HORIBA

Explore the future

HORIBA Scientific

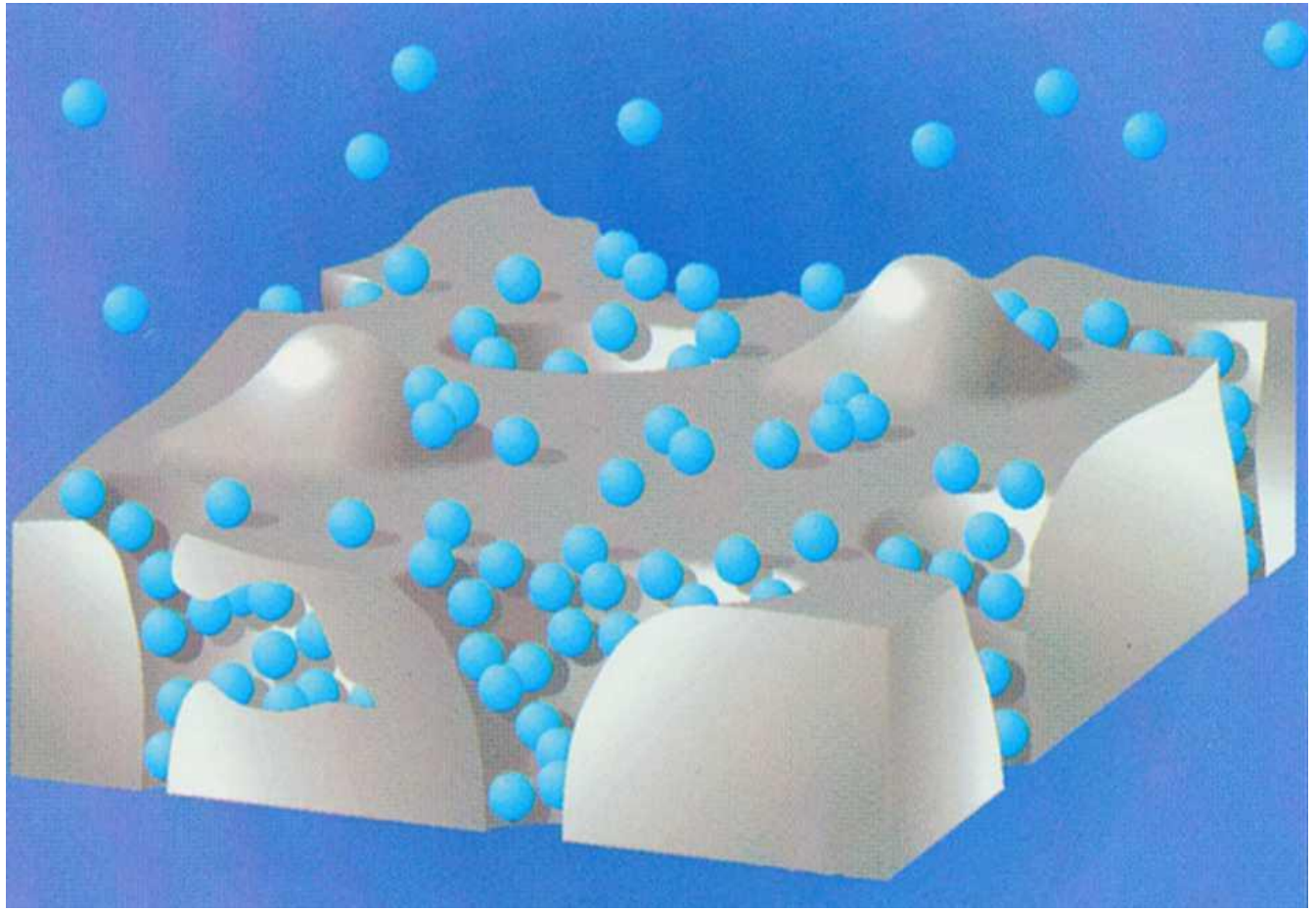
Particle Analysis

Carl Lundstedt

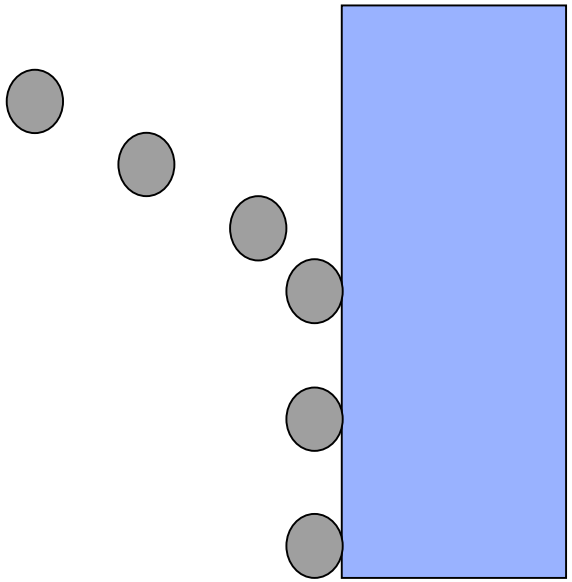
BET Theory and how its used to calculate surface area

August 4th, 2020

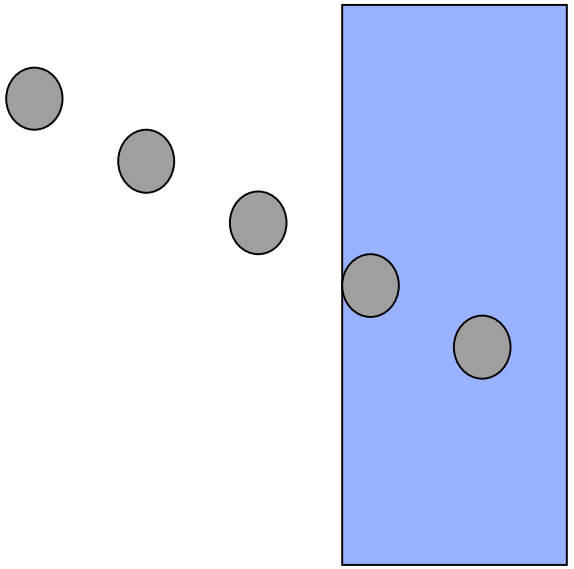
BET Theory seeks to explain the physical adsorption of gas molecules onto solid surfaces



