A model for extreme values of concentration in turbulent dispersion

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- Short-range dispersion of toxic/flammable gases: high concentrations important for hazard assessment

- 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

- 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, distribution of a random variable takes asymptotic form of Generalised Pareto Distribution (GPD):

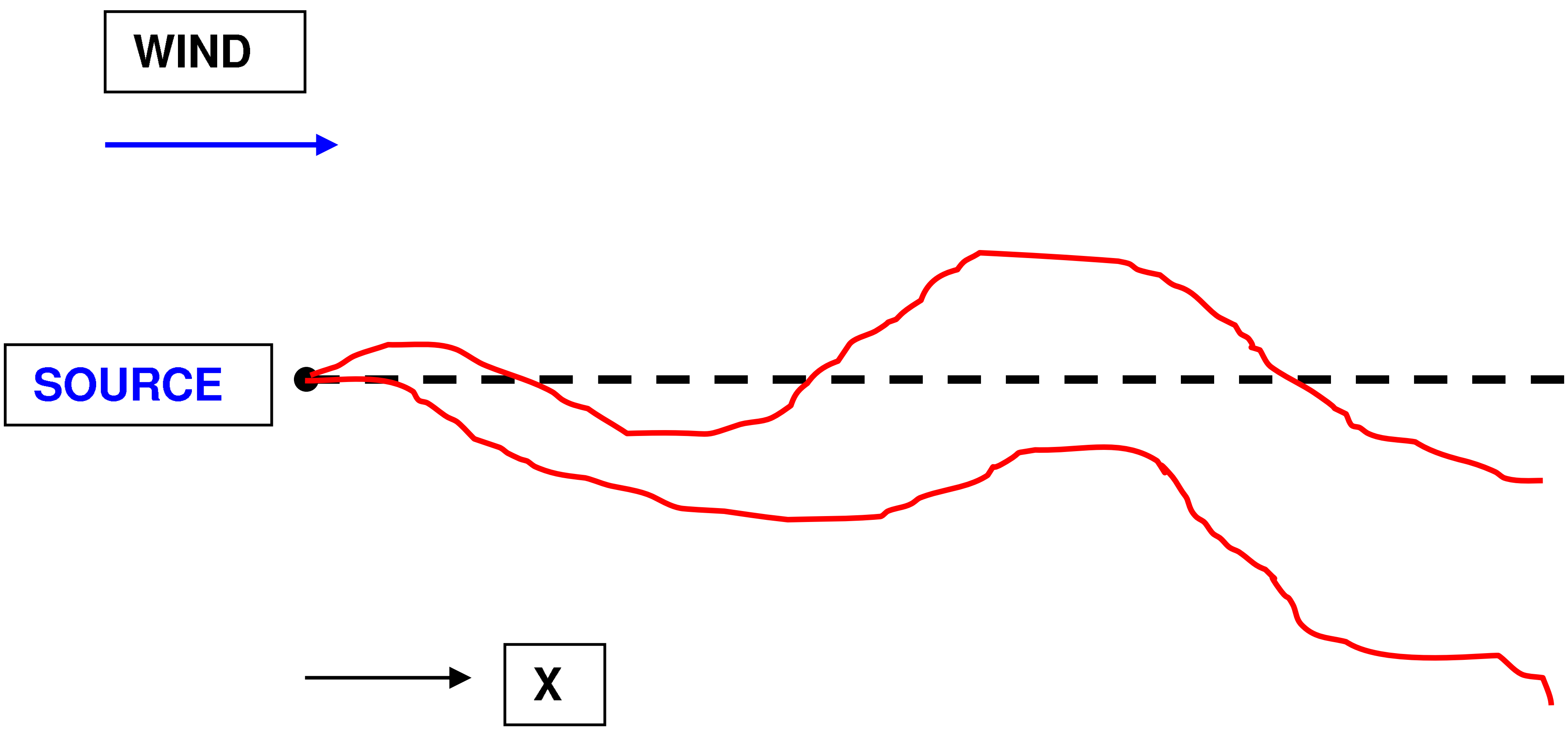
$$g(\theta) = \frac{1}{a}\left(1 - \frac{k\theta}{a}\right)^{1/k-1}, \qquad a > 0$$

  Finite maximum possible concentration

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

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

Plume from steady point or line source



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

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

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

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

(skewness K_3, kurtosis K_4)

Model

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):

