Percolation

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1 Permeability modification Model

The polymers passing through pores are dragged by the flow. There are two forces competing when a polymer adheres to the surface of a pore (1) The drag force on the particle coming from flow, and (2) ionic/VanderWaals or whatever force that tries to adhere the particles to the surface. A particle attaches to the surface if the drag force exerted by the fluid flow around it is smaller than the VanderWaals/ionic force.

For simplicity, I assume that the force is ionic with a force distance profile of $F = K/X^2$, where K is a constant and X is the distance. I assume that polymers have an effective radius of d_p and fluid viscosity is μ and the flow rate is Q. This model states that the particle attaches to the surface when

$$F_{\text{drag}} \leq F_{\text{ionic}} \tag{1}$$

$$6\pi\mu d_p \frac{2Q}{\pi R^2}\left(1 - \frac{r^2}{R^2}\right) \leq \frac{K}{(R-r)^2} \tag{2}$$

$$1 - \frac{r^2}{R^2} \leq \left(\frac{K}{12\mu d_p Q}\right)\frac{1}{(1-r/R)^2} \tag{3}$$

$$1 \leq \frac{r^2}{R^2} + \alpha\frac{1}{(1-r/R)^2} \tag{4}$$

where $\alpha = K/\left(12\mu d_p Q\right)$ is a factor that compares the ionic force and viscous force. Note that it depends on the flux rate. If we define $x = 1 - r/R$ we obtain

$$1 \leq (1-x)^2 + \frac{\alpha}{x^2} \tag{5}$$

$$x^2 - x^2(1-x)^2 \leq \alpha \tag{6}$$

$$x^2(1-(1-x)^2) \leq \alpha \tag{7}$$

$$x^3(2-x) \leq \alpha \tag{8}$$

$$\text{if } x \ll 1 \rightarrow x \leq \left(\frac{\alpha}{2}\right)^{1/3} \tag{9}$$

As a result the distance is proportional to $\alpha^{1/3}$. Note that α depends on $1/Q$. Now, lets

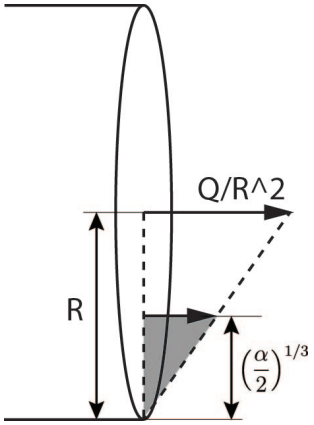

Figure 1: Flow in the pipe

find the flux passing through this adsorbtion layer (any polymer in this layer would attach to the surface)

$$\text{volume/time} = \frac{1}{2}R\alpha^{1/3} \cdot \frac{Q}{R^3}R\alpha^{1/3} \cdot 2\pi R = \pi Q\alpha^{2/3} = \pi \left(\frac{K}{12\mu d_p}\right)^{2/3} Q^{1/3} \tag{10}$$

$$\text{volume/time} \propto Q^{1/3} \tag{11}$$

Now, if we assume that the number of polymers passing through the area cause clogging of the pipe and change the total area of the pipe, then we find that

$$d(\pi R^2) \propto Q^{1/3} \quad \rightarrow \quad RdR \propto Q^{1/3} \tag{12}$$

We also know that $k = \pi R^4/8l^2$, as a result

$$dk \propto R^3 dR \tag{13}$$

$$dk \propto R^2 Q^{1/3} \tag{14}$$

$$dk \propto Q^{1/3} \tag{15}$$

Experimental Results

In Shima's paper, we report a figure that shows the evolution of permeability k per volume of polymer V_{pol} that passes through the porous media. Basically we are plotting Δk versus Q passing through the porous media. The figure and best polynomial fit is shown blow

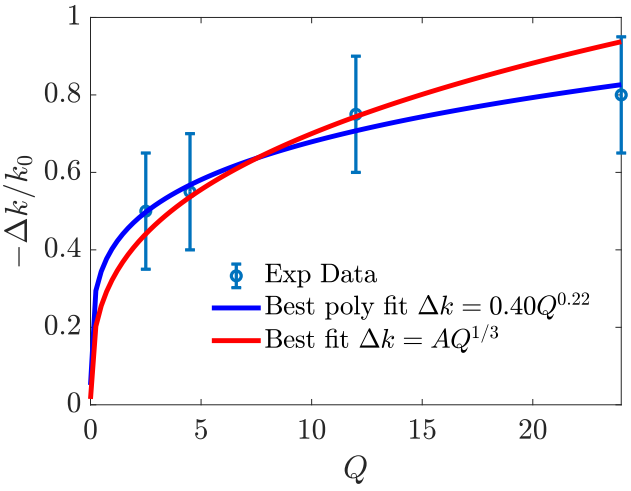

Figure 2: k versus volume of fluid

2 Universality argument

If the pdf of q follows an exponential tail, we have

$$f(q) \propto e^{-q/\lambda} \tag{16}$$

Doing the normalization, we find that

$$f(q) = \frac{1}{\lambda} e^{-q/\lambda} \text{such that} \int f(q)dq = 1 \tag{17}$$

Setting the average $\langle Q \rangle = Q_0$, we obtain

$$\int q f(q)dq = \lambda = Q_0 \tag{18}$$

We then obtain

$$f(q) = \frac{1}{Q_0} e^{-q/Q_0} \tag{19}$$

This means that as long as Q_0 is fixed, then the probability distribution is fixed. However, the observation is that as the clogging happens, the $f(q)$ broadens!

3 Random Resistor Networks

Consider the following random network The diameter of each pipe is randomly chosen from a distribution distribution. The Darcy law in each pipe reads as

$$\frac{\Delta P}{L} = \frac{128}{\pi} \frac{\mu Q}{d^4} \tag{20}$$

where ΔP is the pressure difference on both sides of the pipe, L is the length of the pipe, μ is viscosity, and d is the diameter of the pipe.

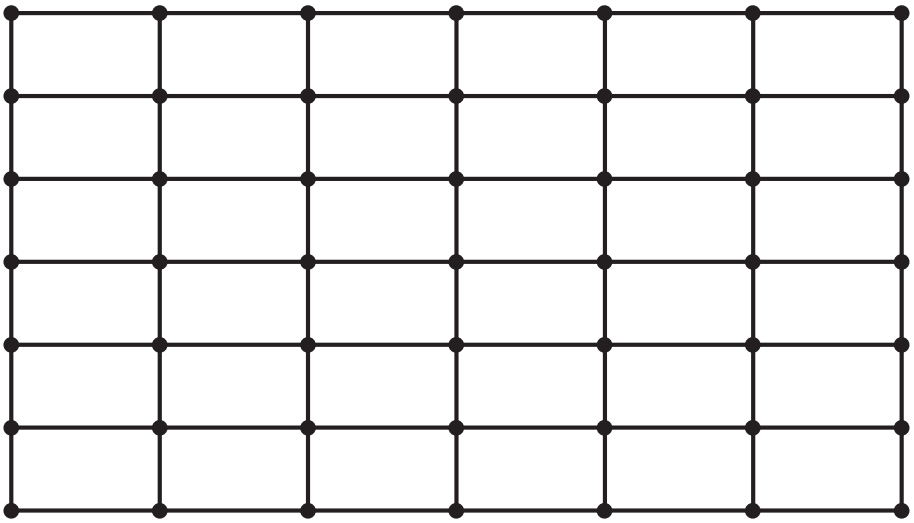

Figure 3: A random grid of pipes

4 Analysis

Consider the following random network of pipes At each level, at each node, the flow from

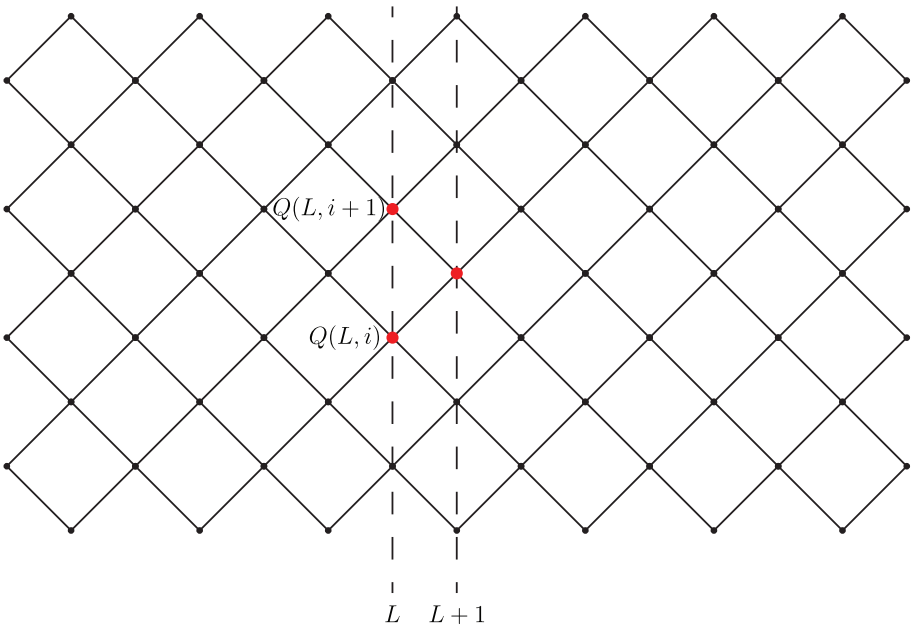

Figure 4: A random grid of pipes

previous layers into that node is considered as $Q(L, i)$. This flow goes to the next layer through the pipes that it is connected to. Some portion of it flows through each pipe as

$$Q(L+1, j) = \sum_i w_{ij} Q(L, i) = w_{i,i+1} Q(L, i+1) + w_{i,i} Q(L, i) \tag{21}$$

such that $\sum_j w_{ij} = 1$. Assuming that these w_{ij} are coming from a distribution $\eta(w)$, we know that

$$\boxed{\int \eta(w)dw = 1} \tag{22}$$

and from $\sum_j w_{ij} = 1$, we can conclude that

$$\sum_j w_{ij} = 1 \rightarrow NE[w_{ij}] = 1 \rightarrow E[w_{ij}] = 1/N \rightarrow \boxed{\int w\eta(w)dw = 1/N} \tag{23}$$

