Physical Chemistry of Surfaces
Homework3
Evaluation of low temperature N_2 vapour adsorption isotherms

Deadline of submission: 8 April

You use the same dataset.

1. As it was shown in the last week material (#6) the limits of the Kelvin equation define the limits of the pore size marking the mesopore range.

2. From the Kelvin equation calculate the relative pressure values corresponding to the narrowest and widest mesopores. The surface tension of liquid nitrogen is 8.94 mN/m. You can calculate the molar volume of nitrogen from the density of liquid nitrogen given in homework 1. (0.808 g/cm^3). The contact angle is 0.

3. Using your isotherm data, calculate pore volume corresponding to the mesopore range, supposing that all the gas adsorbed is in liquid form.

1. As it was shown in the last week material (#6) the limits of the Kelvin equation define the limits of the pore size marking the mesopore range.

The limits of the Kelvin equation are r_{min} =1nm and r_{max} = 25 nm

Table 1 Constant values.

Constants and given
Gas constant (R) = 8.314 J/K mol = 8.314 Nm/K mol
STP ≡ Standard Temperature (T) = 273 K, and standard pressure (p) = 101325 Pa (N/m^2)
Molecular weight (Mwt) of N_2 = 28 g/mol
Liquid density (ρ) of N_2 = 0.808 g/cm^3

2. From the Kelvin equation calculate the relative pressure values corresponding to the narrowest and widest mesopores. The **surface tension of liquid nitrogen is 8.94 mN/m**. You can calculate the molar volume of nitrogen from the density of liquid nitrogen given in homework 1. (**0.808 g/cm³**). **The contact angle is 0**.

$$V_m = \frac{M_{wt}[\frac{g}{mol}]}{\rho[\frac{g}{cm^3}]} \qquad V_m = \frac{28\,[\frac{g}{mol}]}{0.808[\frac{g}{cm^3}]}$$ **= 34.7 cm³/mol**

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Pore size distribution can be deduced with Kelvin equation

$$\ln\frac{p}{p_0} = -\frac{2\gamma^{LV}V^L{}_m}{r_K RT}\cos\theta$$

Surface tension of liquid nitrogen is 8.94 mN/m

molar volume V_m **= 34.7 cm³/mol**

With the given condition, i.e., **the contact angle is 0,**

the equation becomes:

$$r_K = 1\,nm \qquad \ln\frac{p}{p_0} = -\frac{2\times 8.94\,mN/m\times 34.7cm^3/mol}{1nm\times 8.314\,Nm/Kmol\times 77.350K}\times 1$$

$$\ln\frac{p}{p_0} = -\frac{2\times 8.94\times 10^{-3}N/m\times 34.7\times 10^{-6}\,m^3/mol}{1\times 10^{-9}m\times 8.314\,Nm/K\,mol\times 77.35\,K} = -0.97356$$

$$\frac{p}{p_0} = 0.378$$

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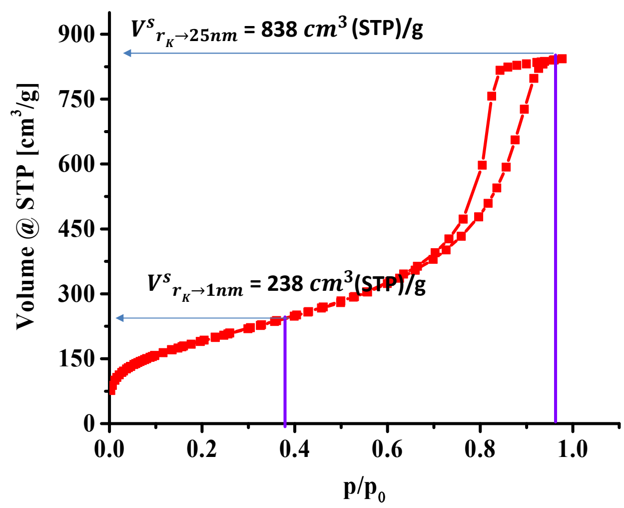
$$r_K = 25\ nm \qquad \ln\frac{p}{p_0} = -\frac{2\times 8.94\ mN/m\times 34.7cm^3/mol}{25nm\times\ 8.314Nm/Kmol\times 77.350K}\times 1$$

$$\ln\frac{p}{p_0} = -\frac{2\times 8.94\ \times 10^{-3}\cancel{N}/\cancel{m}\times 34.7\times 10^{-6}\ \cancel{m^3}/\cancel{mol}}{25\times 10^{-9}\cancel{m}\times 8.314\ \cancel{Nm}/\cancel{K}\ \cancel{mol}\times 77.350\ \cancel{K}} = -0.03894$$

$$\frac{p}{p_0} = 0.962$$

3. Using your isotherm data, calculate pore volume corresponding to the mesopore range, supposing that all the gas adsorbed is in liquid form.



$$n = \frac{pV}{RT},\ m_{nitrogen} = n$$

$$[\text{mol}] \times M_{wt}\left[\frac{g}{mol}\right],\ V_{liquid\ nitogen} = \frac{m_{nitrogen}}{\rho}$$

$$V_{liquid\ nitrogen\ when\ rK=1nm} = \frac{101325\ \cancel{N}/\cancel{cm^2}\,238cm^3/g \times 28\ \cancel{g}/\cancel{mol}}{10^6 \times 8.314\frac{\cancel{Ncm}}{\cancel{Kmol}} \times 273\cancel{K} \times 0.808\ \cancel{g}/\cancel{cm^3}} =$$

$$0.3681\cancel{863}\ \frac{cm3}{g} = 0.368\ \frac{cm3}{g}$$

$$V_{liquid\ nitrogen\ when\ rK=25nm} = \frac{101325\ \cancel{N}/\cancel{cm^2}\,838cm^3/g \times 28\ \cancel{g}/\cancel{mol}}{10^6 \times 8.314\frac{\cancel{Ncm}}{\cancel{Kmol}} \times 273\cancel{K} \times 0.808\ \cancel{g}/\cancel{cm^3}} =$$

$$1.29\cancel{63869}\ \frac{cm3}{g} = 1.30\ \frac{cm3}{g}$$

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$$Mesopore\ volume =$$

$$V_{liquid\ nitrogen\ at\ rK=25nm} - V_{liquid\ nitrogen\ at\ rK=1nm}$$

$$Mesopore\ volume =$$

$$1.30\ \frac{cm3}{g} - 0.368\ \frac{cm3}{g} = 0.932\ \frac{cm3}{g}$$

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Summary table.

Table 2

Sample name: Silica6

Type of the isotherm: IV

Model	Kelvin	Unit
Relative pressure range for mesopores	0.378-0.962	-
Volume of mesopores	0.932	cm^3/g