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

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

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

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

Large n $\Rightarrow$ m_n dominated by large concentrations

Large concentrations GPD

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

Model parameters

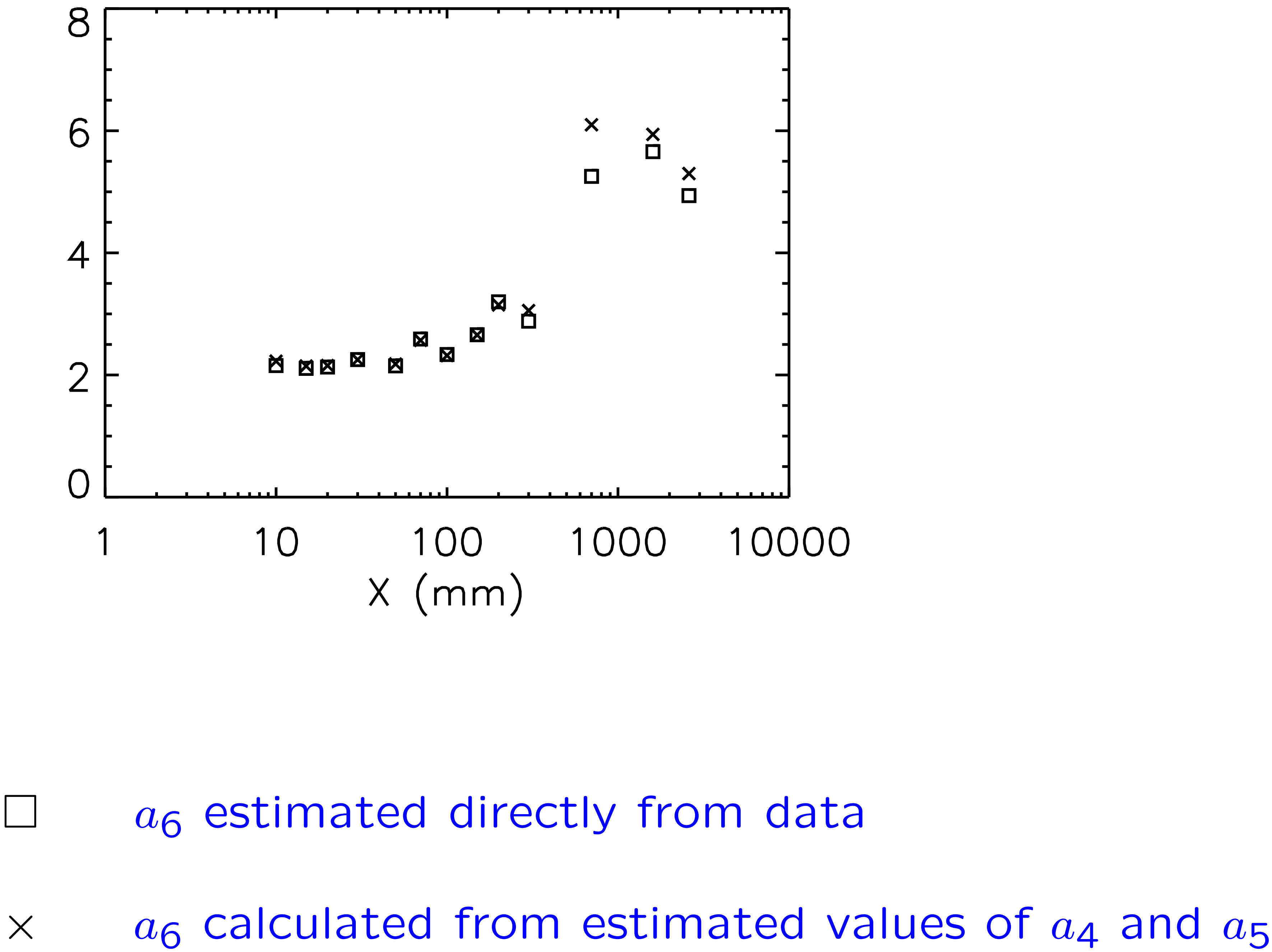
Far from centreline $\frac{C}{C_0} \to 0$

$$\Rightarrow K_n \approx \frac{\lambda_n^{n-1}}{\widehat{C}^{(n-2)/2}} \gg 1 \qquad \Rightarrow K_n \approx a_n K_3^{n-2}$$

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

GPD for high order moments

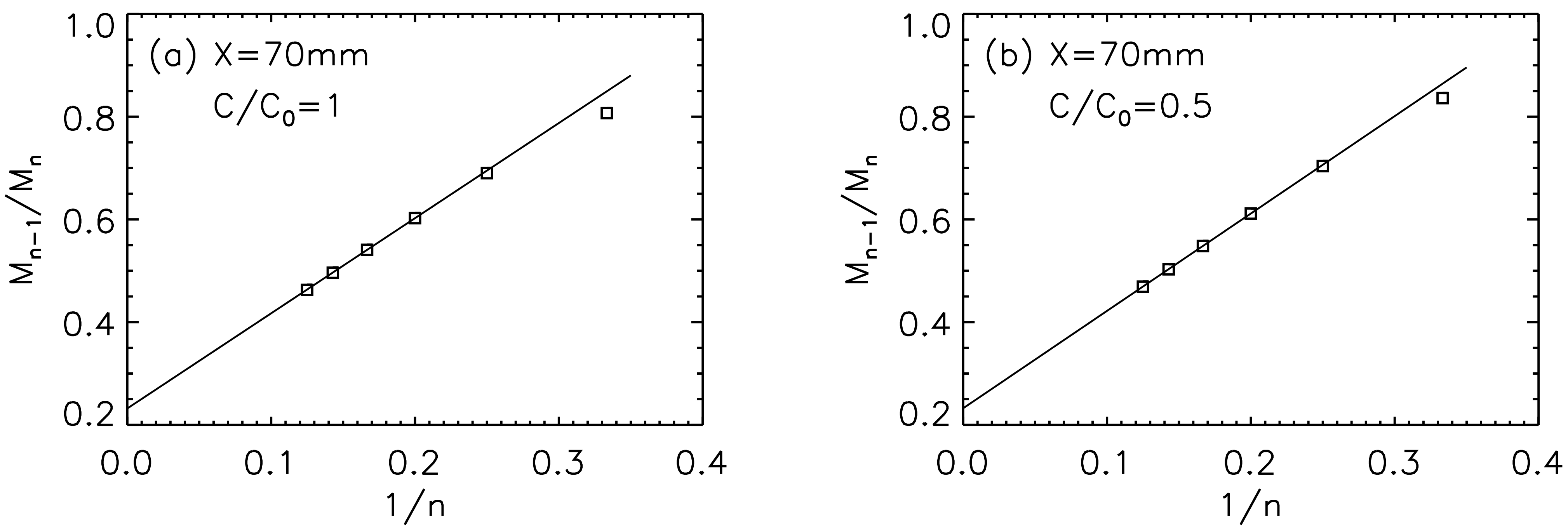
$$\Rightarrow a_6 = \frac{3a_4 a_5^2}{5a_4^2 - 2a_5} \qquad + \text{ similar for } a_7, a_8, \ldots$$


