DÉPARTEMENT MFEE
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Toulouse INP – ENSEEIHT

TRANSFERS IN POROUS MEDIA
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Examination – Correction

Exercise 1 : Bio-reactive nutrient transport in a yeast clog 20 points

Darcy flow in the clog

0.5 pt 1. $\Delta P = R_h(t)Q$.

1 pt 2. The previous relation is valid in the clog with a pressure drop through the clog $\Delta P_c < \Delta P$. Flow rate is conserved. As the clog is homogeneous, the Darcy's law writes $V(t) = \frac{\eta}{k}\frac{\Delta P}{L_c(t)}$. Thus, after multiplying by the cross-section Wh we get

$$R_c(t) = \frac{\eta L_c(t)}{kWh}. \tag{1}$$

1.5 pt 3. We have two resistances in series : the clog's one, and the portion of empty channel of length $L - L_c(t)$. The hydraulic resistance of the empty portion of the channel is $Re(L - L_c)/L$. Thus we get :

$$R_h(t) = \frac{\eta L_c(t)}{khW} + R_e\frac{L - L_c(t)}{L}. \tag{2}$$

1 pt 4. The resistance of the empty portion of the channel must be very small compared to the clog's one. That means $\frac{\eta L_c(t)}{khW} \gg R_e\frac{L-L_c(t)}{L}$. This leads to

$$\frac{L_c(t)}{L} \gg \frac{R_e}{\frac{\eta L}{kWh} + R_e} \Leftrightarrow \frac{L_c(t)}{L} > 10\frac{R_e}{\frac{\eta L}{kWh} + R_e}. \tag{3}$$

In the first picture of Figure 1 we can see that $L_c \approx 0.15L$ so this condition is checked. Consequently,

$$R_h(t) \approx \frac{\eta L_c(t)}{khW}. \tag{4}$$

Bio-reactive transport in the clog

0.5 pt 5. $C(y,t) = \langle C_{loc}\rangle^\alpha = \dfrac{1}{V_\alpha}\int_{V_\alpha} C_{loc}(\overrightarrow{r}, t)dV$.

1 pt 6. This is the volume-averaged version of the advection-reaction-dispersion equation, see lecture. Given the data provided and the problem geometry we get

$$\varepsilon\frac{\partial C(y,t)}{\partial t} = \varepsilon\bar{\bar{D}}\Delta C(y,t) + \overrightarrow{V}(t)\cdot\overrightarrow{\text{grad}}C(y,t) + \varepsilon Q_s(C), \tag{5}$$

2 pts 7. We have Taylor-Aris dispersion, leading to an effective diffusion coefficient $D_{eff} = D_m(1 + Pe^2/48)$ where D_m is the bulk diffusion coefficient and Pe the Péclet number. Then we have classical molecular diffusion modulated by the tortuosity with an effective diffusion coefficient $D_m^{eff} = D_m/\tau$ with τ the tortuosity. Finally we have mechanical dispersion which leads to dispersion due to local porous microstructure. The diffusivity tensor can be written

$$\bar{\bar{D}} = \begin{pmatrix} D_{k_\parallel} + D_m^{eff} & 0 & 0 \\ 0 & D_{k_\perp} + D_m^{eff} & 0 \\ 0 & 0 & D_{k_\perp} + D_m^{eff} \end{pmatrix} \tag{6}$$

$$\text{with } \begin{cases} D_{k_\parallel} = \alpha_\parallel ||\langle\overrightarrow{v}\rangle|| \\ D_{k_\perp} = \alpha_\perp ||\langle\overrightarrow{v}\rangle|| \end{cases} \quad \text{Scheidegger(1951)} \tag{7}$$

With :

— $D_m^{eff} = \dfrac{D_m}{\tau}$: molecular diffusivity corrected by **tortuosity**

— α : dispersivity ($\alpha_\perp = \alpha_\parallel = \dfrac{a^2||\langle\overrightarrow{v}\rangle||}{48D_m}$ for non-connected cylinder assembly - only Taylor-Aris)

1 pt 8. We get

$$\varepsilon\frac{\partial C(y,t)}{\partial t} - V(t)\frac{\partial C(y,t)}{\partial y} = -\varepsilon\alpha\mu_{max}\frac{C(y,t)}{C(y,t)+K}Y(y,t). \tag{8}$$

Remind that in our configuration, we consider $V(t)$ as positive with $\overrightarrow{V}(t) = -V(t)\overrightarrow{e_y}$ (flow is leftwards).

Asymptotic behaviours

2 pts 9. We start from

$$\frac{dL_c}{dt} = \int_0^{L_c(t)} \mu_{max}\frac{C(y,t)}{C(y,t)+K}dy. \tag{9}$$

As $C(y,t) \gg K$ we can simplify

$$\frac{dL_c}{dt} = \int_0^{L_c(t)} \mu_{max}dy \Rightarrow \frac{dL_c}{dt} = \mu_{max}L_c(t). \tag{10}$$

By solving this differential equation with initial condition we get

$$L_c(t) = L_{c0}\exp(\mu_{max}t). \tag{11}$$

For $V(t)$ we remind that $V(t)Wh = Q = \Delta P/R_h(t)$. With the expression of $R_h(t)$ then the expression of $L_c(t)$ we just got, we reach

$$V(t) = \frac{k}{\eta L_c(t)}\Delta P = \frac{k\Delta P}{\eta L_{c0}}\exp(-\mu_{max}t). \tag{12}$$

1.5 pt 10. For large t, the clog is separated in two zones : proliferating (L_p) and non proliferating. In the first one we consider that the proliferation rate is maximal, μ_{max} while it is 0 elsewhere. Thus, the clog growth expression can be reduced :

$$\frac{dL_c}{dt} = \int_0^{L_c-L_p} 0dy + \int_{L_c-L_p}^{L_c} \mu_{max}dy = \mu_{max}L_p \Rightarrow L_c(t) = \mu_{max}L_pt + A_1, \quad (13)$$

where A_1 is an integration constant.
For the velocity expression we get

$$V(t) = \frac{k}{\eta L_c(t)}\Delta P = \frac{k\Delta P}{\eta(\mu_{max}L_pt + A_1)}. \quad (14)$$

2 pts 11. We get the following plots (sorry for the notations a bit different).