Now we use the technique of mean field analysis for a general distribution of $\eta(w)$ to find the distribution of Q at the layers. The values of $Q(D, i)$ are not independent for neighboring sites; however, the mean field approximation ignores these correlations.

$$P_L(Q) = \prod_{j=1}^{N} \left\{ \int_0^1 dw_j \eta(w_j) \int_0^\infty dQ_j P_{L-1}(Q_j) \right\} \times \delta \left(\sum_j w_j Q_j - Q \right) \tag{24}$$

The constraint that Q's eminating downward should add up to one is in the definition of $\eta(w)$. The only approximation in the above equation is that we neglect the possible correlation between the values of Q among anscestors. If we take the laplace transform of the above equation, we obtain

$$\tilde{P}(s) \equiv \int_0^\infty P(Q)e^{-Qs}dQ \tag{25}$$

$$\xrightarrow{\int_0^\infty (\cdot)e^{-Qs}dQ} P(Q) = \prod_{j=1}^{N} \left\{ \int_0^1 dw_j \eta(w_j) \int_0^\infty dQ_j P(Q_j) \right\} \times \delta \left(\sum_j w_j Q_j - Q \right) \tag{26}$$

$$\tilde{P}(s) = \int_0^\infty \prod_{j=1}^{N} \left\{ \int_0^1 dw_j \eta(w_j) \int_0^\infty dQ_j P(Q_j) \right\} \times \delta \left(\sum_j w_j Q_j - Q \right) e^{-Qs}dQ \tag{27}$$

$$= \prod_{j=1}^{N} \left\{ \int_0^1 dw_j \eta(w_j) \int_0^\infty dQ_j e^{-\sum w_j Q_j} P(Q_j) \right\} \tag{28}$$

$$= \prod_{j=1}^{N} \left\{ \int_0^1 dw_j \eta(w_j) \tilde{P}(sw_j) \right\} \tag{29}$$

$$= \left(\int_0^1 dw \eta(w) \tilde{P}(sw) \right)^N \tag{30}$$

Or to summarize

$$\tilde{P}(s) = \left(\int_0^1 dw \eta(w) \tilde{P}(sw) \right)^N \tag{31}$$

Note that in the above calculation $N = 2$. If we set $\eta(w) = \delta(w - 1/2)$, then the flow at each node has probality of $1/2$ to move up or down. As a result the flow at a given depth L will be homogeneous as $P_L(Q) = \delta(Q - \bar{Q})$ where $\bar{Q}$ is the average of input fluid flow.

$P(Q)$ decays faster than Q^{-n} for any n

We first show that $P(Q)$ decays faster than any power of Q for any weight distributions. We expand the Laplace transform as

$$\tilde{P}(s) = 1 + \sum_j \tilde{P}_j s^j \tag{32}$$

Inserting this expansion into Eq. (31), we obtain

$$1 + \sum_j \tilde{P}_j s^j = \left(\int_0^1 dw \eta(w) \left[1 + \sum_j \tilde{P}_j (sw)^j \right] \right)^N \tag{33}$$

$$= \left(1 + \sum_j \tilde{P}_j \langle w^j \rangle s^j \right)^N \tag{34}$$

where $\langle w^j \rangle = \int_0^1 \eta(w) w^j dw$ is the j-th moment of the weights w. In the above equation we can observe that

$$P_j \left(N \langle w^j \rangle - 1 \right) = G(P_{j-1}, P_{j-1}, \cdots, P_1) \tag{35}$$

In the above equation P_j can only diverge only if $N\langle w^j \rangle - 1$ is zero. If w can only be zero and one, then $\langle w^j \rangle = \langle w \rangle = 1/N$ and the coefficient can become zero! Other than this special distribution where $0 \leq w \leq 1$, then

$$w \in [0,1] \rightarrow w > w^2 > w^3 > \cdots \tag{36}$$

$$\forall k > 1 \rightarrow \langle w^k \rangle < \langle w \rangle = \frac{1}{N} \tag{37}$$

which means that $N\langle w^j \rangle - 1$ is not zero and as a result P_j is finite. P_j on the other hand is the j-th moment or $\langle Q^j \rangle$ and it is finite. If $P \approx Q^{-n}$, then the n-th moment will not be finite i.e. $\langle Q^{n+1} \rangle = P_{n+1}$ is not finite. We can then conclude that $P(Q)$ should go to zero faster than any Q^{-n} as $Q \rightarrow \infty$! In other words $d \log P(Q) / d \log Q \rightarrow -\infty$ as $Q \rightarrow \infty$.

Exponential Decay

Since our calculation is for $N = 2$, the main equation becomes

$$\tilde{P}(s) = \left(\int_0^1 dw \eta(w) \tilde{P}(sw) \right)^2 \tag{38}$$

In order to have an approximation for $\eta(w)$ we do the following:

At each node there are two nodes where the flux is distributed by w_1 and w_2. Lets assume that w_1 is uniformly distributed between 0 and 1. As a result $w_2 = 1 - w_1$ (since conservation

of mass $w_1 + w_2 = 1$). Now $\eta(w)$ can be found as

$$\eta(w) = M \int_0^1 dw_1 \delta(1 - w_1 - w) = M, \tag{39}$$

$$\text{since } \int_0^1 \eta(w) dw = 1 \rightarrow M = 1 \tag{40}$$

$$\eta(w) = 1 \tag{41}$$

Just for completeness, if there are three connections ($N = 3$), then we have

$$\eta(w) = M \int_0^1 dw_1 \int_0^1 dw_2 \delta(1 - w_1 - w_2 - w) \tag{42}$$

$$= M(1 - w) \rightarrow \int_0^1 \eta(w) dw = 1 \rightarrow M = \frac{1}{2} \tag{43}$$

$$\eta(w) = \frac{1}{2}(1 - w) \tag{44}$$

As a result the main equation simplifies to

$$\tilde{P}(s) = \left(\int_0^1 dw \tilde{P}(sw) \right)^2 \tag{45}$$

In order to solve the above equation, we assume $\tilde{V}(s) = \sqrt{\tilde{P}(s)}$.

$$\tilde{V}(s) = \int_0^1 dw \tilde{V}(sw) = \int_0^s \frac{du}{s} \tilde{V}^2(u) \tag{46}$$

$$s\tilde{V}(s) = \int_0^s du \tilde{V}^2(u) \tag{47}$$

$$\tag{48}$$

Taking the defferentiation with respect to s yields

$$\tilde{V}(s) + s\frac{d\tilde{V}(s)}{ds} = \tilde{V}^2(s) \tag{49}$$

$$\frac{d\tilde{V}}{\tilde{V}^2 - \tilde{V}} = \frac{ds}{s} \tag{50}$$

$$\log\left(\frac{1 - \tilde{V}}{\tilde{V}}\right) = \log(s) \tag{51}$$

$$\tilde{V}(s) = \frac{1}{1 + Cs} \tag{52}$$

We set the mean to 1 i.e.,

$$\int_0^\infty QP(Q)dQ = 1 \rightarrow \frac{d\tilde{P}}{ds}|_{s=0} = -1 \tag{53}$$

$$\frac{d\tilde{V}}{ds} = \frac{1}{2\sqrt{\tilde{P}(s)}}\frac{d\tilde{P}(s)}{ds} \rightarrow \frac{d\tilde{V}(s)}{ds}|_{s=0} = \frac{-1}{2} \tag{54}$$

$$\frac{d\tilde{V}(s)}{ds} = \frac{-C}{(1+Cs)^2}|_{s=0} = -C = \frac{-1}{2} \rightarrow C = \frac{1}{2} \tag{55}$$

As a result, we have

$$\tilde{P}(s) = \left(\frac{1}{1+s/2}\right)^2 \tag{56}$$

$$P(Q) = 4Qe^{-2Q} \tag{57}$$

5 Continuous Model

6 Analysis

Consider the following random network of pipes In the previous descrete model we found that

$$Q(i,j+1) = w_{i-1,j}Q(i-1,j) + w_{i+1,j}Q(i+1,j) \tag{58}$$

with the constraint that

$$w_{i-1,j} + w_{i+1,j} = 1 \tag{59}$$

Lets now assume that

$$w_{i\pm1,j} = \frac{1}{2}(1 \pm v_{i\pm1,j}) \tag{60}$$

with th abive assumption, we find that

$$Q(i,j+1) = \frac{1}{2}\left(1 - v_{i-1,j}\right)Q(i-1,j) + \frac{1}{2}\left(1 + v_{i+1,j}\right)Q(i+1,j) \tag{61}$$

$$\begin{aligned} Q + L_y\frac{\partial Q}{\partial y} + L_y^2\frac{\partial^2 Q}{\partial y^2} = &\frac{1}{2}(1 - v + L_x\frac{\partial v}{\partial x})\left(Q - L_x\frac{\partial Q}{\partial x} + \frac{1}{2}L_x^2\frac{\partial Q^2}{\partial x^2}\right) \\ &+ \frac{1}{2}(1 + v + L_x\frac{\partial v}{\partial x})\left(Q + L_x\frac{\partial Q}{\partial x} + \frac{1}{2}L_x^2\frac{\partial^2 Q}{\partial x^2}\right) \end{aligned} \tag{62}$$

$$L_y\frac{\partial Q}{\partial y} = L_x v\frac{\partial Q}{\partial x} + L_x\frac{\partial v}{\partial x}Q + \frac{L_x^2}{2}\frac{\partial^2 Q}{\partial x^2} \tag{63}$$

$$\frac{\partial Q}{\partial y} = \frac{L_x}{L_y}\frac{\partial}{\partial x}(vQ) + \frac{L_x^2}{2L_y}\frac{\partial^2 Q}{\partial x^2} \tag{64}$$

Assuming that $L_x = L_y(?)$, we find that

$$\frac{\partial Q}{\partial y} = \frac{\partial}{\partial x}(vQ) + D\frac{\partial^2 Q}{\partial x^2} \tag{65}$$

7 Polymer Adsorption Rate

These polymers (particles) in the tube are dragged by the flow. There are two forces competing when a polymer adheres to the surface (1) The drag force on the particle coming from flow, and (2) ionic/VanderWaals or whatever force that tries to adhere the particles to the surface. A particle attaches to the surface if the drag force exerted by the fluid flow around it is smaller than the VanderWaals/ionic force.