8
6
4
2
0
1
10
100
1000
10000
X (mm)
a_6 estimated directly from data
a_6 calculated from estimated values of a_4 and a_5

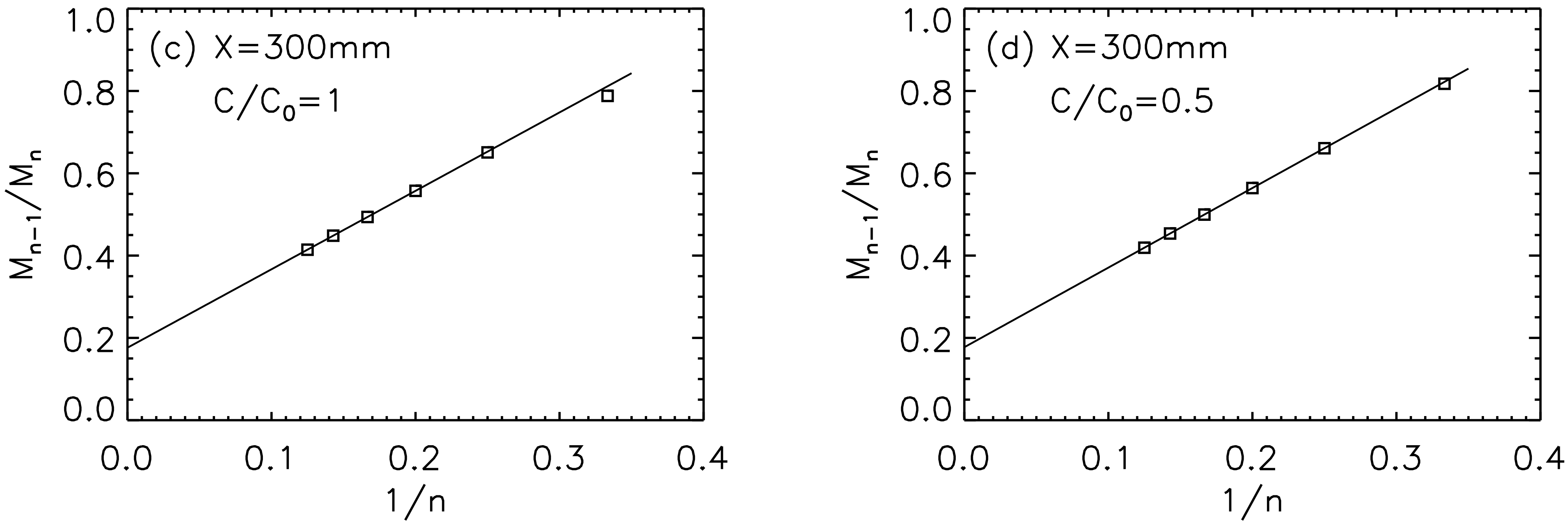
$$\frac{\theta_{\mathrm{max}}}{C_0} \approx \frac{\alpha\beta\lambda_3^2 a_4 a_5}{5a_4^2 - 4a_5} + (1-\beta)\frac{C}{C_0}$$

