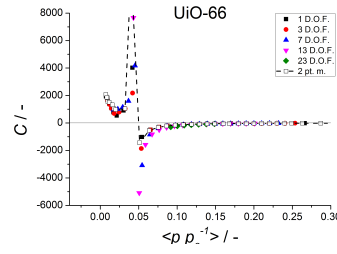
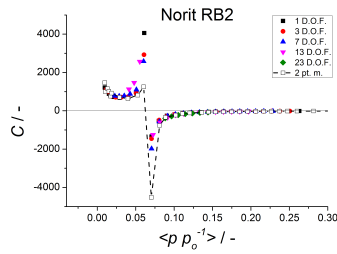


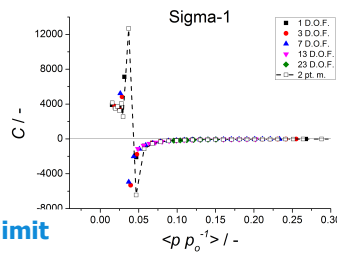
## BET and microporous materials – Upper limit ?



### 'Two-point BET'

Calculate C for two consecutive data points:

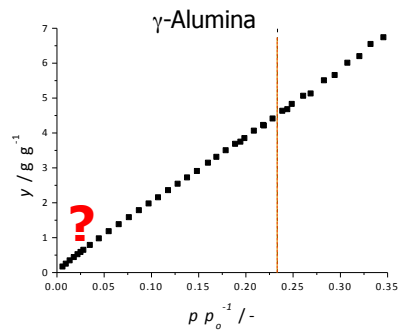
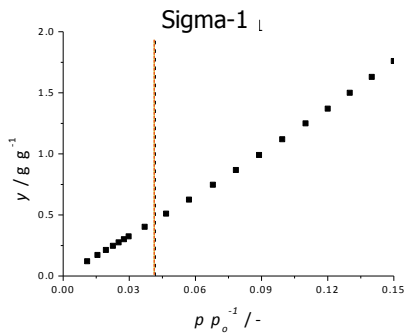
$$y_i = \left( \frac{1}{Cq_m} \right) + \left( \frac{C-1}{Cq_m} \right) x_i \iff C_i = \frac{I_i + s_i}{I_i}$$



Transition determines upper  $p/p_0$  limit  
Easy implementation

## Linearized BET

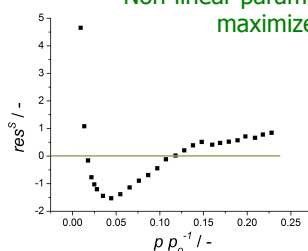
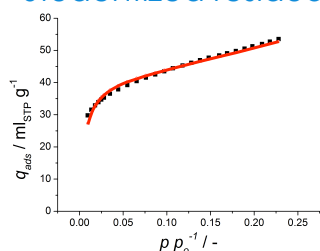
### 2-point BET: upper limit lower limit $p/p_0$ ?



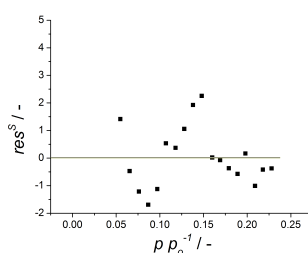
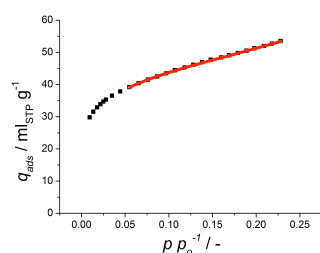
# BET – How to apply to mesoporous materials?