This means that for a particle to adhere to the surface needs to be at a distance from the surface such that the drag force is smaller than the Van-der-Waals force (say F_0). If this happens then the polymer with some probability can adhere to the surface and the flow will not drag it away. This means that particles below this critical velocity.

$$v_{\text{cr}} = \frac{F_0}{6\pi\mu d} \tag{66}$$

Now, we know that the velocity profile is as

$$v(r) = \frac{2Q}{\pi R^2}\left(1 - \frac{r^2}{R^2}\right) \tag{67}$$

$$v_{\text{cr}} = \frac{2Q}{\pi R^2}\left(1 - \frac{r_{\text{cr}}^2}{R^2}\right) \tag{68}$$

$$\frac{r_{\text{cr}}^2}{R^2} = 1 - \frac{v_{\text{cr}}\pi R^2}{2Q} \tag{69}$$

We are interested in the rate of volume of fluid passing between r_{cr} and the boundary of the

wall. This becomes

$$\text{volume/time} = \int_{\text{cr}}^{R} \frac{2Q}{\pi R^2}\left(1-\frac{r^2}{R^2}\right)2\pi r dr \tag{70}$$

$$= \left(\int_0^R - \int_0^{r_{\text{cr}}}\right)\frac{2Q}{\pi R^2}\left(1-\frac{r^2}{R^2}\right)2\pi r dr \tag{71}$$

$$= Q - 2Q\frac{r_{\text{cr}}^2}{R^2}\left(1-\frac{r_{\text{cr}}^2}{2R^2}\right) \tag{72}$$

$$= Q - Q\left(1-\frac{v_{\text{cr}}\pi R^2}{2Q}\right)\left(1+\frac{v_{\text{cr}}\pi R^2}{2Q}\right) \tag{73}$$

$$= Q - Q\left(1-\frac{v_{\text{cr}}^2\pi^2 R^4}{4Q^2}\right) \tag{74}$$

$$= Q\left(1-1+\frac{v_{\text{cr}}^2\pi^2 R^4}{4Q^2}\right) \tag{75}$$

$$= \frac{v_{\text{cr}}^2\pi^2 R^4}{4Q} \tag{76}$$

Another easy way to reach to the above calculation is the following The shaded area

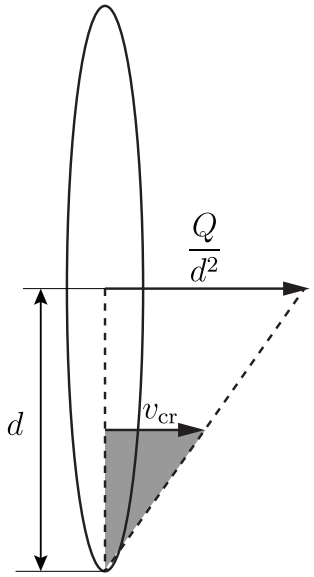

Figure 5: Flow in the pipe

around the tube can be calculated as

$$\text{volume/time} = \frac{1}{2}v_{\text{cr}}\cdot\left(\frac{v_{\text{cr}}}{q/d^2}d\right)2\pi d = \frac{\pi v_{\text{cr}}^2 d^4}{q} \tag{77}$$

which is upto a factor close to what we obtained earlier.

7.1 Modifying the model

For simplicity, let's assume that the force is ionic as $F = K/x^2$. Our model says that

$$6\pi\mu d\frac{2Q}{\pi R^2}\left(1-\frac{r^2}{R^2}\right) \leq \frac{K}{(R-r)^2} \tag{78}$$

$$1-\frac{r^2}{R^2} \leq \left(\frac{K\pi}{12\mu\pi dQ}\right)\frac{1}{(1-r/R)^2} \tag{79}$$

$$1 \leq \frac{r^2}{R^2}+\alpha\frac{1}{(1-r/R)^2} \tag{80}$$

where α is a factor that compares the ionic force and viscous force and it depends on the flux rate. If we define $x = 1 - r/R$ we obtain

$$1 \leq (1-x)^2+\frac{\alpha}{x^2} \tag{81}$$

$$x^2 - x^2(1-x)^2 \leq \alpha \tag{82}$$

$$x^2(1-(1-x)^2) \leq \alpha \tag{83}$$

$$x^3(2-x) \leq \alpha \tag{84}$$

$$\text{if} x \ll 1 \rightarrow x \leq \left(\frac{\alpha}{2}\right)^{1/3} \tag{85}$$

As a result the distance is proportional to $\alpha^{1/3}$. Therefore, we obtain

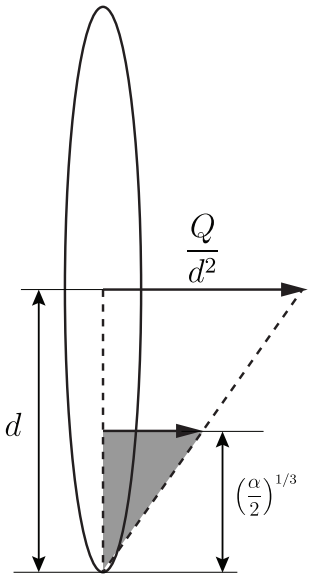

Figure 6: Flow in the pipe

$$\text{volume/time} = \frac{1}{2}\left(\frac{\alpha}{2}\right)^{1/3}\cdot\frac{Q}{d^3}\left(\frac{\alpha}{2}\right)^{1/3}\cdot 2\pi d = \frac{\pi}{2^{2/3}}\frac{Q\alpha^{2/3}}{d^2} \tag{86}$$

Note that in here α scales with $1/Q$.

8 Derivation of Kozeny-Carman Equation

Assuming a proous material we have

$$Q = -k\frac{A}{\mu}\frac{\Delta P}{L} \tag{87}$$

where Q is the flow rate, ΔP is the pressure difference, A is the cross-sectional area, μ is the fluid viscosity, and L is the sample length and k is called permeability.

The Kozney-Carman (KC) assumes that a porous media can be represented by a solid block permeated by parallel cylindrical tubes whose axes may be at an angle to the pressure gradient, so that the length of an individual pipe is larger than that of the block. To relate permeability k to porosity in such idealized porous media we need to relate Q to ΔP. Each cylindrical pipe is circular with radius r. Poisulle flow for a pipe says

$$Q = -\frac{\pi r^4}{8\mu}\frac{\Delta P}{l} \tag{88}$$

where r is the radius of the pipe and l is the length of the pipe. The porosoity ϕ and specific surface area S can be related as

$$\phi = \frac{\pi r^2 l}{AL} = \frac{\pi r^2}{A}\tau \tag{89}$$

where τ is known as tortuosity (ratio of total flow path length to length of the sample). The surface area is then

$$S = \frac{2\pi r l}{AL} = \frac{2\pi r^2 \tau}{A}\frac{1}{r} = \frac{2\phi}{r} \tag{90}$$

Using Poisulle flow in a tube we have

$$Q = -\frac{\pi r^4}{8\mu}\frac{\Delta P}{l} = -\frac{\pi r^4}{8A}\frac{L}{l}\frac{A}{\mu}\frac{\Delta P}{L} \tag{91}$$

As a result the permeability becomes

$$k = \frac{\pi r^4}{8A}\frac{L}{l} = \frac{\pi r^4}{8A\tau} = \frac{1}{8}\frac{\pi r^2 \tau}{A}\frac{1}{\tau^2}r^2 \tag{92}$$

$$= \frac{1}{8}\phi\frac{1}{\tau^2}\left(\frac{2\phi}{S}\right)^2 = \frac{\phi^3}{2S^2\tau^2} \tag{93}$$

where remember that S is the ratio of the total pore surface to the total volume of the porous sample, and τ is turtosity l/L.

Now assume n spherical grains with radius r, the total volume is $n4\pi R^3/3$ and the total surface area is $n4\pi R^2$. These grains occupy $1-\phi$ of the total volume. As a result we have

$$S = \frac{n4\pi R^2}{4/3 \cdot n \cdot \pi R^3/(1-\phi)} = \frac{3(1-\phi)}{R} \tag{94}$$

putting all back into the equation, we obtain

$$k = \frac{\phi^3}{2S^2\tau^2} = \frac{\phi^3 R^2}{2 \cdot 9(1-\phi)^2\tau^2} = \frac{R^2}{18\tau^2}\frac{\phi^3}{(1-\phi)^2} \tag{95}$$

As we can see in the simulations, the radius of the tubes does not change that much. If you make this equivalency for the tubes, we find that

$$S = S \rightarrow \frac{2\phi}{r} = \frac{3(1-\phi)}{R} \tag{96}$$

$$\phi = 0.48, \quad R = 75\mu m \tag{97}$$

$$r = 44\mu m \tag{98}$$

Looking at the voids, we see that the average pore radius in the experiment is only $13\mu m$. How that can be? How can a tube with 3 times the radius represent an average pore size of $13\mu m$. I argue that the void volume should be equal in these two cases.