5 parameters: α, β, λ_3, a_4, a_5

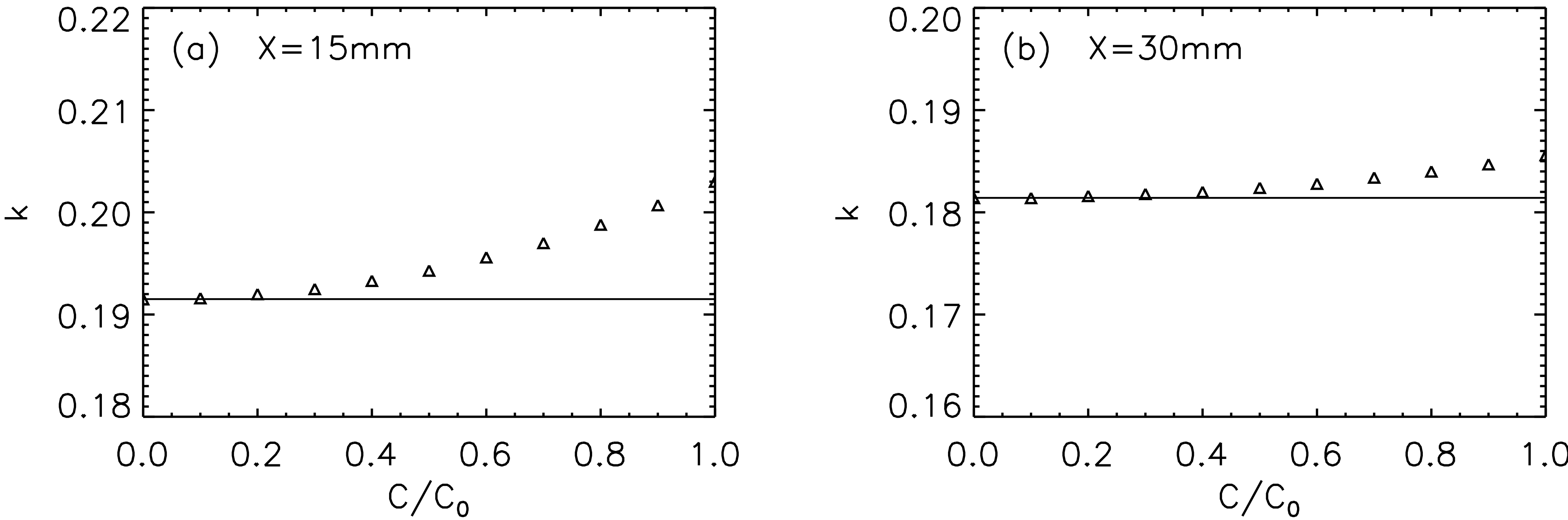
Weak dependence on C/C_0



Linear fits to the moment ratios from model



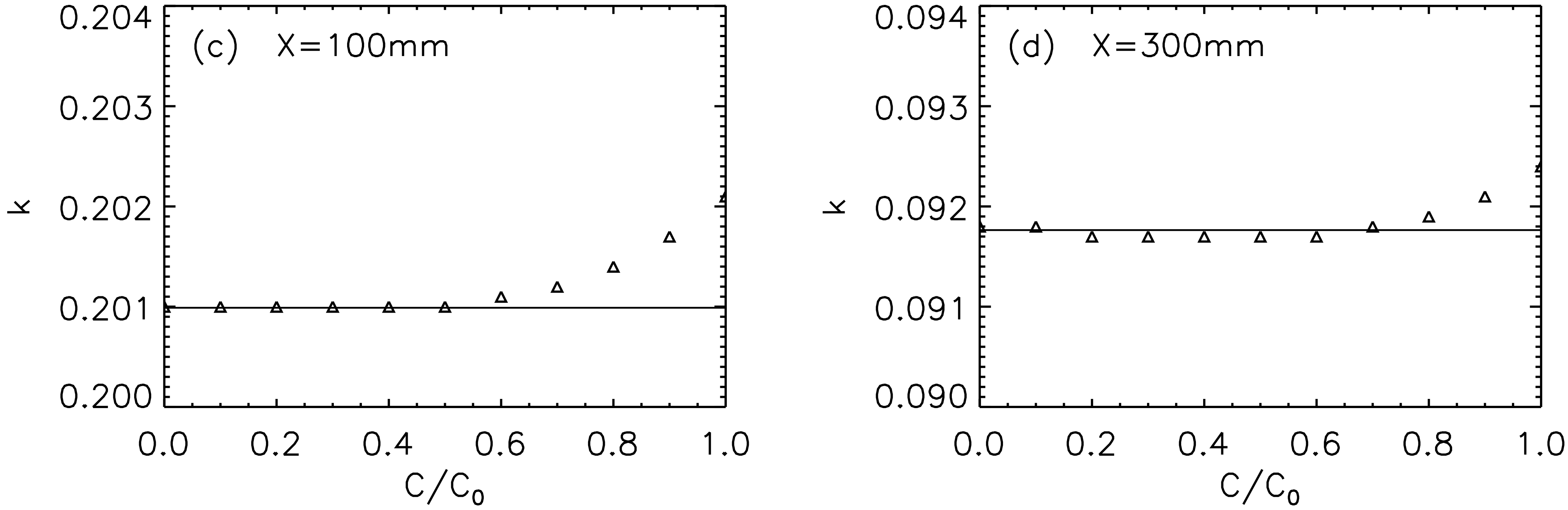
(c) X=300mm
$C/C_0=1$
(d) X=300mm
$C/C_0=0.5$
M_{n-1}/M_n
1/n
0.0
0.1
0.2
0.3
0.4
0.6
0.8
1.0