## Studentized residuals

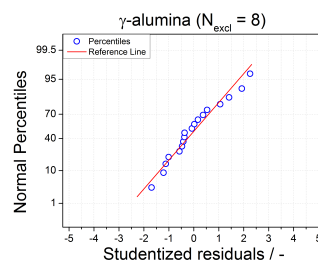
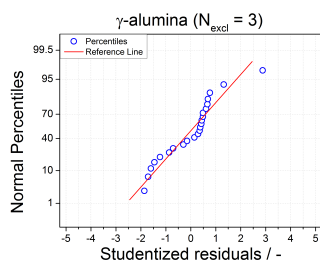
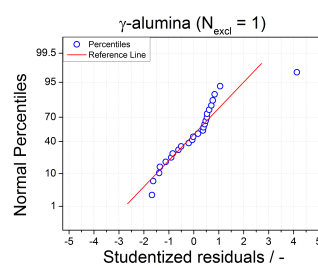
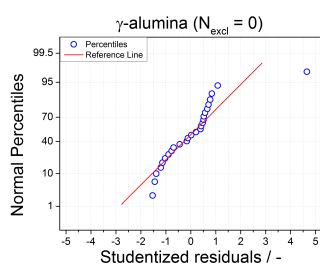
Non-linear parameter estimation  
maximize # data points

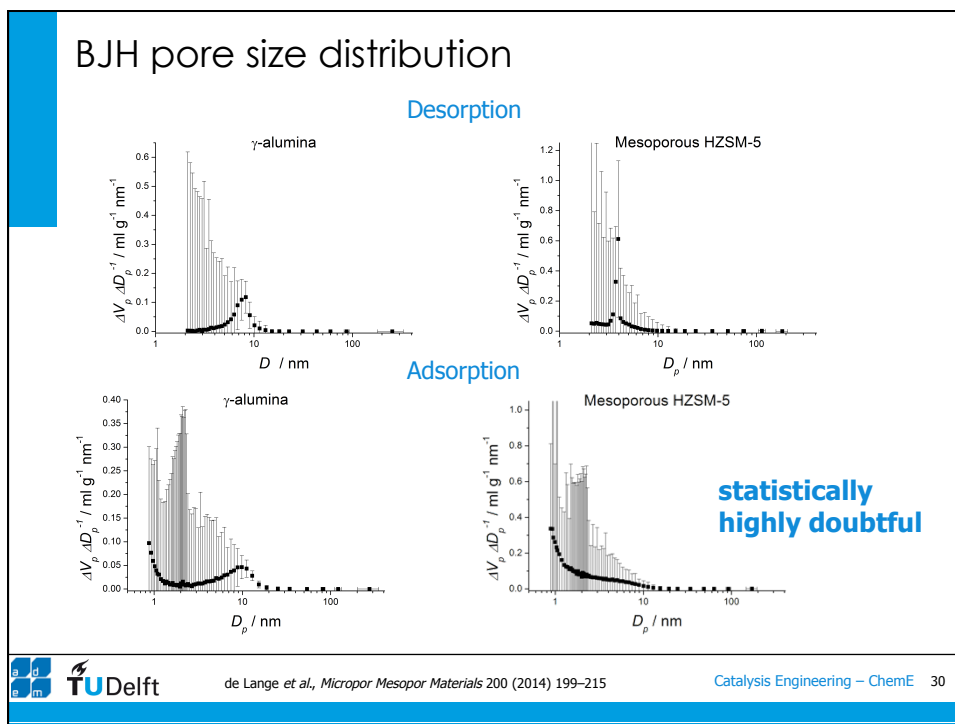
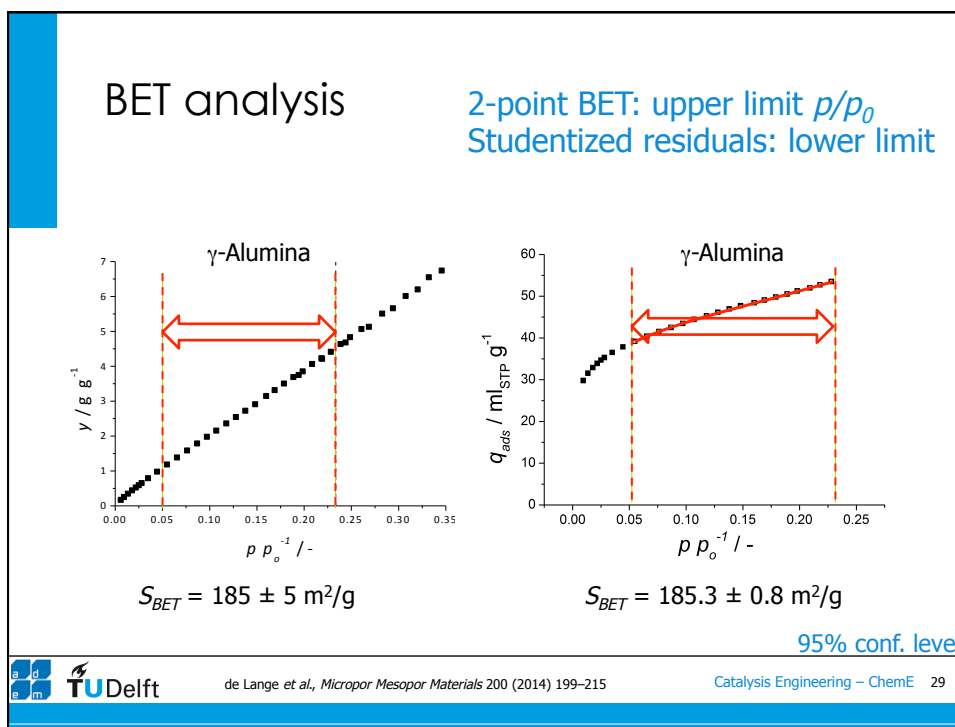