Adsorption differs from absorption, which deals with permeation of surfaces

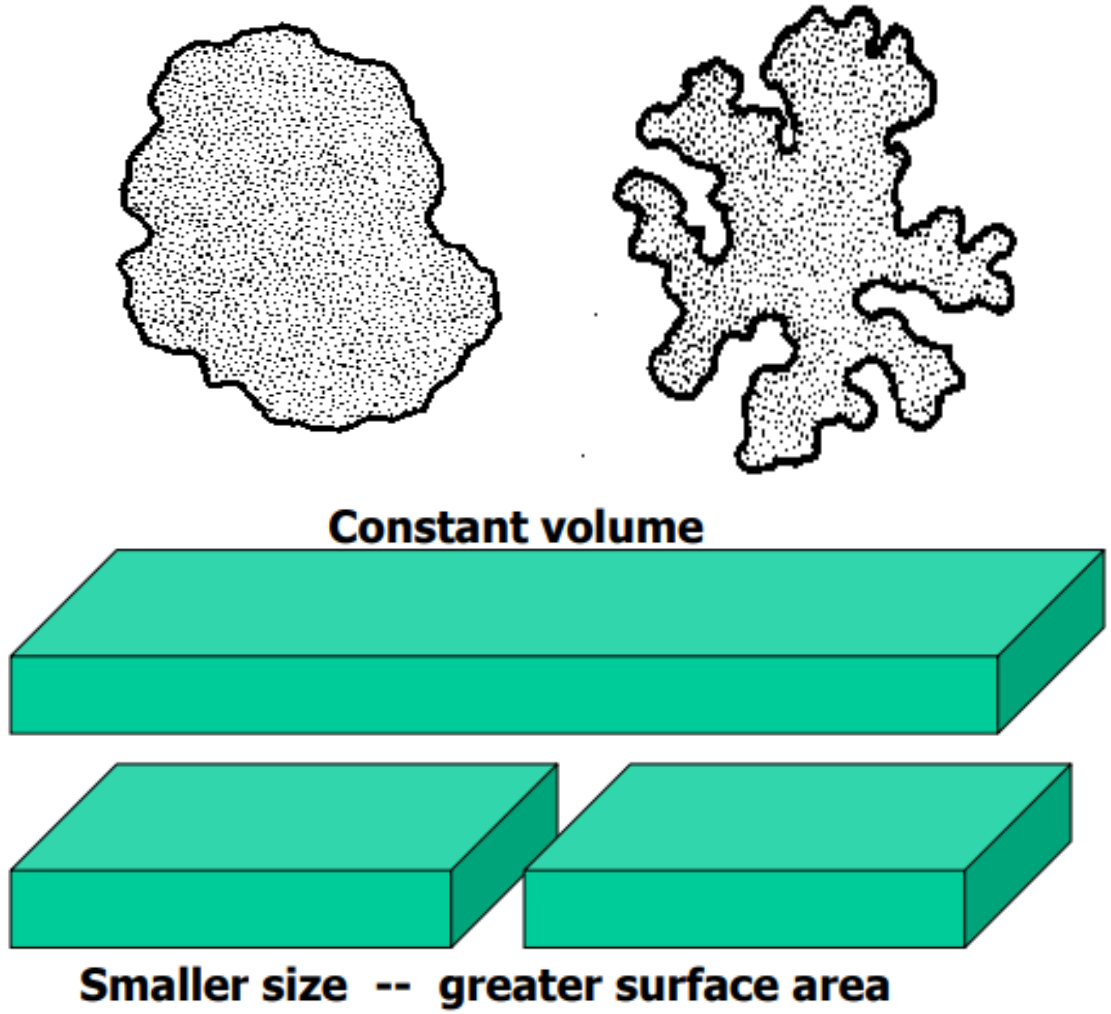


ADsorption



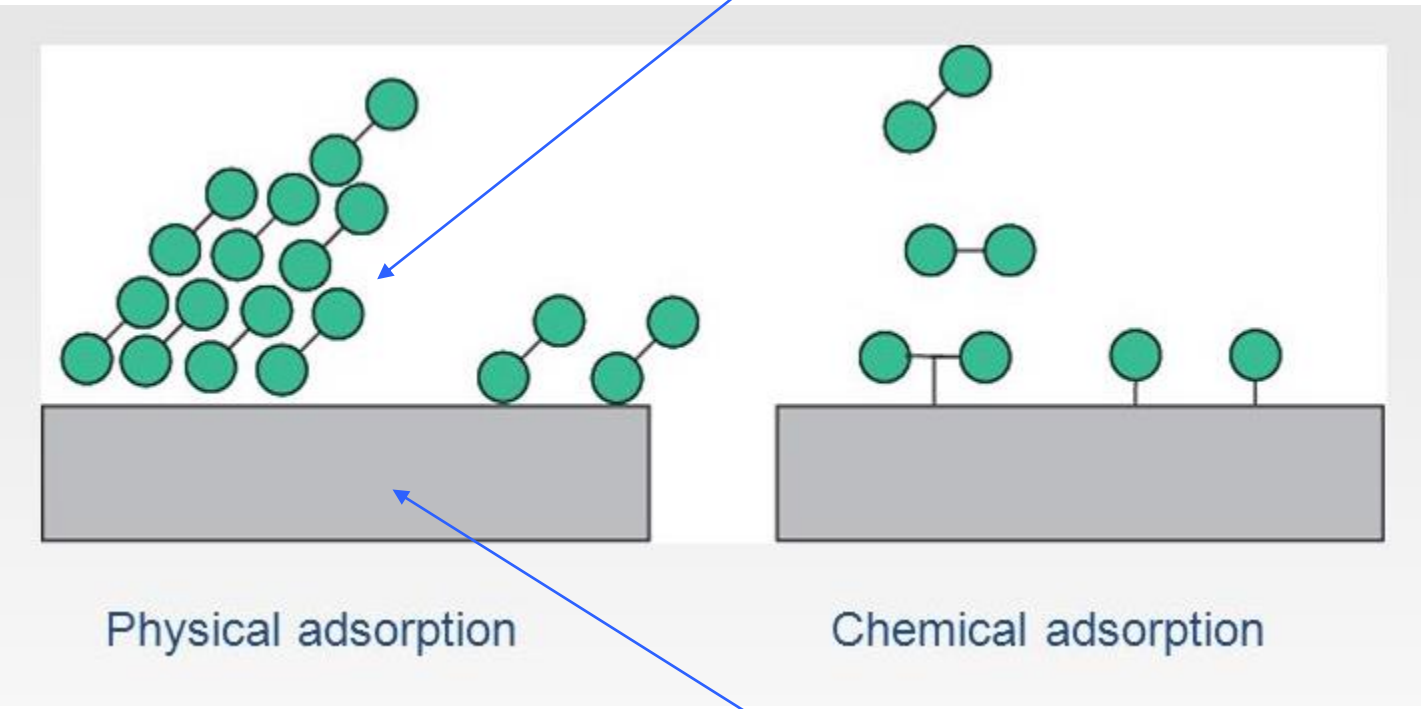
ABsorption

Particles of similar size can vary drastically in surface area



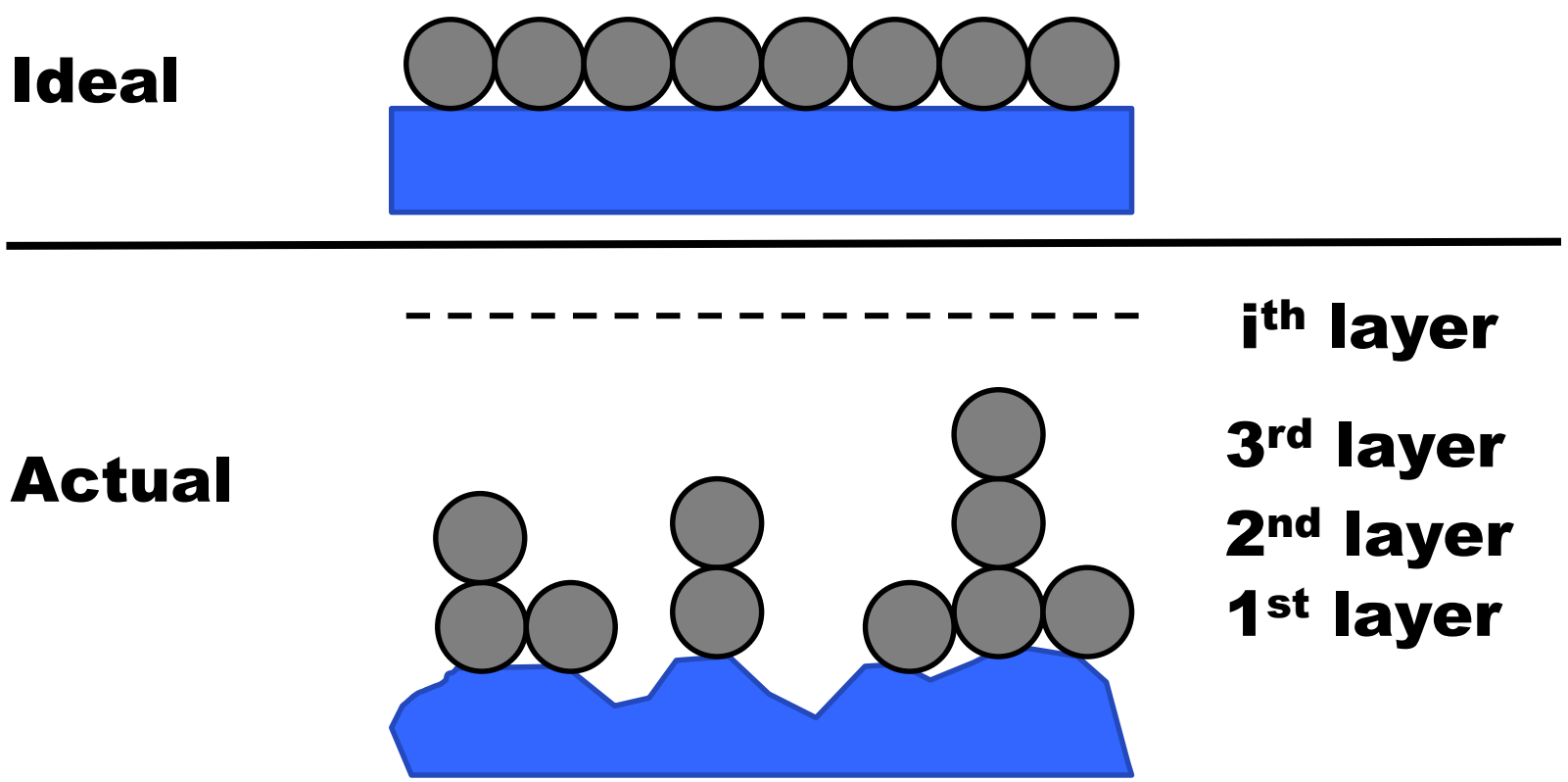
Physical adsorption occurs due to Van der Waals forces when at low temperatures and without chemical reactions