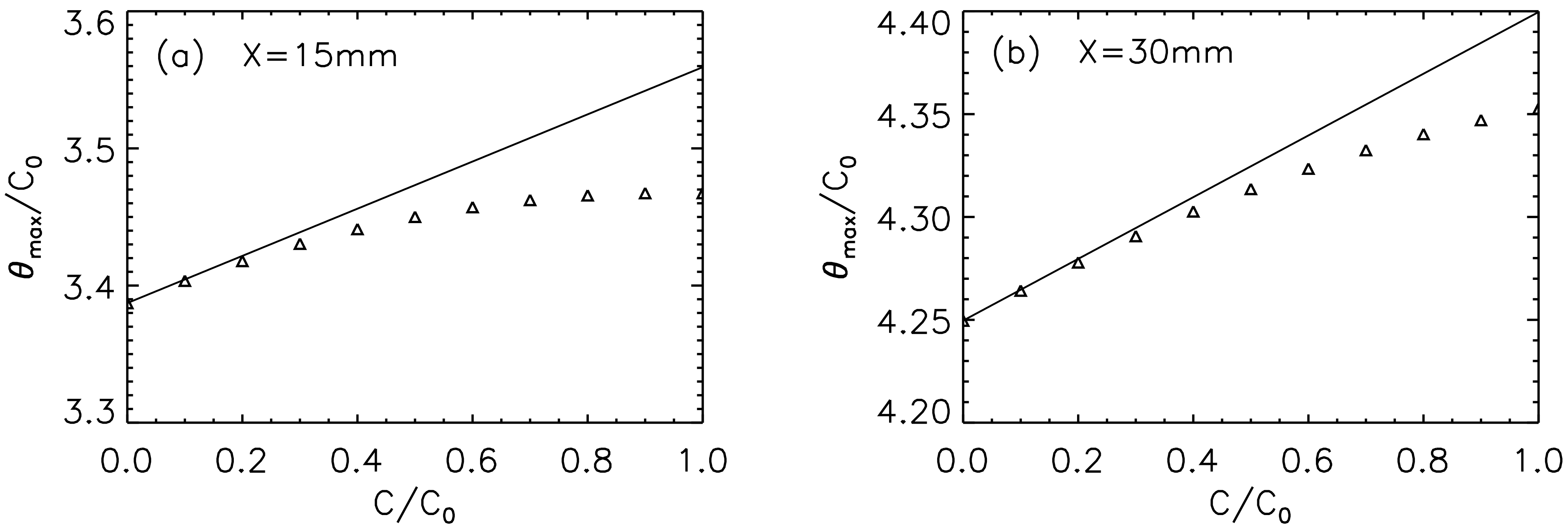


k

Line: from asymptotic approximation

△ from full model calculation

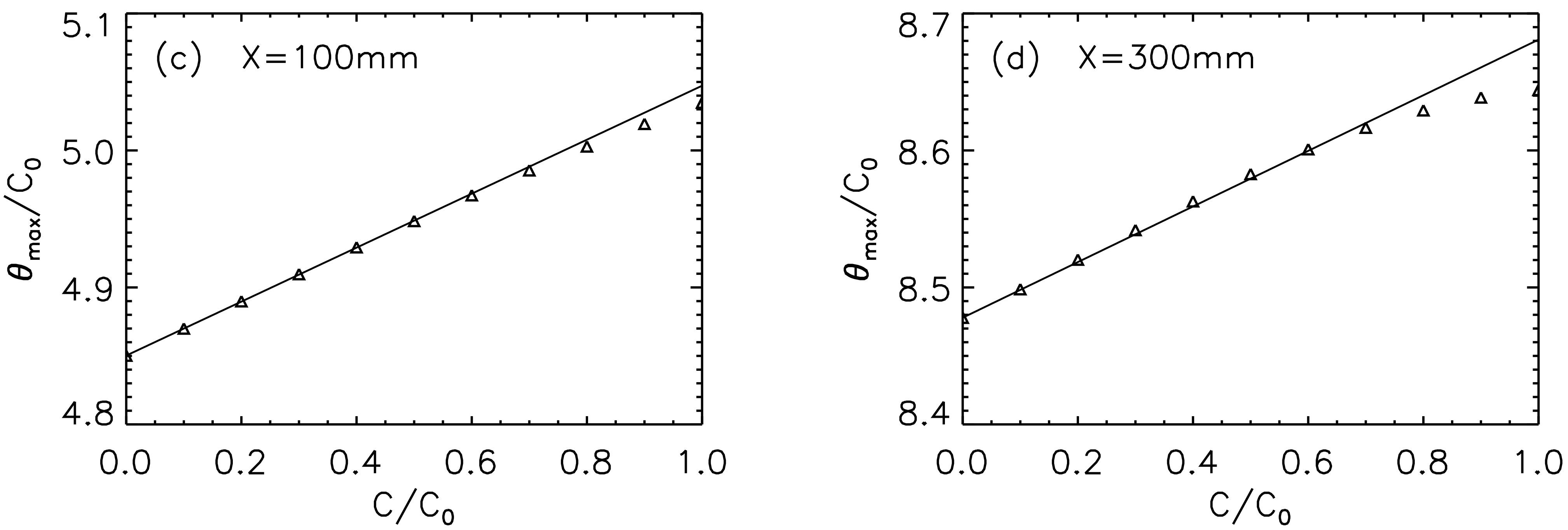

(c) X=100mm
k
0.204
0.203
0.202
0.201
0.200
0.0
0.2
0.4
0.6
0.8
1.0
C/C0
(d) X=300mm
k
0.094
0.093
0.092
0.091
0.090
0.0
0.2
0.4
0.6
0.8
1.0
C/C0