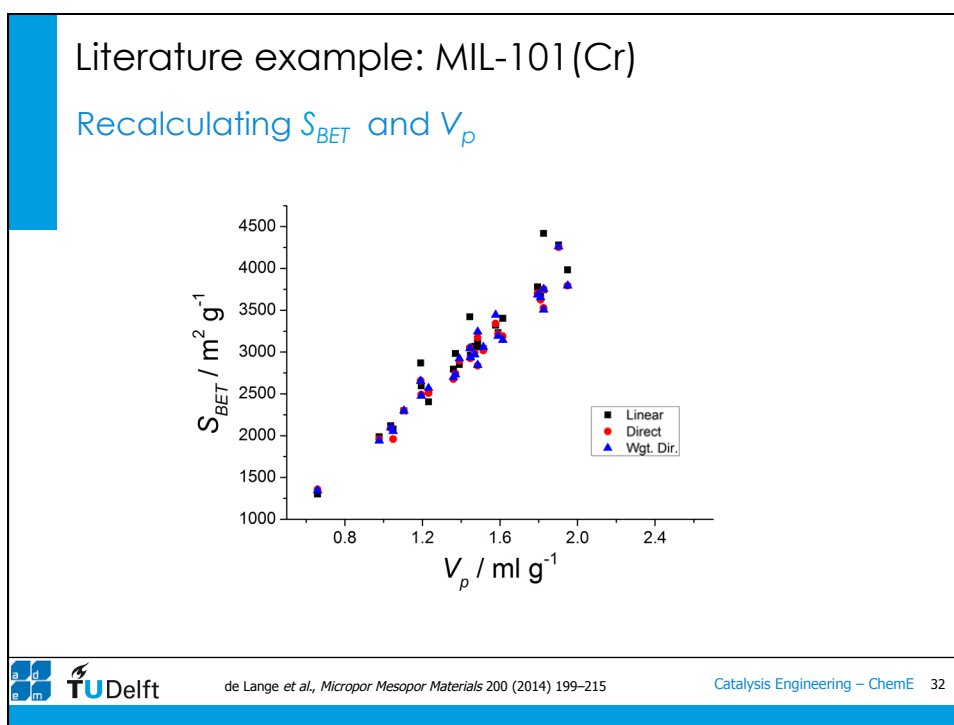
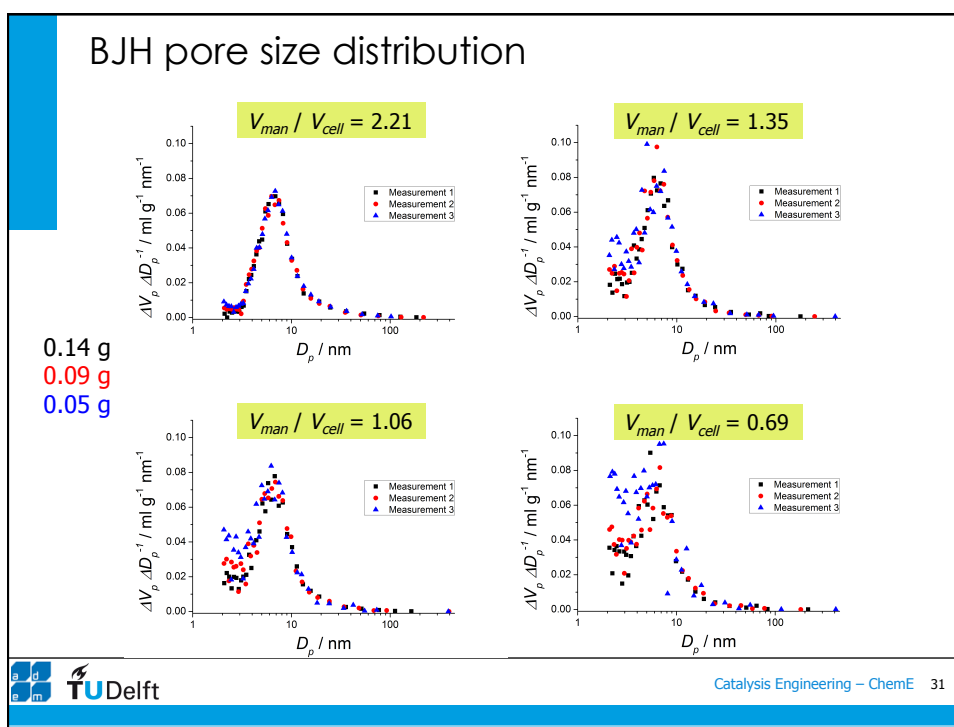
all data points