9 My Model

$$Q_{\text{tube}} = -\frac{\pi r^4}{8\mu}\frac{\Delta P_{\text{tube}}}{l_{\text{tube}}} \tag{99}$$

Fore each tube. In total we know that

$$Q_{\text{tot}} = n\frac{\pi r^4}{8\mu}\frac{\Delta P_{\text{tube}}}{l_{\text{tube}}} \tag{100}$$

where n is the density of the tubes. This density should be proportional to the area divided by the distance between these tubes.

$$Q = \frac{1}{l^2}\frac{\pi r^4}{8}\frac{A}{\mu}\frac{\Delta P}{L} \tag{101}$$

As a result the permeability is

$$k = \frac{\pi r^4}{8l^2} \tag{102}$$

The question now is how to relate this r and l to porosity and radius of packing objects.

$$\phi = \frac{\frac{A}{l^2}\pi r^2 L}{AL} = \frac{\pi r^2}{l^2} \tag{103}$$

As a result

$$k = \frac{l^2}{\pi}\phi^2 \tag{104}$$

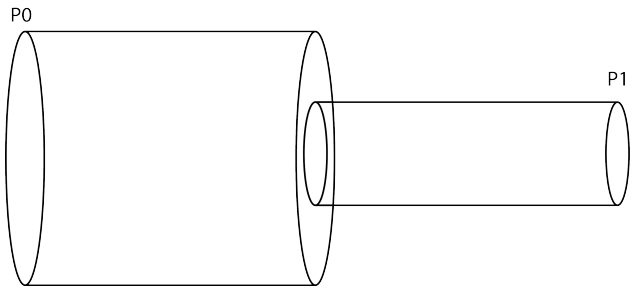

Figure 7: Two pipe model

10 Two pipe model

In order to simplify the calculations, we run the two pipe model. Assume the followig pipe structure The ODE set is

$$P - P_0 = R(d_1)Q \tag{105}$$
$$P_1 - P = R(d_2)Q \tag{106}$$
$$R(d) = \frac{c}{d^4} \tag{107}$$

which results in the following equation

$$P_1 - P_0 = \left(R(d_1) + R(d_2)\right) Q \tag{108}$$
$$\text{set } P_0 = 0 \quad \rightarrow \quad P_1 = \left(R(d_1) + R(d_2)\right) Q \tag{109}$$

11 Numerical Simulation From the paper

11.1 manuscript

We further develop a numerical model to examine the introduced normalization in a random network of tubes and to obtain insights on the dynamics of local pore size changes. It has been shown that at low porosities $\phi < 0.6$, a network of tubes with random diameters correctly captures flow behaviors of a porous medium **?**. We consider a network of tubes with a random distribution of diameters as shown in Fig. **??**b. Assuming Poiseuille flow and solving for conservation of mass at all nodes, the fluid flow velocity in each tube is obtained (see supplementary material for details). Considering different distribution of diameters (uniform, log-normal, or truncated normal) in 2D or 3D, an exponential tail for probability distribution function (PDF) of magnitude of fluid flow is observed which is in agreement with previous studies **?**. We now model a gradual polymer retention in the network of tubes with gradual reduction of tubes' diameters in iterations. We consider different diameter reduction rates: a (i) constant rate, or a rate proportional to the (ii) local flux, (iii) local shear rate, or (iv) local velocity. Among these different cases, we observe that a constant rate or a rate proportional to the local flux behaves similar to the experimental results. The gradual reduction of diameters broadens the PDF of velocity and furthermore

the normalization of interstitial velocity using bulk permeability results in a decent collapse of probability distribution functions. (See Fig. **??**c,d). In addition to the collapse of PDFs, changes in permeability, porosity, and average change of velocity are also consistent with the experimental results (see supplementary material for details). Although the numerical results closely approximate the experimental results, it should be noted that the study here is insufficient to conclude any definite answer for the precise mechanism of diameter reduction.

11.2 supplumentary

We use our approximate numerical model as a proxy to investigate the polymer adsorption rate in the pores. We gradually reduce tubes' diameters through iterations while we monitor changes in the distribution of fluid flow velocity and examine if such changes preserve the scaling law introduced earlier. The rate of tube's diameter reduction δ, which represent the polymer deposition in the pores, can be considered (i) constant ($\delta \propto 1$), (ii) proportional to the flux rate in the tube ($\delta \propto q$), (iii) proportional to shear rate at tube's wall ($\delta \propto q/d^3$), or even (iv) proportional the the velocity in the tube ($\delta \propto q/d^2$). For each process, we pick a uniform distribution of diameters with $\langle d \rangle = 10, \sigma_r = 0.5$ and obtain the flow rates throughout the pipes. We then reduce the tubes diameter $d_{\text{new}} = d_{\text{old}} - \alpha\delta$ where α is a constant chosen such that the normalized average of diameter reduction be 0.2% i.e., $\langle \alpha\delta \rangle / \langle d \rangle = 0.2\%$. After this small diameter reduction, we recalculate the flow in the tubes and reiterate the process. Each iteration is indexed by m and the result for different diameter reduction procedures are shown in Fig. 8 a,c,e,g. In the case of constant diameter reduction or diameter reduction proportional to the local flux, the probability distribution for magnitude of velocity remains exponential and the tail of distribution broadens slowly (see Fig. 8a,c). However, when diameter reduction is proportional to shear rate or velocity, the distribution starts to diverge from an exponential and extreme large values in the tail is observed (see Fig. 8e,g). The results for normalizing the interstitial velocity using permeability values are shown in 8 b,d,f,h for different cases. When the diameter reduction is at a constant rate or proportional to the local flux, the scaling law is conserved (see Fig. 8 b,d); however, when the diameter reduction is proportional to the shear rate or tube's velocity the tail of the probability distribution fails to collapse on a single curve. Based on the above numerical experiments, the dynamics of polymer retention is consistent with the models of diameter reduction either at a constant rate or at a rate proportional to the local flux. We further compare the details of changes where in the experiments we found that the permeability decreases by 60%, while porosity only decreases by 20%, and average velocity increases by 70%. In the case where diameter reduces proportional to the local flux, we find that after $m = 55$ iterations the permeability reduces by 60%, while the porosity decreases by 20% and average velocity increases by 67%; while in the case of constant diameter reduction after $m = 100$ iterations, the permeability reduces by 60%, the porosity decreases by 30%, while the average velocity increases by 50%. As a result, the diameter reduction proportional to the flux rate better matches with the experimental results.

12 Percolation

Percolation theory is about emergent conectivity properties of large number of objects. The objects are extended spatially and the positioning are statistically prescribed.

Definition: A cluster is a group of nearest neighboring occupied sites.

Definition: The cluster number $n_s(p)$ denotes the number of s-clusters per lattice site.

Definition: The percolation threshold p_c is the concentration (occupation probability) p at which an infinite cluster appears for the first time in an infinite lattice.

Definition: If $\Pi(p, L)$ denotes the probability that a lattice of linear size L percolates at concentration L, then

$$\lim_{L\to\infty} \Pi(p, L) = \begin{cases} 0 & \text{if } p < p_c \\ 1 & \text{if } p \geq p_c \end{cases} \tag{110}$$

13 Percolation in 1D

Consider a 1d lattice of size L where each site is occupied with the probability p. Since the probability of occupying the sites are independent, then the probability of all sites being occcupied is

$$\Pi(p, L) = p^L \tag{111}$$

therefore

$$\lim_{p\to\infty} \Pi(p, L) = \lim_{L\to\infty} p^L = \begin{cases} 0 & \text{if } p < 1 \\ 1 & \text{if } p = 1 \end{cases} \tag{112}$$

This implies that $p_c = 1$.

The number of s-clusters can be found as

$$n_s(p) = (1-p)p^s(1-p) \tag{113}$$

This expression can be re-written as

$$\begin{aligned} n_s(p) &= (1-p)p^s(1-p) && (114)\\ &= (1-p)^2 p^s && (115)\\ &= (1-p)^2 \exp(s\log(p)) && (116)\\ &= (p_c - p)^2 \exp(-\frac{s}{s_\zeta}) && (117) \end{aligned}$$

where

$$s_\zeta = -\frac{1}{\log(p)} = -\frac{1}{\log(p_c - (p_c - p))} \tag{118}$$

As a result, when $p \to p_c$, then

$$s_\zeta \to \frac{1}{p_c - p}, \qquad p \to p_c. \tag{119}$$

Therefore the $n_s(p)$ as $p \to p_c$ becomes

$$n_s(p) \to (p_c - p)\exp(-(p_c - p)s) \tag{120}$$

therefore if we plot $s^2 n_s(p)$ versus $s^2(p_c - p)$ all the graphs should collapse on each other if $p \to p_c$.

Definition: The critical exponent $\sigma$is defined as

$$s_\zeta \propto (p_c - p)^{\frac{1}{\sigma}}, \qquad p \to p_c \tag{121}$$

Next, we want to prove that

$$\sum_{s=1}^{\infty} s n_s(p) = p \tag{122}$$

In the LHS, the $sn_s(p)$ is the probability that an arbitrary site belongs to a s-cluster size. If we add these probabilities for all cluster sizes, it should become the probability of the site being occupied. To show this, we have

$$\sum_{s=1}^{\infty} s n_s(p) = \sum_{s=1}^{\infty} s(1-p)^2 p^s \tag{123}$$

$$= \sum_{s=1}^{\infty} (1-p)^2 p \frac{\mathrm{d}}{\mathrm{d}p} p^s \tag{124}$$

$$= (1-p)^2 p \frac{\mathrm{d}}{\mathrm{d}p} \sum_{s=1}^{\infty} p^s \tag{125}$$

$$= (1-p)^2 p \frac{\mathrm{d}}{\mathrm{d}p} \frac{p}{1-p} \tag{126}$$

$$= p. \tag{127}$$

The next question is, how large on average clusters are? At first, we need to see what is the probability of a cluster with size s? We know that the probability of a site belonging to a cluster size s is $sn_s(p)$, and the probability of that point belongs to any cluster size is p. Therefore each point has the probability of $w_s = sn_s(p)/p$ belonging to a cluster size s among all clusters. Therefore

$$w_s = \frac{s n_s(p)}{p} = \frac{s n_s(p)}{\sum_{s=1}^{\infty} s n_s(p)} \tag{128}$$

Now, we can calculate the mean cluster size as

$$S(p) = \sum_{s=1}^{\infty} s w_s(p) = \frac{\sum_{s=1}^{\infty} s^2 n_s(p)}{\sum s n_s(p)} \tag{129}$$

$$= \frac{1}{p}(1-p)^2 (p\frac{\mathrm{d}}{\mathrm{d}p})(p\frac{\mathrm{d}}{\mathrm{d}p}) \sum_{s=1}^{\infty} p^s \tag{130}$$

$$= \frac{1+p}{1-p} \tag{131}$$

Definition: The correlation funtion or pair conectivity $g(r)$ is the probability that a site at position r from an occupied site belongs to the same finite cluster. Note that clearly $g(r=0) = 1$ since the site is already occupied.

In 1D, the correlation function is calculated as

$$g(r) = p \cdot p \cdot \cdots \cdot p = p^r \tag{132}$$

We normally express this in an exponential form and find the critical exponent as

$$g(r) = p^r = \exp(r \log(p)) = \exp(-\frac{r}{\zeta}) \tag{133}$$

$$\zeta = -\frac{1}{\log(p)} = -\frac{1}{\log\left[p_c - (p_c - p)\right]} \to (p_c - p)^{-1}, \quad p \to p_c \tag{134}$$

The value of ζ is known as correlation length which diverges as $p \to p_c$. In 1D, we found that $\zeta = s_\zeta$, where it is not normally true; normally $s_\zeta \propto \zeta^D$ where D is the fractal dimention.