Adsorbate

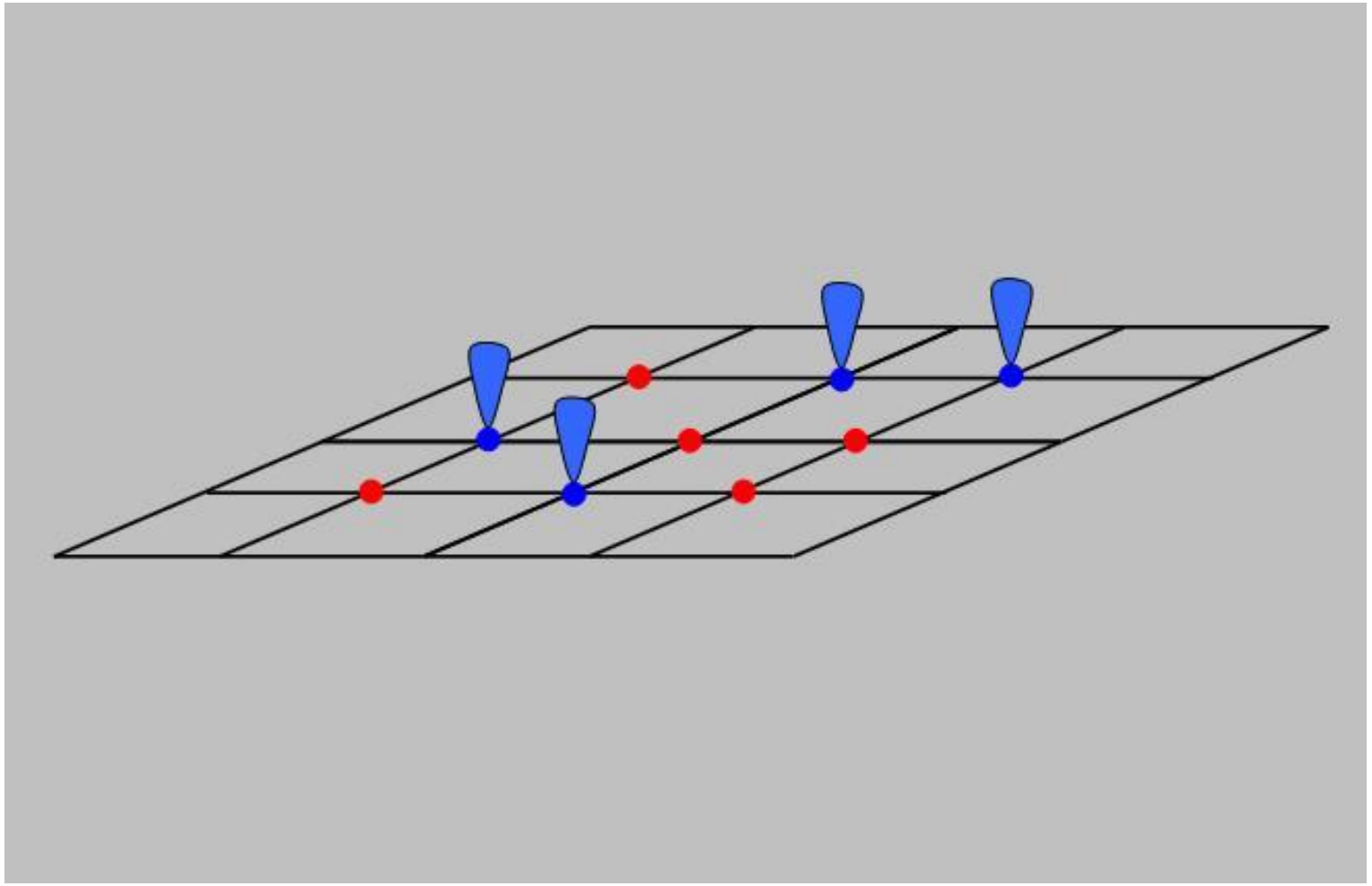


Adsorbent (Substrate)

BET Theory extends the Langmuir theory from monolayer adsorption to multilayer adsorption

