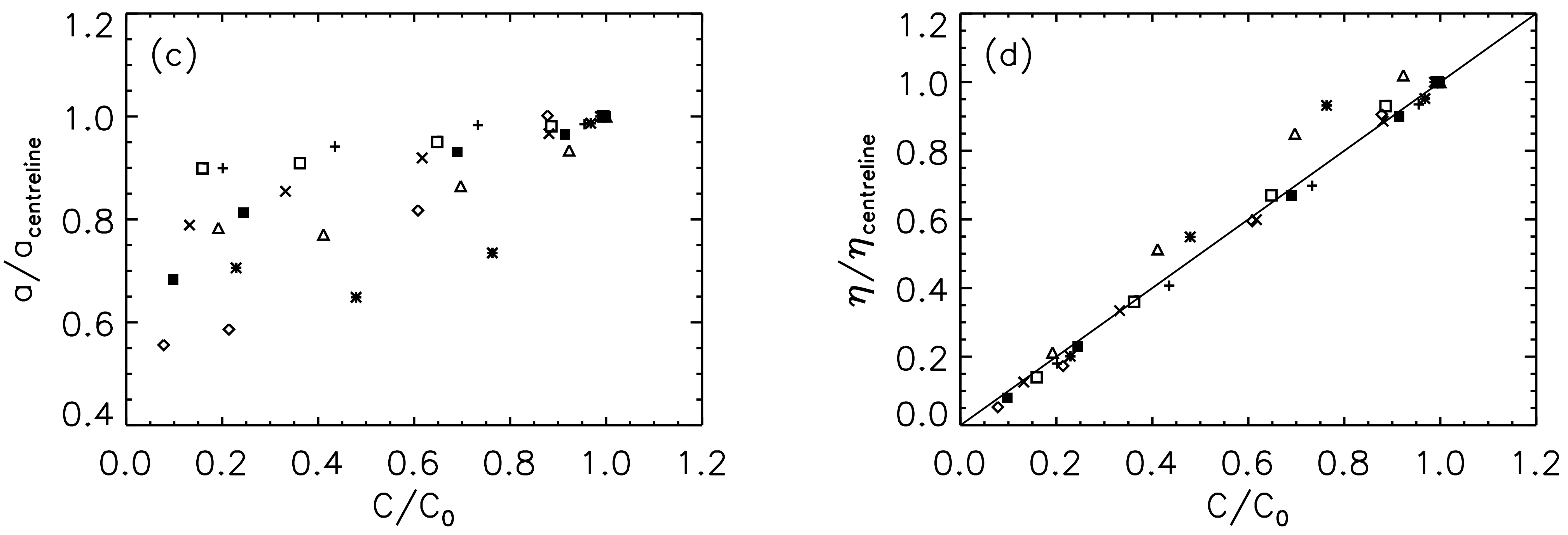
□ Least squares fit to $n = 4, \ldots, 8$



2.0
1.5
1.0
0.5
0.0
a/C0
1
10
100
1000
10000
X (mm)



(a)
θmax/(θmax)centreline
C/C0
(b)
k/kcentreline
C/C0
X = 10 mm
X = 30 mm
X = 100 mm
X = 150 mm
X = 300 mm
X = 1600 mm
X = 2600 mm