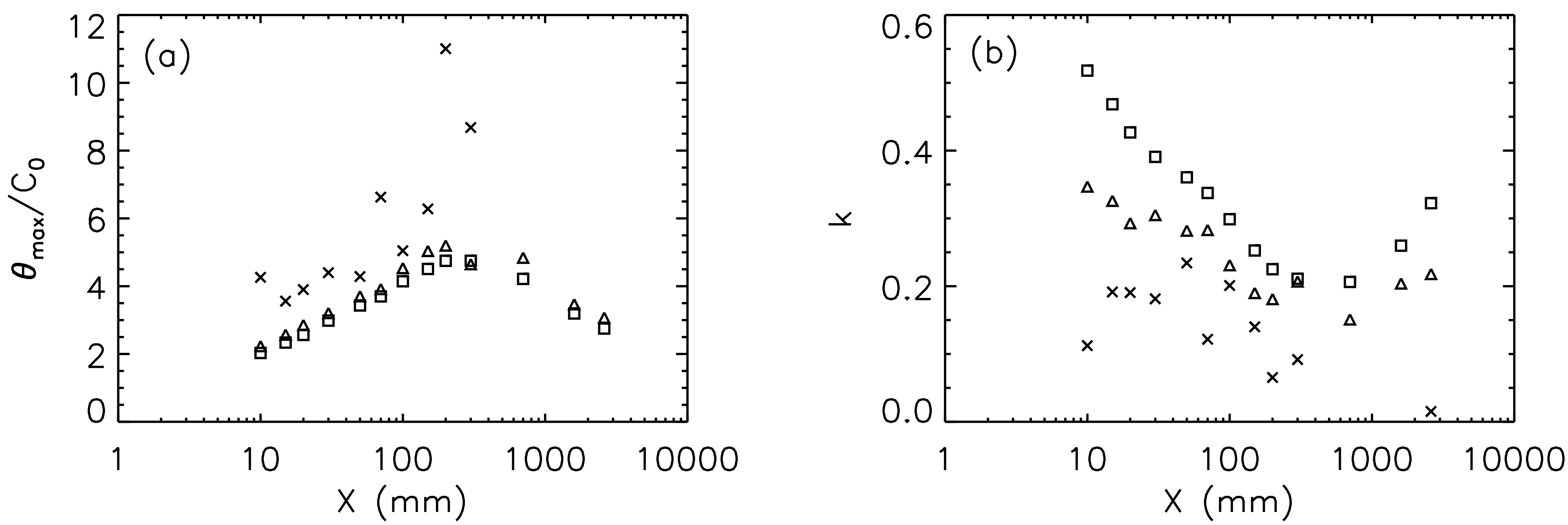


$\theta_{\mathrm{max}}/C_0$

Line: from asymptotic approximation

△ from full model equations

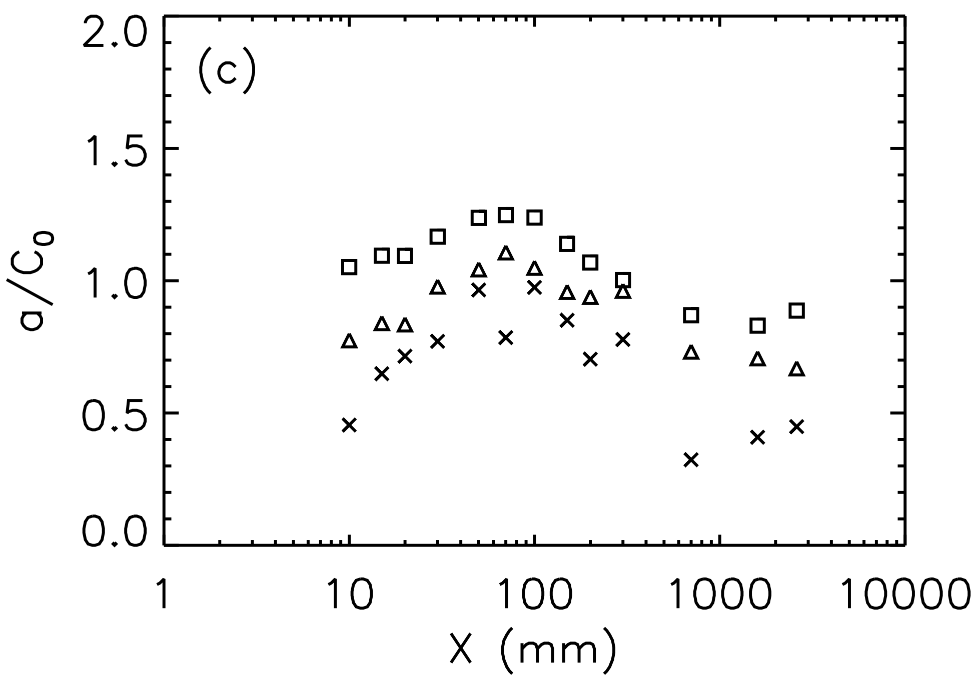

(c) X=100mm
θmax/C0
C/C0
5.1
5.0
4.9
4.8
0.0
0.2
0.4
0.6
0.8
1.0
(d) X=300mm
θmax/C0
C/C0
8.7
8.6
8.5
8.4
0.0
0.2
0.4
0.6
0.8
1.0