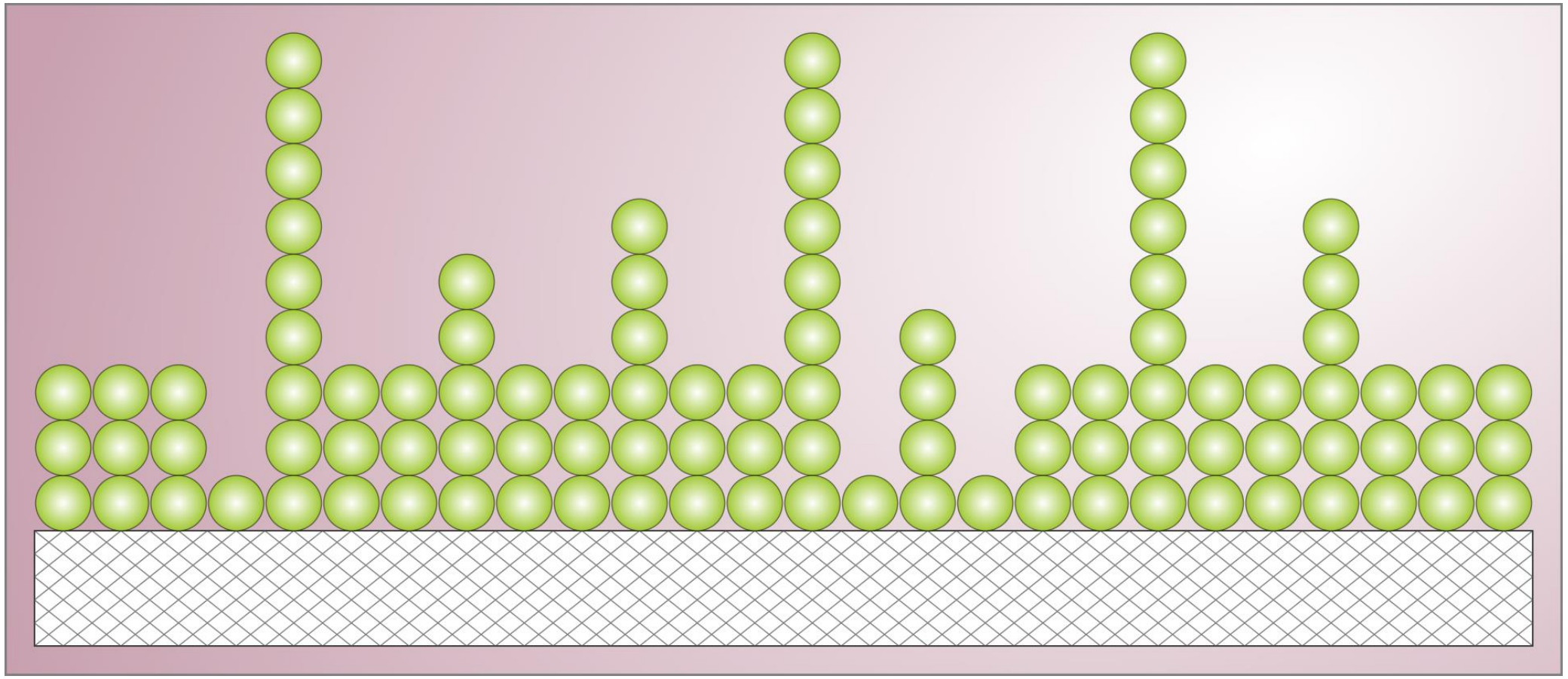


Langmuir adsorption model



By SmugBoy - Own work, CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=5164981

BET model



By Life of Riley - Own work, CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=10137983

We use the BET equation to determine the monolayer absorbed gas volume (v_m)

$$\frac{1}{v[(p_0/p) - 1]} = \frac{c - 1}{v_m c}\left(\frac{p}{p_0}\right) + \frac{1}{v_m c}$$

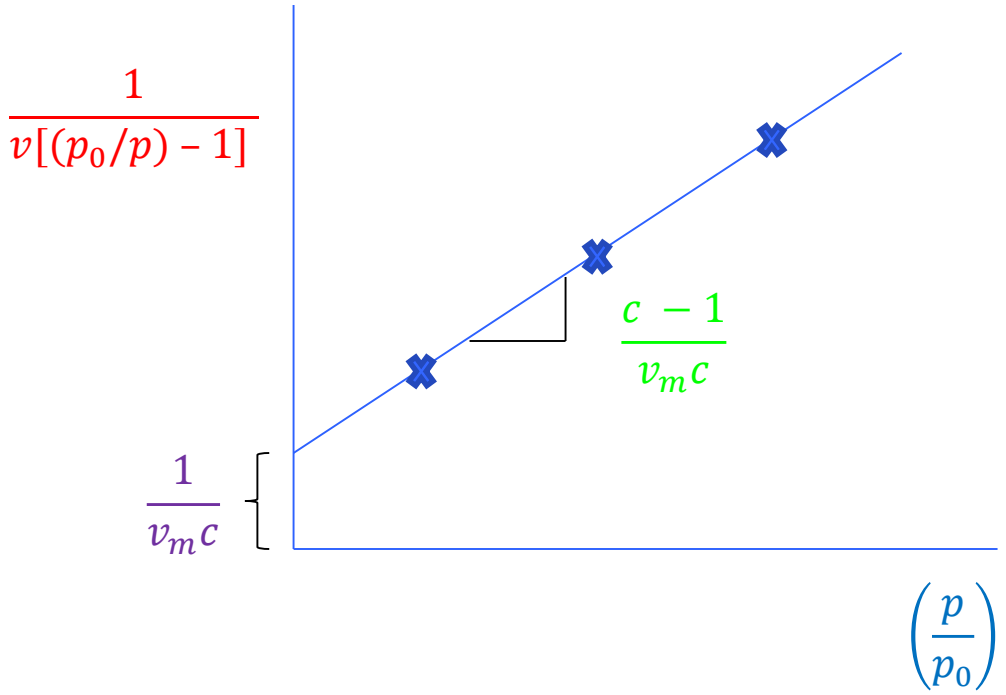
v = adsorbed gas quantity
p_0 = saturation pressure of adsorbate
p = equilibrium pressure of adsorbate
c = BET constant = $\exp\left(\frac{E_1 - E_L}{RT}\right)$

E_1 = heat of adsorption for the first layer
E_L = heat of vaporization

BET equation can be plotted to determine monolayer adsorbed gas quantity and the BET constant

$$\frac{1}{v[(p_0/p) - 1]} = \frac{c - 1}{v_m c}\left(\frac{p}{p_0}\right) + \frac{1}{v_m c}$$

$$y = mx + b$$



Take numerical values for slope and intercept to solve for v_m and c

$$slope = \frac{c - 1}{v_m c}$$

$$\text{intercept} = \frac{1}{v_m c}$$

$$v_m = \frac{1}{slope + intercept}$$

$$c = 1 + \frac{slope}{intercept}$$

From the monolayer absorbed gas volume (v_m), we can determine total and specific surface area