8 points removed







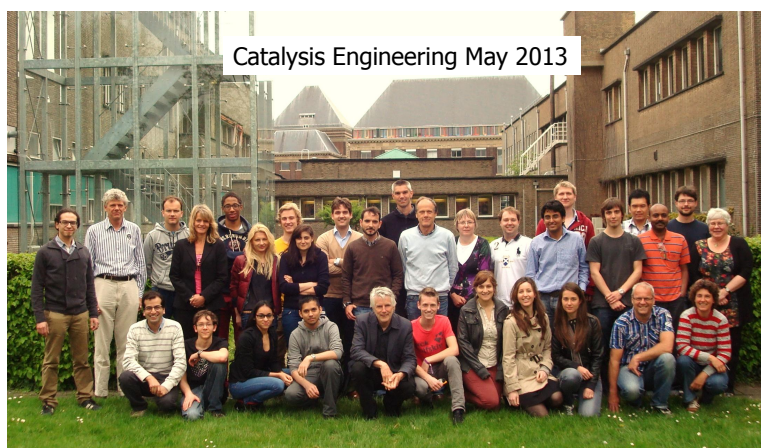
## Recommendations N<sub>2</sub> adsorption @77 K

- Regarding **isotherm measurement and pore volume**
  - Use  $2 \leq V_{man} / V_{cell} \leq 3$  (e.g., by using glass filler rods):
    - Minimal uncertainty
    - Less artificially enlarged desorption hysteresis
- Regarding **BET surface area**
  - Use direct fitting method (**nonlinear parameter estimation**)
  - Relative pressure
    - upper limit by **two-point BET calculation**
    - lower limit (**mesoporous**) Use residual distributions
- Regarding **BJH-pore size distribution**
  - Compare PSD from adsorption and desorption to check for artifacts
  - Do not apply below  $p/p_0 = 0.42$  (desorption)
  - Interpret data only qualitatively
- When **reporting**
  - State exact determination procedure
  - Don't exaggerate accuracy (# significant digits)

pressure accuracy  
manifold volume

confidence limits

## Thanks to.....



## Thank you for your attention