(c)
a/a_centreline
C/C_0
(d)
η/η_centreline
C/C_0

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

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

5 parameters: α, β, λ_3, a_4, a_5

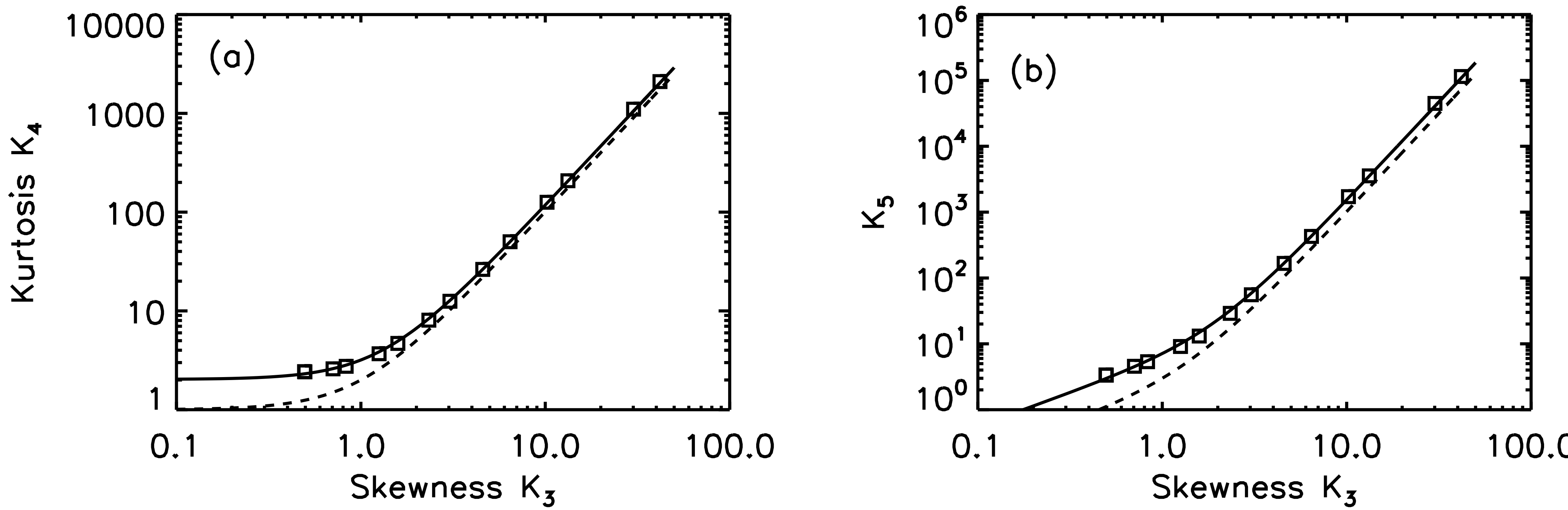
Weak dependence on C/C_0

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

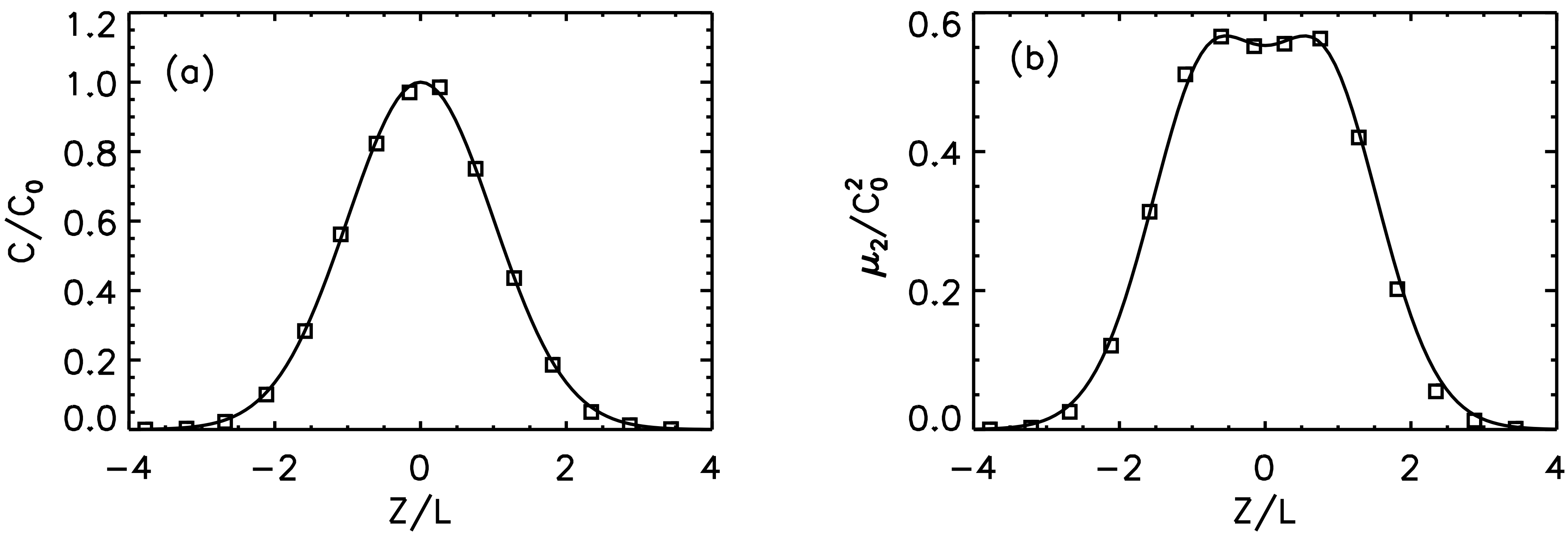
- Large concentrations deserving of more research effort