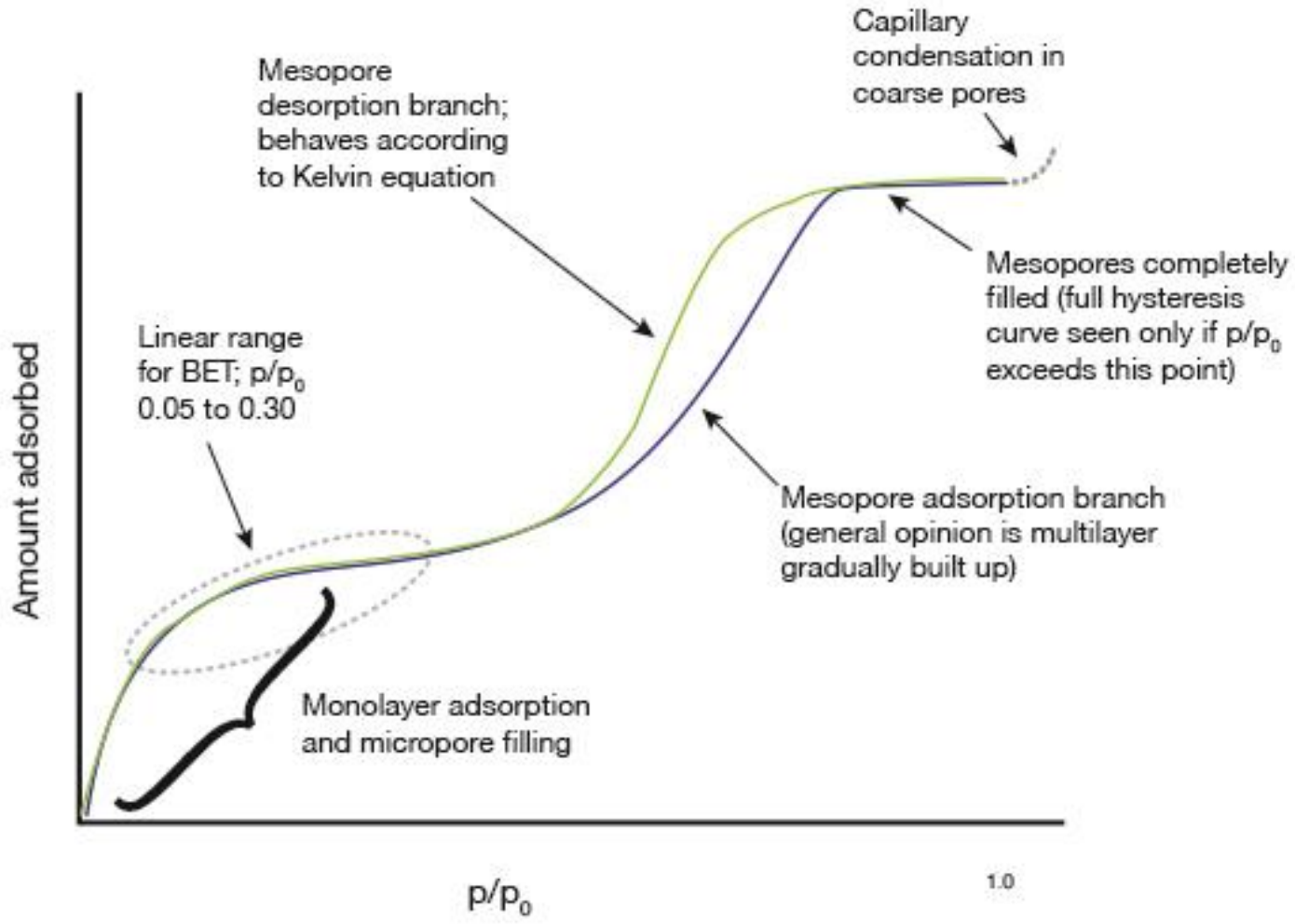
$$S_t = \frac{v_m N s}{V}$$

S_t = total surface area of sample material
v_m= monolayer absorbed gas volume
N = Avogadro's number = 6.02 x 10^{23} molecules/mol
s = cross-sectional area of adsorbed gas molecule (0.162 nm^2 for N^2)
V = molar volume of adsorbed gas

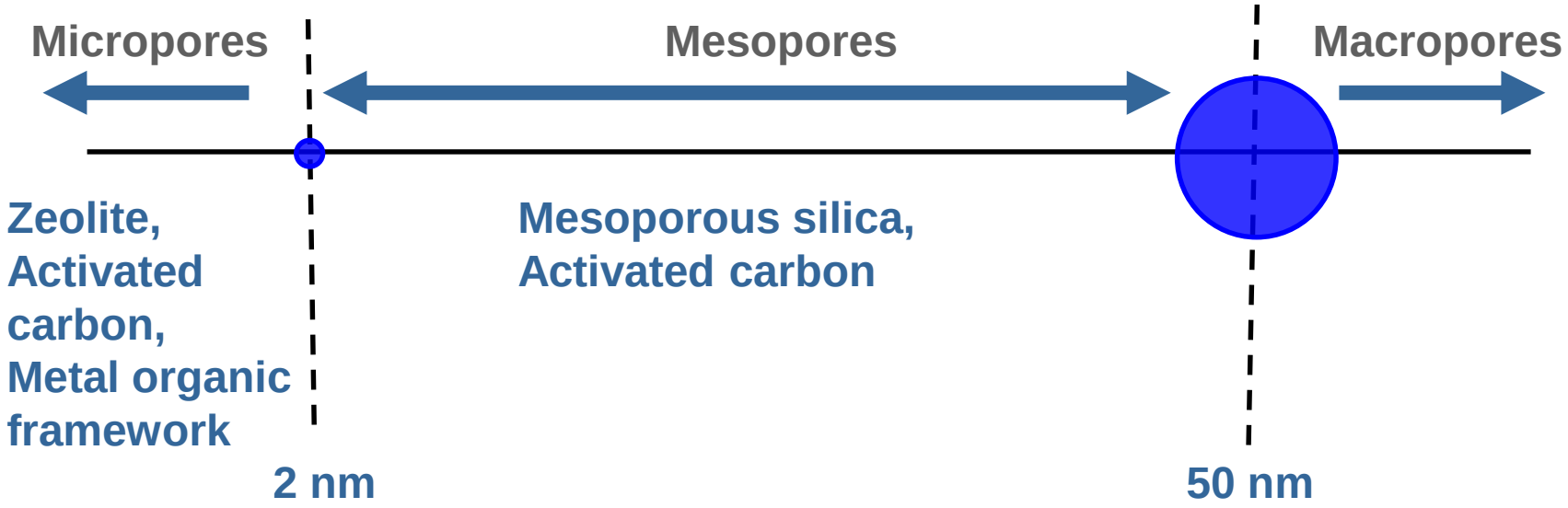
$$S_{BET} = \frac{S_t}{a} \text{ [=] } m^2/g$$

S_{BET} = specific surface area
a = mass of sample

Can only assume linear relationship for adsorption isotherms in the range of 0.05 < p/p_0 < 0.30



Pore width can make a big difference on the shape of the isotherm

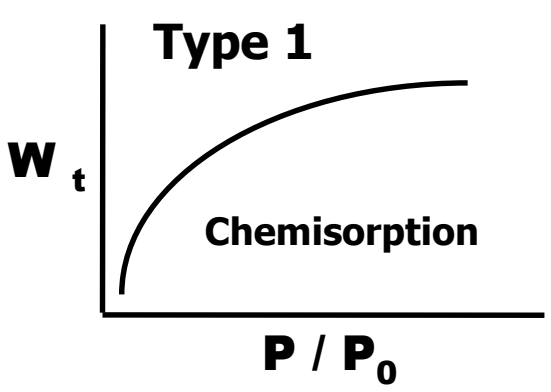


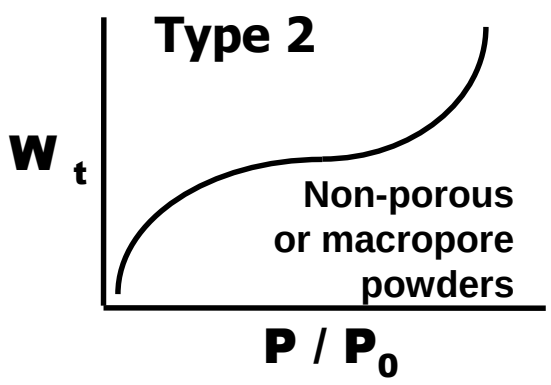
Usually apply BET theory to Type 2 and Type 4 isotherms, apply to Type 1 with caution

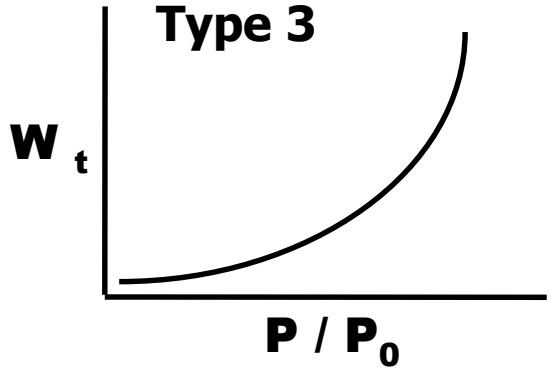
Microporous or chemisorption (C > 150)

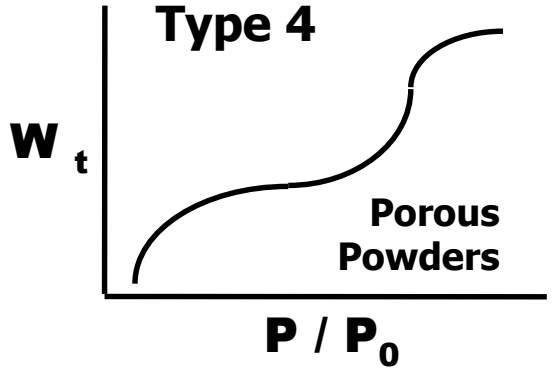
Macroporous/non-porous (C > 80)

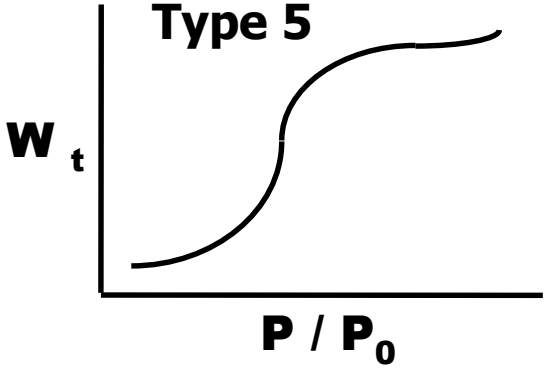
(C < 2)