Definition: The critical exponent ν is defined by

$$\zeta \propto |p_c - p|^\nu, \qquad p \to p_c \tag{135}$$

??????? I don't know why, but it is aruged that

$$\sum_r g(r) = S(p) \tag{136}$$

14 Infinite Dimension

Percolation in 1D and infinite dimension can be solved analytically. The infinte dimension is similar to the Beth lattice.

14.1 Beth Lattice

In Beth lattice, each site (vortex) is connected to z neighbors (vortices). As a result each branch (edge) is connected to $z-1$ other branches.

The 1D case that we studied is essentially a Beth lattice with $z = 2$. The next question is why Beth lattice corresponds to $d = \infty$? The reasons are

- (a) The number of surface sites relative to total number of sites approaches a constant as $d \to \infty$.

  The total number of sites in Beth lattice are number of sites from generation 0 plus number of sites in generation 1 added together. Assume we have a Beth lattice with $z = 3$, and we go upto g generations then

$$\begin{aligned} \text{total number of sites} &= 1 + 3 + 3 \cdot 2 + 3 \cdot 2^2 + \cdots + 3 \cdot 2^{g-1} && (137) \\ &= 1 + 3(1 + 2 + 2^2 + 2^3 + \cdots + 2^{g-1}) && (138) \\ &= 1 + 3\frac{2^g - 1}{2 - 1} = 3 \cdot 2^g - 2 && (139) \end{aligned}$$

  while the total number of surface sites (sites at the outer most boundary) are $3 \cdot 2^{g-1}$. Therefore

$$\frac{\text{Number of surface sites}}{\text{Total Num of sites}} = \frac{3 \cdot 2^{g-1}}{3 \cdot 2^g - 2} \to \frac{1}{2}, \qquad g \to \infty \tag{140}$$

  Generally, the numbers are a s

$$\begin{aligned} \text{total number of sites} &= 1 + z(1 + (z-1) + (z-1)^2 + \cdots + (z-1)^{g-1}) && (141) \\ &= 1 + z\frac{(z-1)^g - 1}{z - 2} && (142) \end{aligned}$$

  therefore

$$\begin{aligned} \frac{\text{Number of surface sites}}{\text{Total Num of sites}} &= \frac{z \cdot (z-1)^{g-1}}{1 + z\frac{(z-1)^g - 1}{z-2}} && (143) \\ &= \frac{(z-1)^g + (z-1)^{g-1}}{\frac{z - 2 + (z-1)^{g+1} + (z-1)^g - z}{z-2}} && (144) \\ &\to \frac{(z-2)(z-1)^g}{(z-1)^{g+1}} = \frac{z-2}{z-1} && (145) \end{aligned}$$

  In a hypercube lattice of linear size L when $d \to \infty$, the surface in a d dimension is proportional to L^{d-1} and the volume is proportional to L^d, therefore

$$\text{Surface} \propto \text{Volume}^{\frac{d-1}{d}} = \text{Volume}^{1 - \frac{1}{d}} \tag{146}$$

  therefore as $d \to \infty$, the ration of the surface to volume becomes a constant.

- (b) There are no closed loops in Bethe lattice. In a hypercube lattice the probability of finding a close loop is zero. Assume a d dimension hypercube and a particle centered at a site. There are $2d$ nearest sites that the next particle can be placed. The next particles can be placed at $2d - 1$ positions. Therefore assuming a 4 point lattice, there are $2d(2d-1)^2$ possibilities. If now we want to put these 4 points in a lattice, we have $2d$ for the second particle, $2d - 2$ positions for the third particle and only 1 position for the last particle. Therefore

$$\frac{\text{Number of loops}}{\text{Total number of chains}} = \frac{2d \cdot (2d-2) \cdot 1}{2d(2d-1)^2} \to 0, \qquad d \to \infty \tag{147}$$

For these two reasons, a Bethe lattice is considered as infinite dimension lattice.

Question. What is the occupation probability to make sure an infinite path occurs in a Bethe lattice? Starting from the center, there are $z-1$ neighbors, and assuming an occupation probability of p, we have $p(z-1)$ occupied sites. We need to make sure that at least one occupied site exists, therefore

$$p_c(z-1) = 1 \to p_c = \frac{1}{z-1} \tag{148}$$

Definition: The strength of an infinite cluster $P(p)$ is the probability that an arbitrary site belongs to an infinite cluster.

15 Random Walk

15.1 Random Walk and Diffusion Equation

If at time t the probability distribution is as $p(\mathbf{r}, t)$. Now assume τ time later, we need to integrate over all the space. We have

$$p(\mathbf{r}, t+\tau) = \int p(\mathbf{r}-\mathbf{l}, t) g(\mathbf{l}) \mathrm{d}\mathbf{l} \tag{149}$$

To proceed we do the Taylor expansion, we find that

$$p(\mathbf{r}-\mathbf{l}, t) \approx p(\mathbf{r}, t) - \nabla p \cdot \mathbf{l} + \frac{1}{2} \sum_{ij} \frac{\partial^2 p}{\partial x_i \partial x_j} l_i l_j \tag{150}$$

$$p(\mathbf{r}, t+\tau) = p(\mathbf{r}, t) + \tau \frac{\partial p}{\partial t} \tag{151}$$

Therefore,

$$p(\mathbf{r}, t) + \tau \frac{\partial p}{\partial t} = \int \left[p(\mathbf{r}, t) - \nabla p \cdot \mathbf{l} + \frac{1}{2} \sum_{ij} \frac{\partial^2 p}{\partial x_i \partial x_j} l_i l_j \right] g(\mathbf{l}) \mathrm{d}\mathbf{l} \tag{152}$$

$$p(\mathbf{r}, t) + \tau \frac{\partial p}{\partial t} = p(\mathbf{r}, t) - \nabla p \cdot \int \mathbf{l} g(\mathbf{l}) \mathrm{d}\mathbf{l} + \int \frac{1}{2} \sum_{ij} \frac{\partial^2 p}{\partial x_i \partial x_j} l_i l_j g(\mathbf{l}) \mathrm{d}\mathbf{l} \tag{153}$$

If the diffusion process is isotropic, then there is no difference between $\pm\mathbf{l}$, therefore the second term on the RHS vanishes as

$$\int \mathbf{l} g(\mathbf{l}) \mathrm{d}\mathbf{l} = 0 \tag{154}$$

The relation therfore summarizes to

$$\tau \frac{\partial p}{\partial t} = \frac{1}{2} \int \sum_{ij} \frac{\partial^2 p}{\partial x_i \partial x_j} l_i l_j g(\mathbf{l}) \mathrm{d}\mathbf{l} \tag{155}$$

If we assume that the diffusion is isotropic, i.e., $g(x, y, z) = g(-x, y, z)$ and etc., then only the diagonal terms survive and we obtain

$$\tau \frac{\partial p}{\partial t} = \frac{1}{2} \int \sum_{i} \frac{\partial^2 p}{\partial x_i \partial x_i} l_i^2 g(\mathbf{l}) \mathrm{d}\mathbf{l} \tag{156}$$

$$\tau \frac{\partial p}{\partial t} = \frac{1}{2} \sum_{i} \frac{\partial^2 p}{\partial x_i \partial x_i} \int l_i^2 g(\mathbf{l}) \mathrm{d}\mathbf{l} \tag{157}$$

We furthermore have that

$$\int l_i^2 g(\mathbf{l}) d\mathbf{l} = \frac{1}{3} \int \mathbf{l} \cdot \mathbf{l} g(\mathbf{l}) d\mathbf{l} = < \mathbf{l}^2 > \tag{158}$$

Therefore, we finally obtain

$$\tau \frac{\partial p}{\partial t} = \frac{1}{6} \nabla^2 p < \mathbf{l}^2 > \tag{159}$$

$$\frac{\partial p}{\partial t} = \frac{< \mathbf{l}^2 >}{6\tau} \nabla^2 p \tag{160}$$

where we can summarize the final equation as

$$\frac{\partial p}{\partial \tau} = D \nabla^2 p \tag{161}$$

in which $D = < \mathbf{l}^2 > /6\tau$ is the diffusion constant.

15.2 Normal Diffusion

There are various approaches to the diffusion equation.

15.2.1 Fick's law

Diffusion was pioneered by Fick motivated by a biological application (transport through membranes). By conservation law for total number of particles, he derived the diffusion equtaion for concentration of species as

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \tag{162}$$

The derivation is as follows: Assume we have $N(x)$ particles at position x, and $N(x + \Delta x)$ at position $x + \Delta x$. The cross section area in between these points is A. The question is how

many particles will pass through this cross sectional area. Half of the particles at x move to right and the other half to the left. Same story for the particles at $x + \Delta x$. Therefore the flux of molecules J through the area A during a short time τ is

$$J = \frac{-\frac{1}{2}(N(x + \Delta x) - N(x)}{A\tau} \tag{163}$$

we define concentration $c \equiv N(x)/A\Delta x$, therefore the flux becomes

$$J = -\frac{\Delta x^2}{2\tau}\frac{c(x + \Delta x) - c(x)}{\Delta x} = -D\frac{\partial c}{\partial x} \tag{164}$$

therefore the flux is proportional to the diffusion constant $D \equiv \Delta x^2/2\tau$ and the gradient of concentration. Since the total number of particles are conserved, then

$$\frac{c(t + \Delta t) - c(t)}{\Delta t} = \frac{1}{\Delta t}\frac{(J(x) - J(x + \Delta x))\, A\Delta t}{A\Delta x} = -\frac{J(x + \Delta x) - J(x)}{\Delta x} \tag{165}$$

Therefore the results summarizes to

$$\frac{\partial c}{\partial t} = -\frac{\partial J]}{\partial t}, \qquad J = -D\frac{\partial c}{\partial x} \tag{166}$$

or in one diffusion equation as

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial t^2} \tag{167}$$

Observations:

- The same equation holds for the probability density (PDF) $p(x, t)$ to find a particle at position x and time t
- The PDF of the position of particles starting from a concentrated droplet in an unbounded medium is Gaussian with variance $2Dt$
- It means that the particles mean squared displacement (MSD) in the x-direction grows proportionally with time $< x^2 >= 2Dt$, where the coefficient of this proportionality is twice the diffusion constant D
- The same is true for other coordinates, so the toal MSD grows as $< r^2 >= 2dDt$, where d is the dimension of the space.