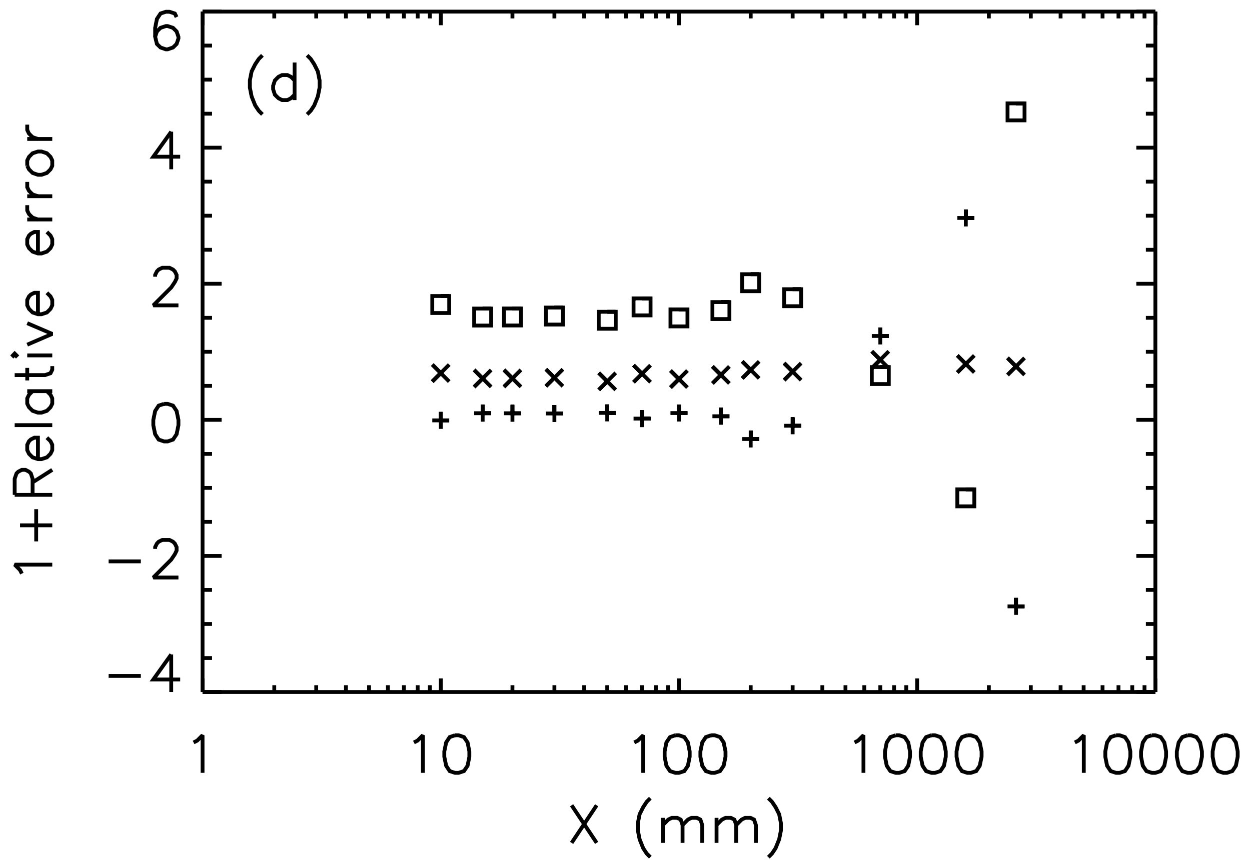


× Model values

□ Calculated directly from measurements: least squares fit to $n = 4, \ldots, 8$

△ Calculated directly from measurements: linear fit through $n = 7, 8$


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



Errors assuming 5% error in a_5

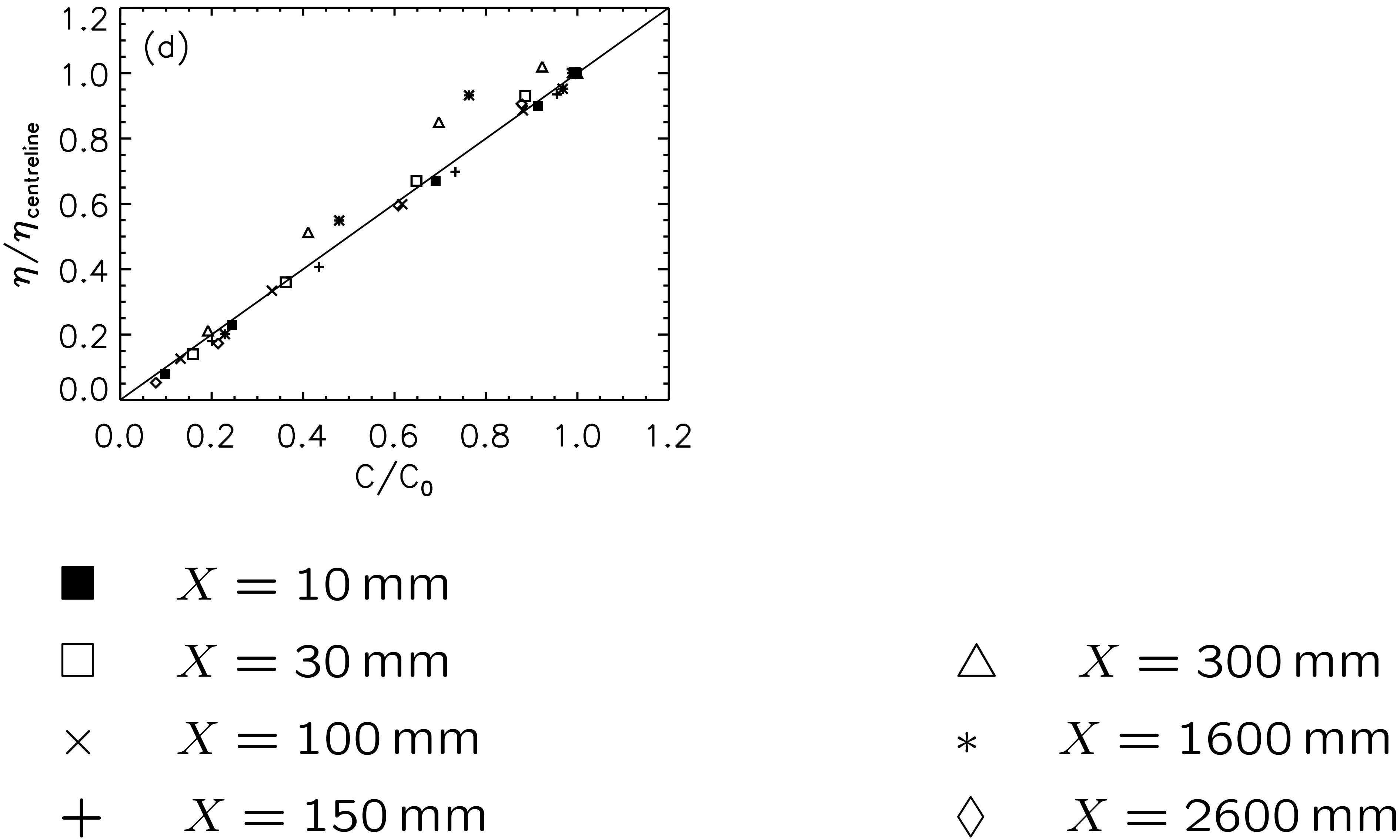
□ θ_{max}/C_0 + k × a/C_0

In principle:

Any model which gives spatial dependence of 2nd–6th moments

$\Rightarrow$ values of $\alpha, \beta, \lambda_3, a_4, a_5$

$\Rightarrow$ values of $\dfrac{\theta_{\mathrm{max}}}{C_0}$



(d)
η/η_centreline
C/C_0
0.0
0.2
0.4
0.6
0.8
1.0
1.2
X = 10 mm
X = 30 mm
X = 100 mm
X = 150 mm
X = 300 mm
X = 1600 mm
X = 2600 mm