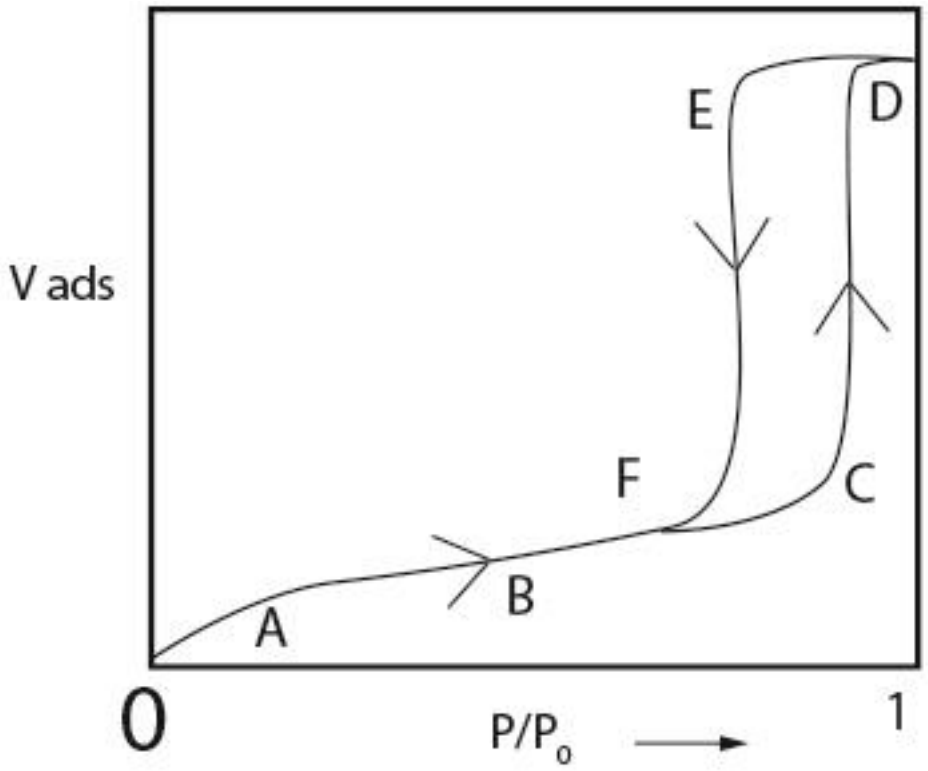


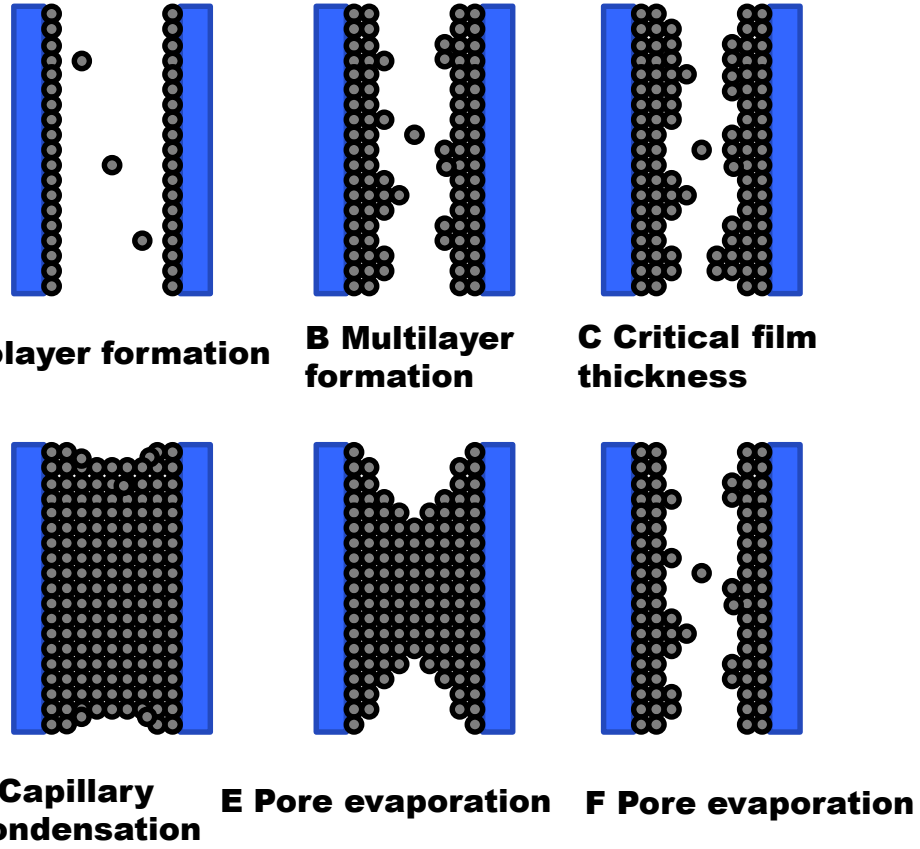


Mesoporous (C > 80)

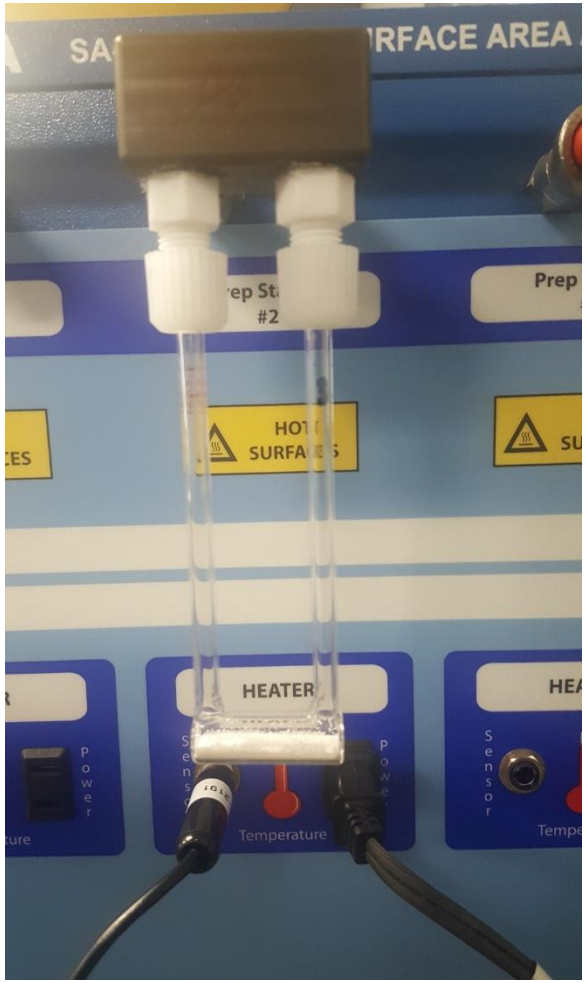
(C < 2)