15.2.2 Microscopic, molecular approach

Done by Einstein! It is essentially a random walk. It samples particles at discrete istant of time separated by interval τ. How does the known MSD behavior in diffusion emerges from such a model?

Assume the particle is taking steps s_i at each time. The particle's displacement is then given by

$$x(t) = \sum_{1}^{N(t)} s_i \tag{168}$$

where $N(t)$ is the total number of steps performed until time t. From this picture, we get

$$\langle x(t)^2 \rangle = \langle \left(\sum_{1}^{N(t)} s_i \right)^2 \rangle = \langle \sum_{i,j=1}^{N(t)} s_i s_j \rangle = \langle \sum_{i=1}^{N(t)} s_i^2 \rangle + \langle \sum_{i \neq j} s_i s_j \rangle \tag{169}$$

So the MSD is expressable through step correlation function $C_{ij} = \langle s_i s_j \rangle$. Since the steps are assumed to be independent and uncorrelated and symmetrically distributed around zero, the last term vanishes . The mean squared displacement of each step is $\langle s_i^2 \rangle = a^2$, thus

$$\langle x(t)^2 \rangle = \sum_{i=1}^{N(t)} \langle s_i^2 \rangle = N(t) a^2 = \frac{a^2}{\tau} t \tag{170}$$

So the diffusion coefficient becomes as $D = a^2/2\tau$. The term $k \equiv 1/\tau$ is the rate of steps or the mean number of steps per unit time.

15.2.3 Langevin Approach

In this approach, paqrticles are moving in a fluid medium following Newtonian Mechanics and under the influence of esxternal forces and friction! The effect of thermal motion of the molecules and of the surrounding medium are modeled with addisional random force term ("noise"). The equation of motion is then

$$m\dot{v} = -\gamma v + f + \zeta(t) \tag{171}$$

where m is the mass, γ is the friction, and ζ is the random force, and f is the external force. From this equation Langevin was able to derive MSD of the particles.

In order to solve the (171) equation, lets first assume there is no external force and no randomness. Therefore, the equation is dominated by the viscous force and we have

$$m\dot{v} = -\gamma v \tag{172}$$

where the solution is

$$v(t) = \exp(-\gamma t/m) v(0) \tag{173}$$

which means that the velocity vanishes. We know that the average of random particles should become $1/2m\langle v^2 \rangle = 1/2k_B T$, so the particles are not only derived by the viscous term. Lets add the random force, we have

$$m\dot{v} = -\gamma v + \zeta(t) \tag{174}$$

Now that we have $\zeta(t)$ on the right hand side, we assume the solution to have the following form

$$v(t) = e^{-\gamma t/m} b(t) \tag{175}$$

replacing back in the governing equation, we obtian

$$\dot{b}(t) = e^{\gamma t/m} \zeta(t)/m \tag{176}$$

Note that the initial condition for $b(0) = v(0)$. The solution of $b(t)$ becomes as

$$b(t) = v(0) + \int_0^t e^{\gamma s/m} \zeta(s)/m \, \mathrm{d}s \tag{177}$$

putting everything together, the solution becomes as

$$v(t) = e^{-\gamma/mt} v(0) + \int_0^t e^{-\gamma(t-s)/m} \zeta(s)/m \, \mathrm{d}s \tag{178}$$

Now lets calculate the mean squared velocity, we have

$$\langle v(t) \rangle^2 = \langle e^{-2\gamma/mt} v(0)^2 \rangle + 2 \langle e^{-\gamma/mt} v(0) \cdot \int_0^t e^{-\gamma(t-s)/m} \zeta(s)/m \, \mathrm{d}s \rangle + \langle \int_0^t \left(e^{-\gamma(t-s)/m} \zeta(s)/m \, \mathrm{d}s \right)^2 \rangle \tag{179}$$

If we assume that $\langle \zeta \rangle = 0$, and $\langle \zeta(t)\zeta(s) \rangle = 2B\delta(t-s)$, therefore the result become as

$$\begin{aligned}
\langle v(t)^2 \rangle &= \langle e^{-2\gamma/mt} v(0)^2 \rangle + \int_0^t \int_0^t e^{-\gamma(t-s)/m} e^{-\gamma(t-s')/m} \frac{\langle \zeta(s)\zeta(s') \rangle}{m^2} \, \mathrm{d}s \, \mathrm{d}s' && (180) \\
&= \langle e^{-2\gamma/mt} v(0)^2 \rangle + \int_0^t \int_0^t e^{-\gamma(t-s)/m} e^{-\gamma(t-s')/m} \frac{2B\delta(s-s')}{m^2} \, \mathrm{d}s \, \mathrm{d}s' && (181) \\
&= \langle e^{-2\gamma/mt} v(0)^2 \rangle + \int_0^t e^{-2\gamma(t-s)/m} \frac{2B}{m^2} \, \mathrm{d}s && (182) \\
&= e^{-2\gamma/mt} v(0)^2 + \frac{B}{\gamma m} \left(1 - e^{-2\gamma t/m} \right) && (183)
\end{aligned}$$

15.3 1D - Random Walk - Characteristic Function

In 1d random walk we have the following

$$x = \begin{cases} 1, & \text{probability } p \\ -1 & \text{probability } q \end{cases} \tag{184}$$

we define the characteristic function $\lambda(\theta) = \langle e^{i\theta x} \rangle$. Therefore,

$$\lambda = p e^{i\theta} + q e^{-i\theta} \tag{185}$$

We can now find the probability of the object being at jth location after n steps by calculating the coefient of

$$P_n(j) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \left(pe^{i\theta} + qe^{-i\theta}\right)^n e^{-ij\theta}\mathrm{d}\theta \tag{186}$$

which is giving out the coefficient corresponding to the jth position. Noting that

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-i\theta n}\mathrm{d}\theta = \delta_{n,0} \tag{187}$$

one can calculate the above expression. In the case of $p = q = 1/2$, the expression reduces to

$$\lambda(\theta) = \cos(\theta). \rightarrow P_n(j) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \cos\theta^n e^{-ij\theta}\mathrm{d}\theta \tag{188}$$

15.3.1 General case

Assume the random walker picks its displacement per step by a probability density function $p(x)$.

16 Poroelasticity

The coupling between changes in stress and changes in fluid pressure forms the subject of poroelasticity

There are two types of coupling:

- Solid-to-Fluid Coupling: a change in applied stress produces a change in the fluid pressure. The magnitude of this coupling depends on the compressibility of the fluid.
- Fluid-to-solid Coupling: A change in Fluid pressure changes the volume of porous material

Assumptions and terms usually used:

- fluid pressure and pore pressure are usually used interchangeably
- elastic wave propagation due to fluid-solid interaction is also usually ignored
- Poroelastic equations were derived by Biot (**???**)

  A review of Biot's approach is as follows:

  - σ: isotropic applied stress, positive if tensile, negative if compressive
  - V: the bulk volume
  - $\epsilon = \delta V/V$ volumetric strain, positive in expansion, negative in contraction
  - ζ increment in fluid content
  - p fluid pressure

  Constitutive relations are

$$\epsilon = a_{11}\sigma + a_{12}p \tag{189}$$
$$\zeta = a_{21}\sigma + a_{22}p \tag{190}$$

16.1 Mandel Cryer Effect

Model is as follows:

$$\sigma - \sigma_0 = \mathbf{C} : (\epsilon - \epsilon_0) - \alpha p \mathbf{I} \tag{191}$$
$$\rho S \frac{\partial p}{\partial t} + \nabla.(\rho \mathbf{q}) = Q - \rho\alpha \frac{\partial \epsilon_v}{\partial t} \tag{192}$$
$$\mathbf{q} = -\frac{k}{\mu}\nabla p \tag{193}$$

where $\mathbf{C}$ is the stiffness tensor, σ is the stress tensor, ϵ is the strain tensor, ρ is fluid density, k is permeability, μ is fluid viscosity, S is the storage parameter, α is the Biot constant, and ϵ_v is the volumetric strain.

17 Percolation and Structural Mechanics

Assume we have a structure made of soft and hard materials on a 2D lattice (see Fig. 12). The proability of a site being occupied as soft material is p and the probability of the site being occupied with hard material is $1-p$. The question is how does the material property changes for different values of p? Obviously when $p=1$, all the material is made of a soft material with its properties and when $p=0$ the material is made of a hard material and its properties is determined with the hard material.

I would expect that the Elasticity of the 2D material have some sort of transition from soft to hard that depends on the probability p.

18 Elasticity

Under action of a force, solid objects deform. Assuming a point in solid at $\mathbf{x}=(x,y,z)$ will come to $\mathbf{X}=(X,Y,Z)$. The vector $\mathbf{u}=\mathbf{x}-\mathbf{X}$ is then known as displacement field. When the solid is elastic and the displacement is small, the relation ship between stress σ, and the strain tensor ϵ is given by Hooke's law as

$$\sigma_{ij}=\lambda\delta_{ij}\nabla.\mathbf{u}+2\mu\epsilon_{ij}(\mathbf{u}) \tag{194}$$

where the strain tensor is given as

$$\epsilon_{ij}(\mathbf{u})=\frac{1}{2}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right) \tag{195}$$

The parameters λ and μ are two constants (known as Lamé constants) that depend on the material properties.

Question. How does Lamé constants relate to the famous Yong and shear modul of elasticity E,G?