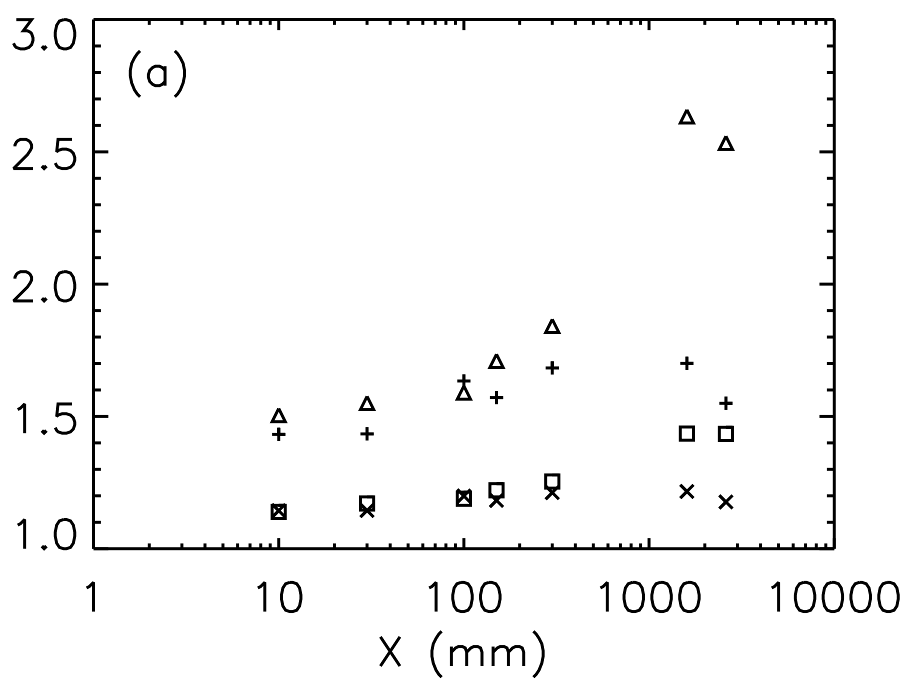
Possible further reduction of no. of parameters:

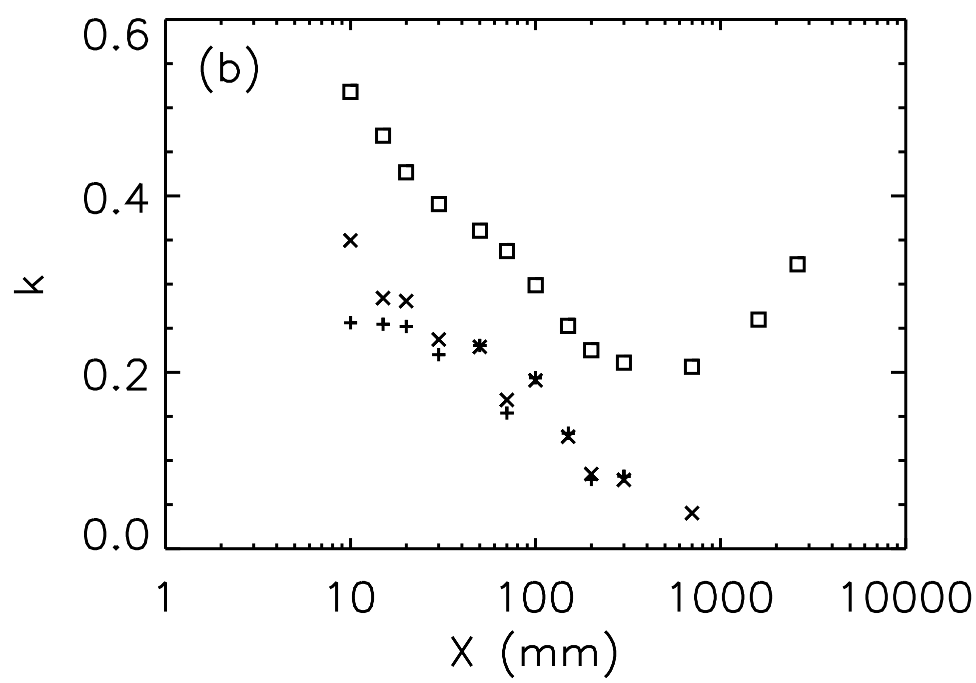
if in tail pdf $\approx \eta g(\theta)$

and $\eta \ll 1$ far from centreline (consistent with data here) then

$$a_4 = \frac{4(1+3k)}{3(1+4k)}$$

$$a_5 = \frac{20(1+3k)^2}{9(1+4k)(1+5k)} = \frac{5a_4^2}{8-3a_4}$$





(a) Measured a_4 ($\square$), modelled a_4 ($\times$), measured a_5 ($\triangle$) and modelled a_5 ($+$)

(b) Measured centreline k ($\square$) and modelled peripheral k using a_4 ($\times$) and a_5 ($+$)

$$k > 0 \qquad \Rightarrow \qquad 1 < a_4 < 4/3, \qquad 1 < a_5 < 20/9$$

(agrees with most data)

$$\boxed{\frac{\theta_{\text{max}}}{C_0} \approx \alpha\beta\lambda_3^2\left(1 + \frac{1}{3k}\right) + (1 - \beta)\frac{C}{C_0}}$$

Conclusions

- For first time (as far as we are aware) derived an explicit expression for $\frac{\theta_{\text{max}}}{C_0}$

  Involves 5 (or 4) parameters which can in principle be modelled

- Agreement with observation reasonable given the relatively large uncertainty in estimates of pdf tail properties

- Method relating properties of high concentrations to moment ratios allows any models which give enough moments to predict $\frac{\theta_{\mathrm{max}}}{C_0}$ etc.

Future work

- Attempt modelling of the parameters and hence $\frac{\theta_{\mathrm{max}}}{C_0}$

- Compare with more experiments