Capillary condensation explains the hysteresis loop in Type 4 isotherms

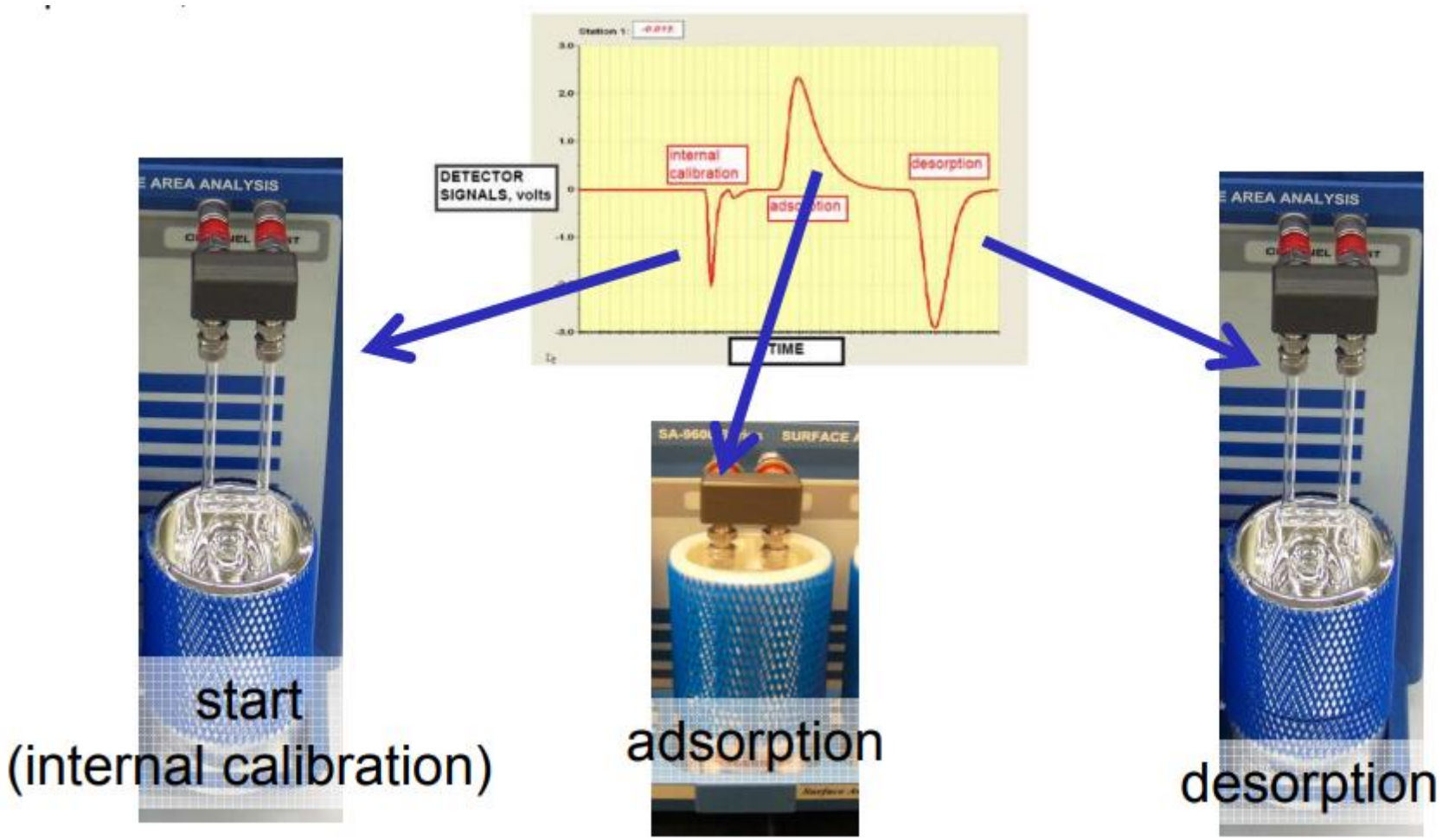




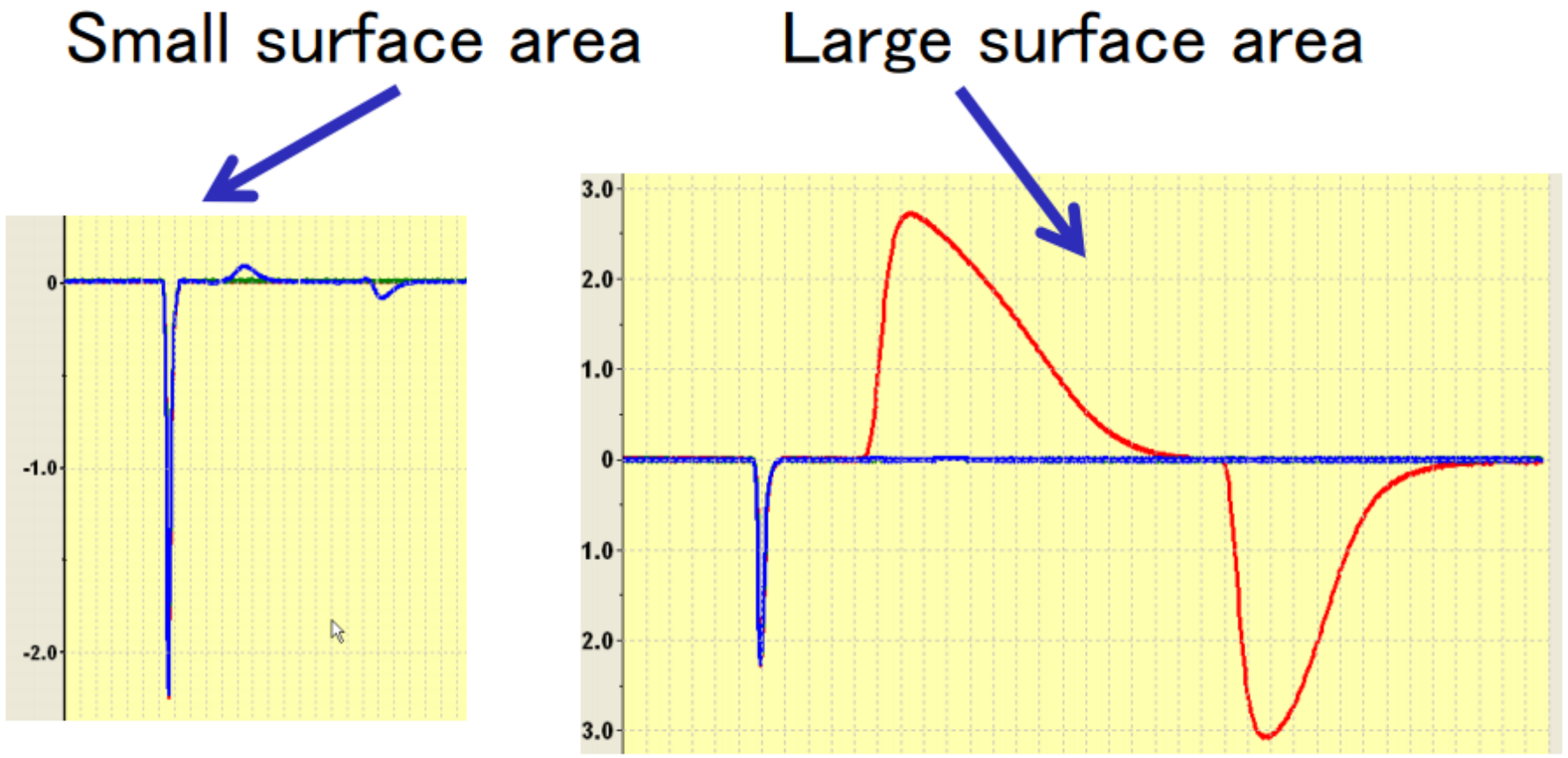
Have to insert sample into cell and degas sample to remove excess moisture on surface