We define $\varepsilon_{ij}=\partial u_i/\partial x_j$. Expanding the relation we had, we see

$$\begin{aligned}\sigma_{11}&=\lambda(\varepsilon_{11}+\varepsilon_{22}+\varepsilon_{33})+\mu\left(\varepsilon_{11}+\varepsilon_{11}\right)\\&=(\lambda+2\mu)\varepsilon_{11}+\lambda\varepsilon_{22}+\lambda\varepsilon_{33}\end{aligned} \tag{196}$$

$$\begin{aligned}\sigma_{12}&=\mu(\varepsilon_{12}+\varepsilon_{21})\\&=2\mu\varepsilon_{12}\end{aligned} \tag{197}$$

On the other hand, by the definition of Yong modulus E and shear modulus G we have

$$\varepsilon_{11}=\frac{1}{E}\left[\sigma_{11}-\nu\left(\sigma_{22}+\sigma_{33}\right)\right] \tag{198}$$

$$\varepsilon_{22}=\frac{1}{E}\left[\sigma_{22}-\nu\left(\sigma_{11}+\sigma_{33}\right)\right] \tag{199}$$

$$\varepsilon_{33}=\frac{1}{E}\left[\sigma_{33}-\nu\left(\sigma_{11}+\sigma_{22}\right)\right] \tag{200}$$

$$\varepsilon_{12}=\frac{\sigma_{12}}{2G},\qquad \varepsilon_{23}=\frac{\sigma_{23}}{2G},\qquad \varepsilon_{13}=\frac{\sigma_{13}}{2G} \tag{201}$$

Comparing these two set of equations, one can find that

$$\mu = G \equiv \frac{E}{2(1+\nu)}, \qquad \lambda = \frac{E\nu}{(1-2\nu)(1+\nu)} \tag{202}$$

19 Equilibrium Equation - Variational Format

The equilibrium equation reads as

$$\frac{\partial \sigma_{ij}}{\partial x_j} + F_i = \ddot{u}_i \rightarrow \frac{\partial \sigma_{ij}}{\partial x_j} + F_i = 0 \tag{203}$$

where the second equation is assuming the static equilibrium. Therefore the equation that we are solving is as

$$\nabla \cdot \sigma + \mathbf{F} = 0 \tag{204}$$

To get the variational form, we multiply both sides by a test function and integrate over a test domain Ω to obtain

$$\int_\Omega (\nabla \cdot \sigma) \cdot \ \mathbf{v} \ \mathrm{d}x + \int_\Omega \mathbf{F} \cdot \mathbf{v} \ \mathrm{d}x = 0 \tag{205}$$

$$\int_{\partial\Omega} (\sigma \mathbf{n}) \cdot \mathbf{v} \ \mathrm{d}s - \int_\Omega \sigma : \nabla \mathbf{v} \ \mathrm{d}x + \int_\Omega \mathbf{F} \cdot \mathbf{v} \ \mathrm{d}x = 0 \tag{206}$$

Note that in the above equations we used the following divergence identity from vector calculus: For an arbitrary domain D, tensor A_{ij} and vector b_i, the following identity holds

$$\int_D (\nabla \cdot \mathbf{A}) \cdot \mathbf{b} \ \mathrm{d}x = \int_{\partial D} (\mathbf{A}\mathbf{n}) \cdot \mathbf{b} \ \mathrm{d}s - \int_D \mathbf{A} : \nabla \mathbf{v} \ \mathrm{d}x \tag{207}$$

where $\mathbf{n}$ is the normal vector to the boundary ∂D and : denotes the double dot product as

$$\mathbf{X} : \mathbf{Y} = \sum_{ij} X_{ij} Y_{ij} \tag{208}$$

and the gradient of the vector defined as

$$(\nabla \mathbf{v})_{ij} = \frac{\partial v_i}{\partial x_j} \tag{209}$$

Now getting back to equation (206), since stress tensor is symmetric we have

$$\int_{\partial\Omega} (\sigma \mathbf{n}) \cdot \mathbf{v} \ \mathrm{d}s - \int_\Omega \sigma : \nabla \mathbf{v} \ \mathrm{d}x + \int_\Omega \mathbf{F} \cdot \mathbf{v} \ \mathrm{d}x = 0 \tag{210}$$

$$\int_{\partial\Omega} (\sigma \mathbf{n}) \cdot \mathbf{v} \ \mathrm{d}s - \int_\Omega \sigma : \frac{1}{2} \left(\nabla \mathbf{v} + \nabla \mathbf{v}^\top \right) \ \mathrm{d}x + \int_\Omega \mathbf{F} \cdot \mathbf{v} \ \mathrm{d}x = 0 \tag{211}$$

$$\int_{\partial\Omega} (\sigma \mathbf{n}) \cdot \mathbf{v} \ \mathrm{d}s - \int_\Omega \sigma : \epsilon(\mathbf{v}) \ \mathrm{d}x + \int_\Omega \mathbf{F} \cdot \mathbf{v} \ \mathrm{d}x = 0 \tag{212}$$

From the previous section we know that

$$\sigma_{ij} = \lambda \delta_{ij} \nabla . \mathbf{u} + 2\mu \epsilon_{ij}(\mathbf{u}) \tag{213}$$

Using the above equation we obtain the following variational form

$$\int_{\partial\Omega} (\sigma \mathbf{n}) \cdot \mathbf{v} \, \mathrm{d}s - \int_{\Omega} \lambda \nabla \cdot \mathbf{u} \nabla \cdot \mathbf{v} \, \mathrm{d}x - \int 2\mu \epsilon(\mathbf{u}) : \epsilon(\mathbf{v}) \, \mathrm{d}x + \int_{\Omega} \mathbf{F} \cdot \mathbf{v} \, \mathrm{d}x = 0 \tag{214}$$

where the first equation is usually handled with the boundary conditions. So, we solve the following variational form equation

$$\int_{\Omega} \lambda \nabla \cdot \mathbf{u} \nabla \cdot \mathbf{v} \, \mathrm{d}x + \int 2\mu \epsilon(\mathbf{u}) : \epsilon(\mathbf{v}) \, \mathrm{d}x - \int_{\Omega} \mathbf{F} \cdot \mathbf{v} \, \mathrm{d}x = 0 \tag{215}$$

$$\text{subject to } \sigma \mathbf{n} = \mathbf{g} \text{ on some boundaries}$$

$$\text{and } \mathbf{u} = \mathbf{u}_0 \text{ on other boundaries} \tag{216}$$

20 Numerical Result

In this section, I implement the finite element code discussed above and test it for various cases.

20.1 Initial Test - Simple tension

The simple geometry is a 2D material in a rectangle shape with size 2×20 (see Fig. 14). The physical constants are

$$E = 10^6, \qquad \nu = 0, \qquad \sigma_0 = 1000 \tag{217}$$

The expected tension at the end of the rod is

$$\delta l = \frac{L\sigma_0}{E} = \frac{20 \times 1000}{10^6} = 0.02 \tag{218}$$

The numerical value I got for the tension at the central point of the material on the right hand side is 0.02.

21 Random Network

Consider the following network of pipes The diameter of each pipe is randomly chosen from a Gaussian distribution. The Darcy law in each pipe reads as

$$\frac{\Delta P}{L} = \frac{128}{\pi} \frac{\mu Q}{d^4} \tag{219}$$

where ΔP is the pressure difference on both sides of the pipe, L is the length of the pipe, μ is viscosity, and d is the diameter of the pipe.

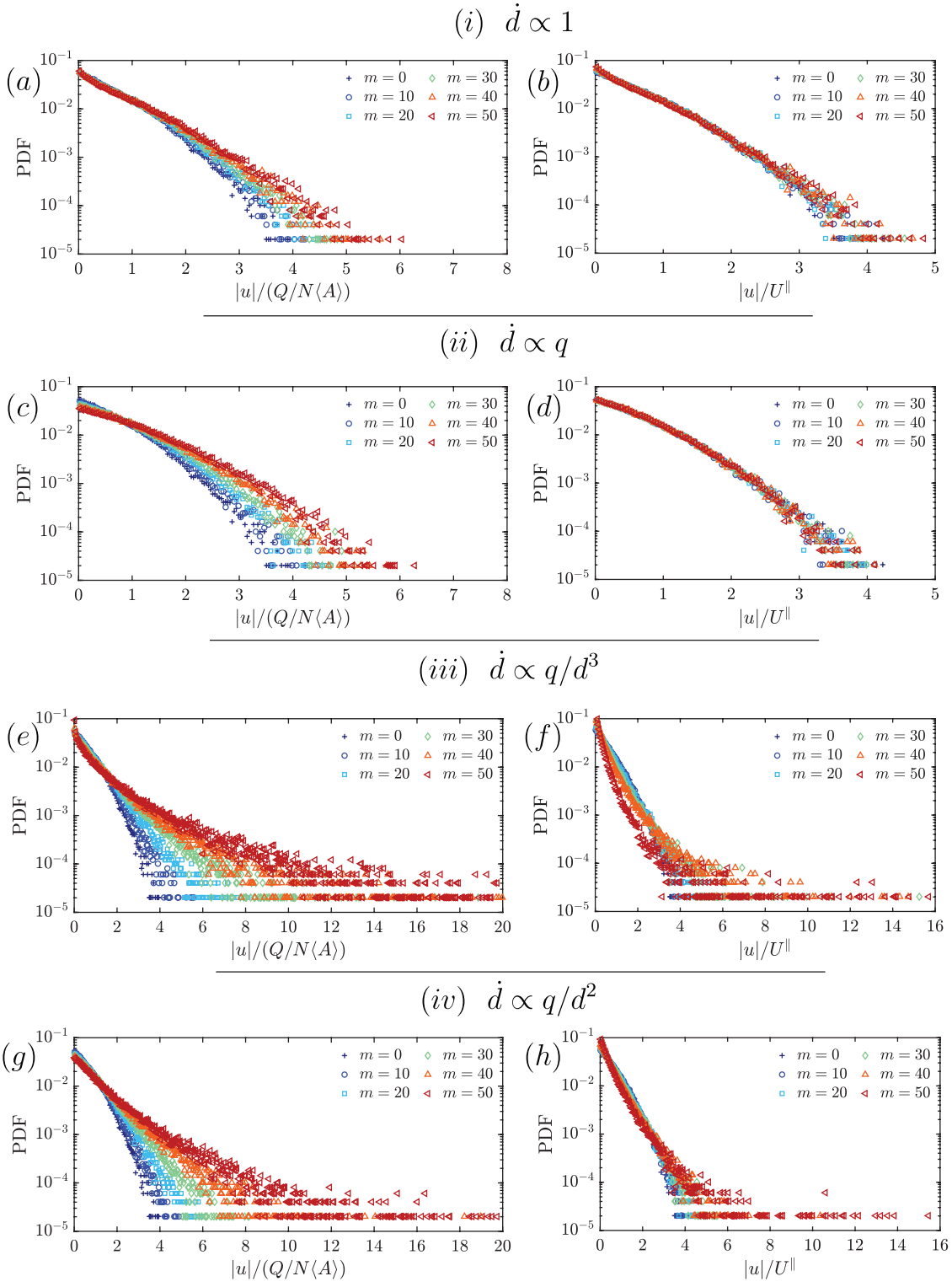

Figure 8: Gradual diameter reduction of tubes (i) at a constant rate, proportional to (ii) the local flux, (iii) local shear rate at the tube's wall, (iv) local velocity. The left figures correspond to gradual changes in probability distribution of magnitude of fluid flow velocity normalized by the interstitial velocity. At each iteration the diameters are reduced as $d_{\text{new}} = d_{\text{old}} - \alpha\delta$ where α is a constant value such that $\langle \alpha d \rangle / \langle d \rangle = 0.02\%$. Iterations are indexed by m. Figures on the right correspond to the collapse of probability distribution curves when normalized by the apparent velocity $U^{\parallel}$ which is calculated using inverse square scaling with the measured permeability.

