Methodology - User definition

The user must define:

- porosity,
- permeability,
- sample dimensions,
- mean coordination number,
- initial pore-to-pore spacing or number of pores.

Estimating mean throat diameter

Hagen–Poiseuille modification:

$$\Delta p = \frac{128 \mu L Q}{N_{pipes} \pi D_t^4}$$

Permeability from Darcy equation:

$$K = \frac{\mu Q L}{A_{in} \Delta p}$$

$$K = \frac{\pi D_t^4 N_{pipes}}{A_{in} 128}$$

$$D_t = \sqrt[4]{\frac{K A_{in} 128}{\pi N_{pipes}}}$$

Estimating mean throat diameter

$$D_t = \sqrt[4]{\frac{K A_{in} 128}{\pi N_{pipes} Z}}$$

Estimating mean pore diameter

$$\phi = \frac{V_{p+t}}{V_{sample}} = \frac{N_p \frac{\pi D_p^3}{6} + \frac{\pi D_t^2 L_t}{4} N_t}{V_{sample}}$$

$$\phi = \frac{V_{p+t}}{V_{sample}} = \frac{N_p \frac{\pi D_p^3}{6} + \frac{\pi D_t^2 L_t}{4} N_p Z}{V_{sample}}$$

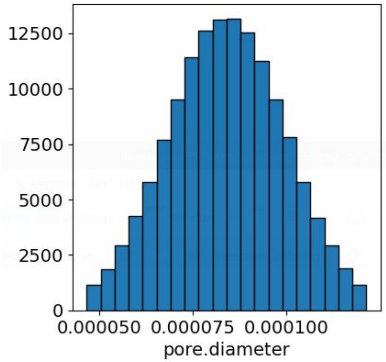
Estimating mean pore diameter

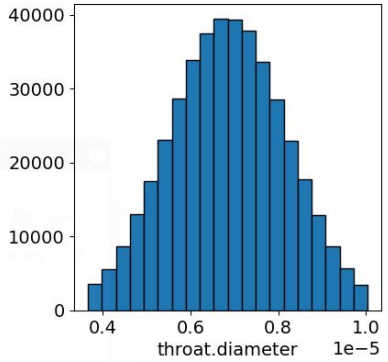
$$L_t = d_{pp} - D_p \qquad\qquad L_t = D_p$$

$$\left(\frac{N_p \pi}{6}\right) D_p^3 - \left(\frac{D_t^2}{4}\right) D_p - \frac{\phi V_{sample}}{N_p \pi} = 0$$

Defining pores and throats size distribution

$$\frac{\sigma_{D_p}}{D_p} = \max\left(0, \min\left(0.3, \left(\frac{d_{pp} - D_p}{D_p}\right)\right)\right)$$





Testing the estimations

	Test 1	Test 2	Test 3
Porosity	0.27	0.15	0.05
Permeability (m^2)	1e-12	7.3e-13	1e-16
Z	7	6	3
d_{pp}	1e-3	5e-4	1e-5
	Relative error		
Porosity error %	**1.62**	**7.62**	**20.1**
Permeability error %	**502.1**	**247.9**	**11.4**

Fine tunning

- scipy optimize root_scalar of porosity and permeability error.
- Correct porosity first and then permeability.
- Three cycles give a relative error of **1e-3%** for both properties. It is necessary 25 s for execution
- On cycle can result in error of **30%** for permeability. 7 s for execution.