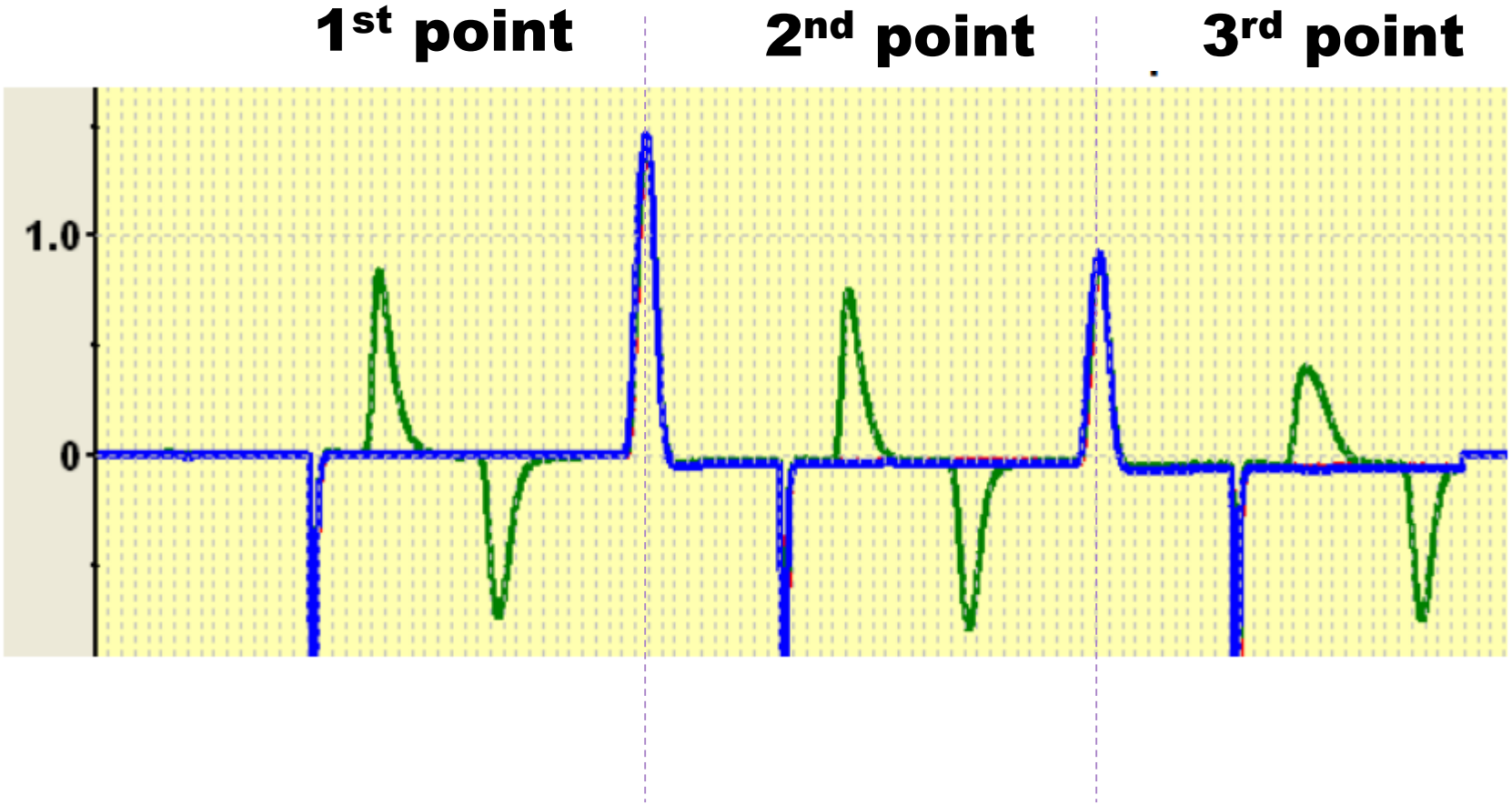
BET measurement includes calibration of 1 cm^3 of nitrogen, adsorption, and desorption



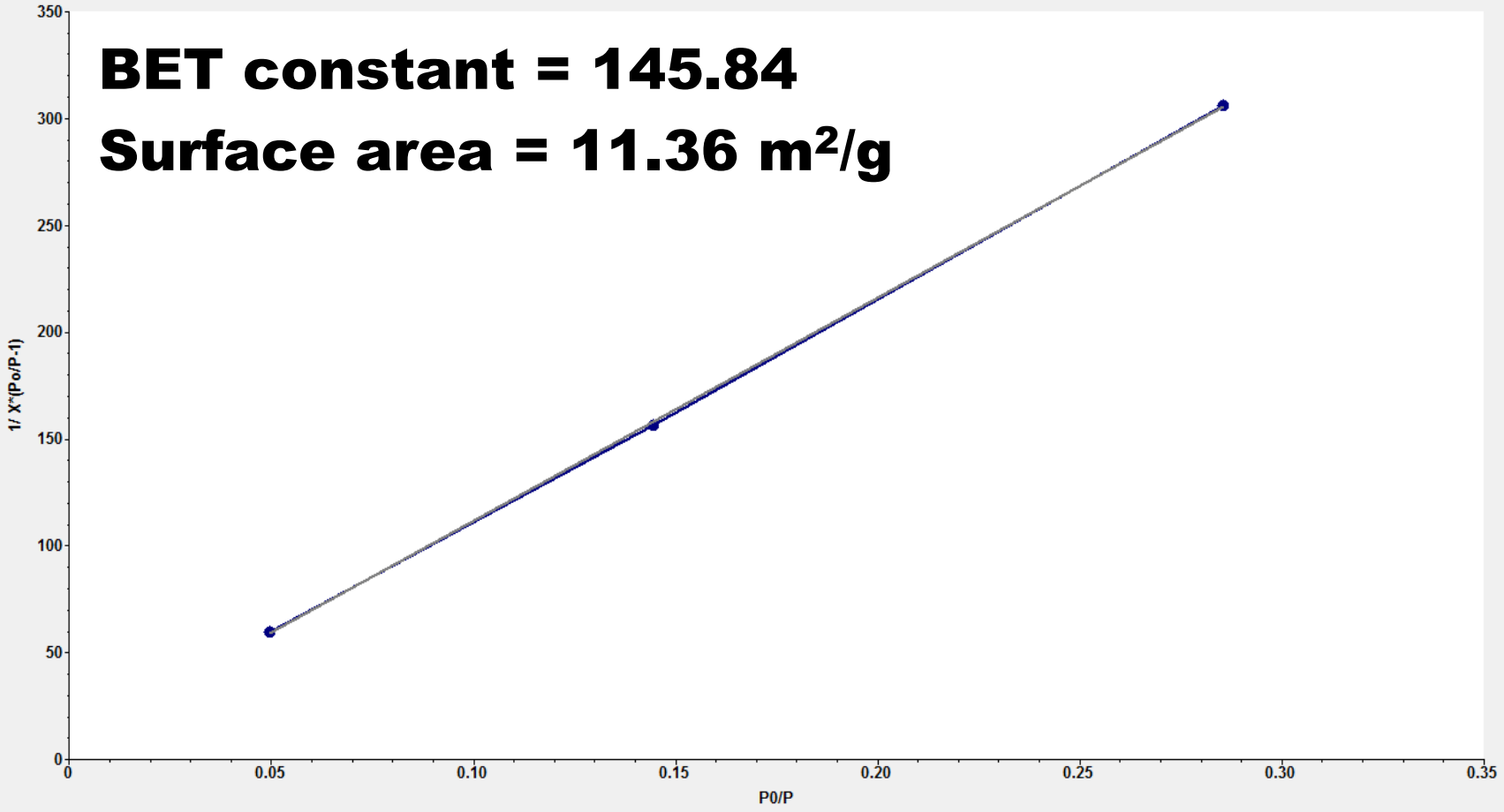
Large surface area samples will adsorb and desorb more nitrogen



BET multipoint measurement example



Plot at least 3 points to obtain multi-point plot, solve for BET constant (c) and V_m (monolayer volume)



Applications

- Cement
- Catalysts
- Activated Carbon
- Pharmaceutical products
- Batteries
- Ceramics

Thank you

Omoshiro-okashiku

Joy and Fun

Terima kasih

Gracias 谢谢

Danke Σας ευχαριστώ πάρα πολύ

Tack ska du ha **THANK YOU** ধন্যবাদ

Grazie ขอบคุณครับ Большое спасибо

ありがとうございました Obrigado Cảm ơn Merci 감사합니다

Dziękuję