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

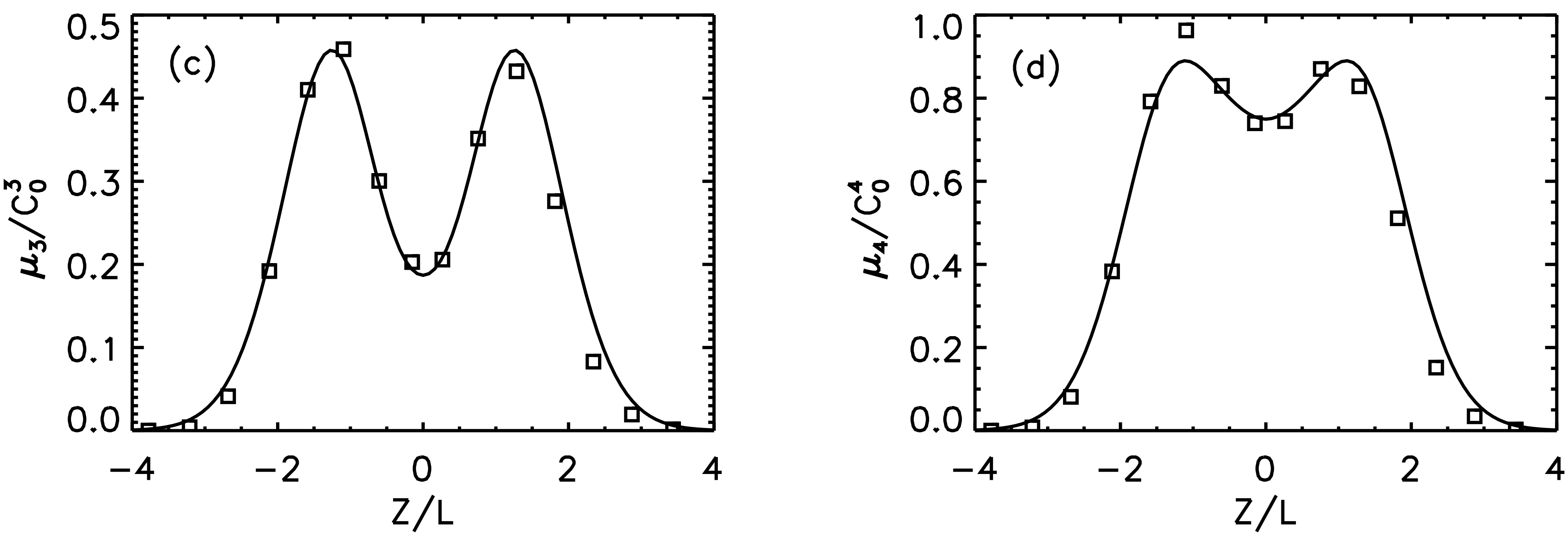
Solid curves: Mole & Clarke (1995) $a_4 = 1.161$, $b_4 = 2.025$, $a_5 = 1.485$, $b_5 = 5.647$

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



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

$\alpha = 1.729$, $\beta = 0.871$, $\lambda_3^2 = 1.161$, $\lambda_4^3 = 1.511$



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