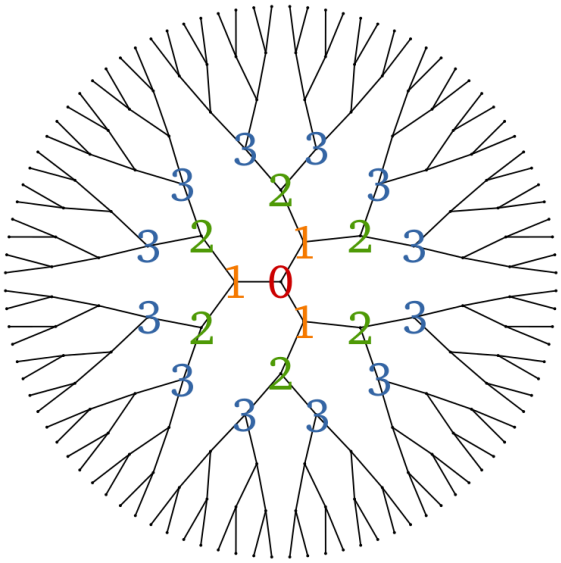

Figure 9: Beth Lattice with $z = 3$. Source: wikipedia

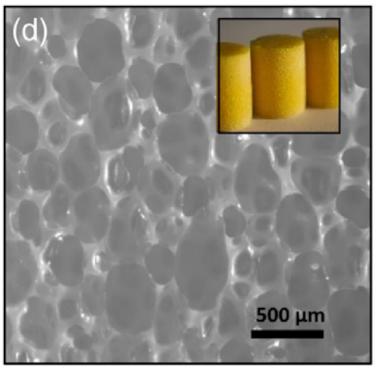

Figure 10: Example of a 2D structure considered for percolation problem, Lahini *et al.*, PRL, 2017

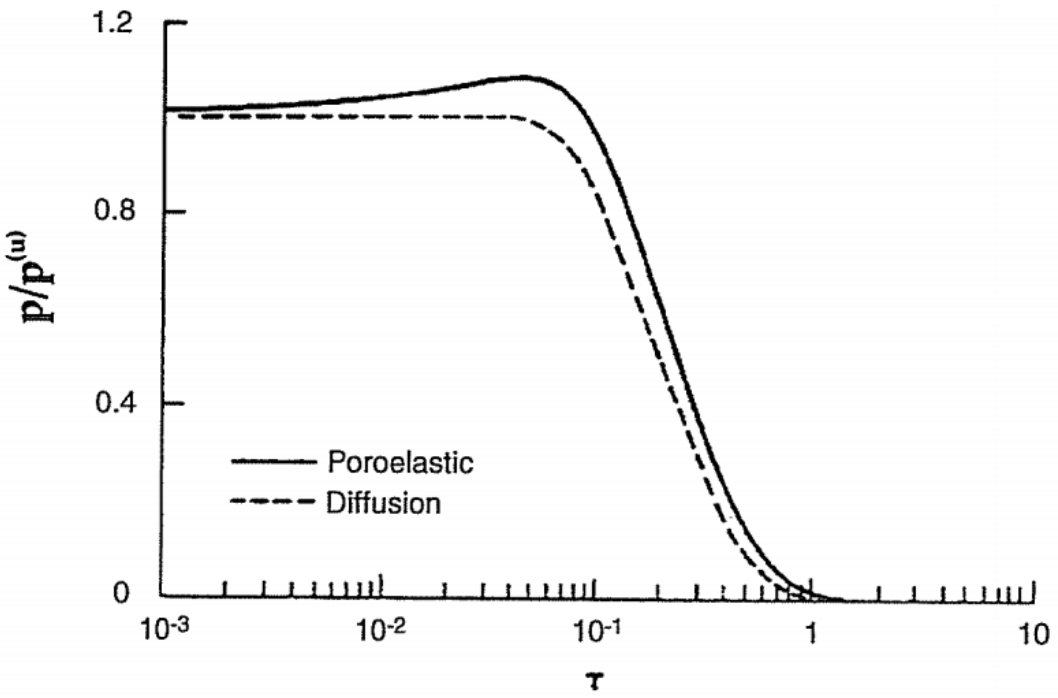

Figure 11: Mandel-Cryer effect. Pore pressure versus time at the center of a poro-elastic cylinder. From p. 196, Herbert Wang, Theory of linear poroelasticity.

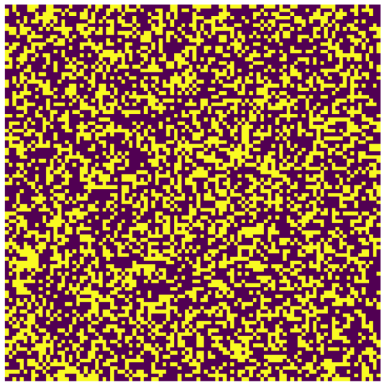

Figure 12: A 2D material with soft (yellow) and hard (black) material next to each other.

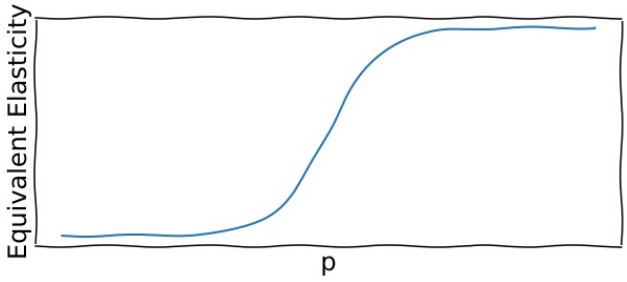

Figure 13: Behavior of elasticity with percolation probability p

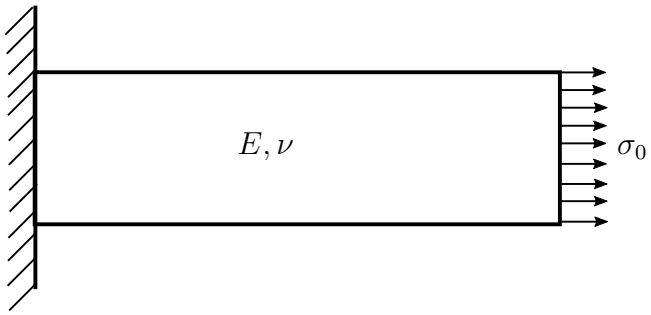

Figure 14: An isotropic material under simple tension

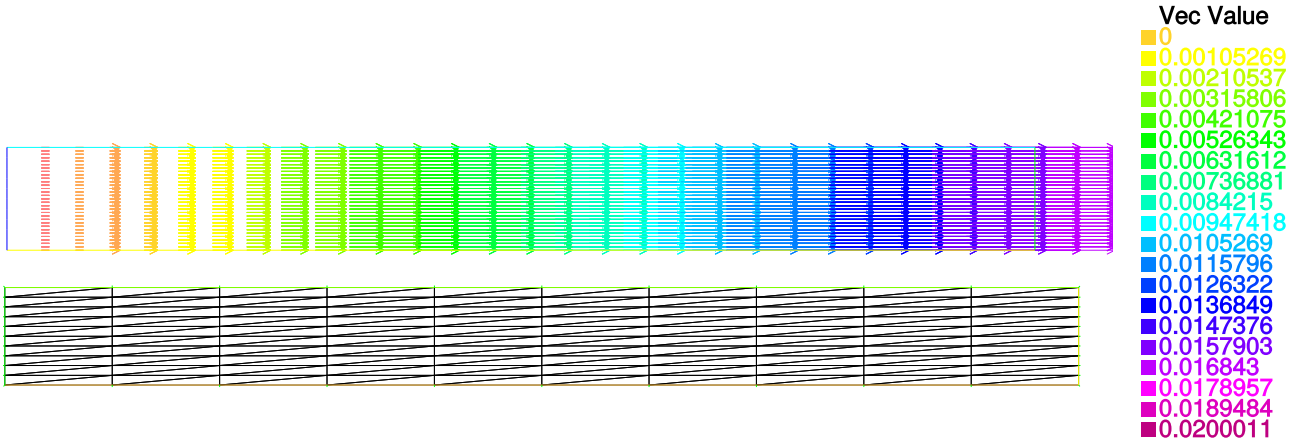

Figure 15: Simulation result of a rod under tension

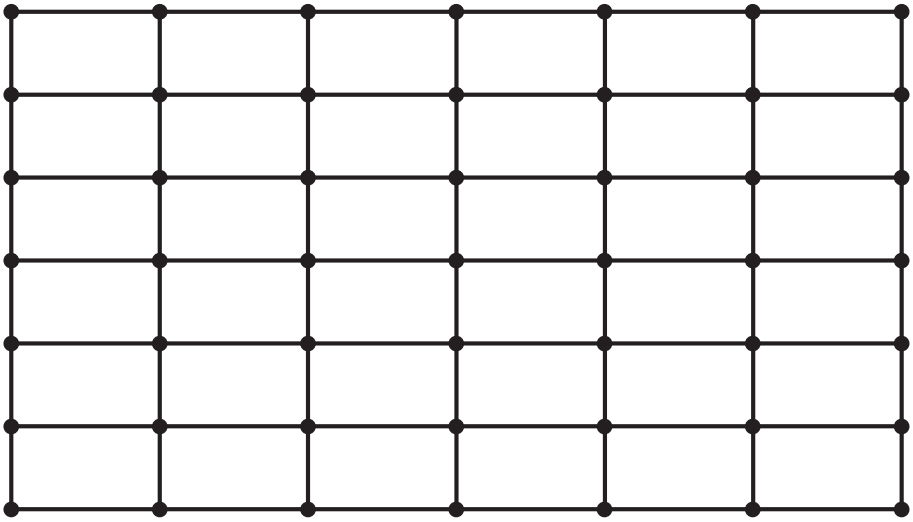

Figure 16: A random grid of pipes