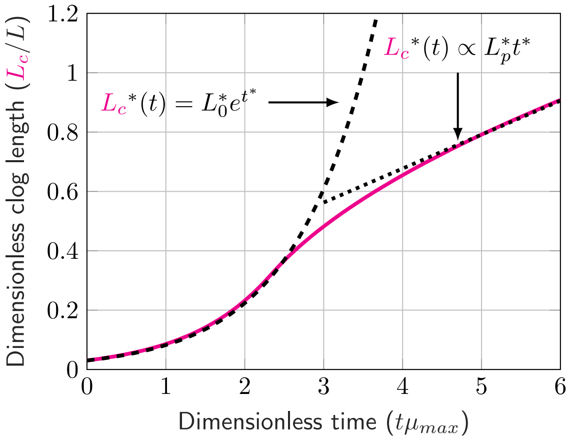

FIGURE 1 – Time evolution of the dimensionless clog length $L_c(t)$.

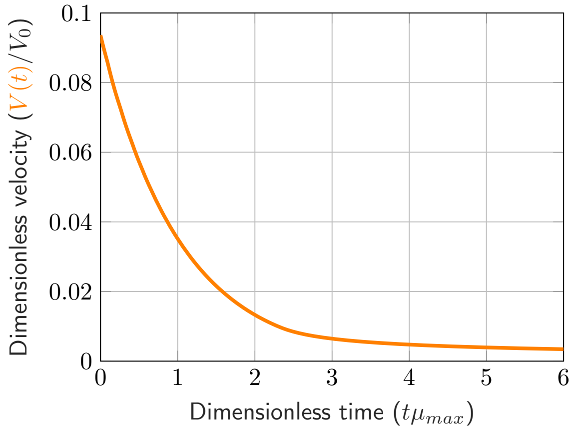

FIGURE 2 – Time evolution of the dimensionless fluid velocity $V(t)$.

Quasi-static resolution

2 pts 12. By separating the variables, we have an equation easy to integrate on y on one hand and C on the other hand. With the boundary condition at $y = L_c$ that leads to :

$$C(y,\tau) - C_{inj} + K\ \ln\left(\frac{C(y,\tau)}{C_{inj}}\right) = -\left[\varepsilon\frac{\alpha\mu_{max}Y_{max}}{V(\tau)}\right](L_c - y) \quad (15)$$

1.5 pt 13. Using the normalizations $\tilde{C} = C/K$ and $\tilde{y} = y/L_c$, we get :

$$\tilde{C} + \ln\tilde{C} = \tilde{C}_{inj} + \ln\tilde{C}_{inj} - \left[\varepsilon\frac{\alpha\mu_{max}Y_{max}L_c(\tau)}{V(\tau)K}\right](1-\tilde{y}). \quad (16)$$

That allows to extract the following Damköhler number

$$Da(\tau) = \left[\varepsilon\frac{\alpha\mu_{max}Y_{max}L_c(\tau)}{KV(\tau)}\right] \approx \varepsilon\frac{\alpha\mu_{max}Y_{max}\eta L_c^2(\tau)}{K\Delta Pk}. \quad (17)$$

1 pt 14. It compares advection through the clog to nutrient consumption in the clog. If $Da \ll 1$, advection dominates; if $Da \gg 1$, consumption dominates. We can see that while L_c rises, Da rises leading to an increase of the influence of nutrient consumption compared to advection.

1.5 pt 15. We observe that the nutrient concentration decreases roughly linearly with the distance from clog surface. When Da increases, the slope is steeper and steeper. A small value for Da implies that the nutrient consumption rate is small or the advection is important. Nutrients travel further through the clog as $Da \to 0$. The nutrient concentration can only remain approximately uniform if the nutrient spread is sufficiently fast and the consumption rate is sufficiently small. In this case we expect an exponential growth rate of the clog.

Exercise 2 : Article analysis — 20 points

Questions

A Generalities about the article

0.25 pt 1. 2021.

0.25 pt 2. Physical Review E.

1.5 pt 3. Authors propose to use numerical lattice-Boltzmann simulations to estimate the permeability to fluid flow of packs of hard spheres of different porosity and polydispersivity. They also want to compare their results to standard models used in literature, such as Kozeny-Carman.

B Introduction and Background

0.5 pt 1. It is the superficial average $\langle u \rangle = \frac{1}{V}\int_{V_\alpha} u dV$.

0.75 pt 2. The other average is the intrinsic one : $\langle u \rangle^\alpha = \frac{1}{V_\alpha}\int_{V_\alpha} u dV$. $\langle u \rangle = \phi \langle u \rangle^\alpha$.

1.5 pt 3. We can base on the slide 10 of the *Upscaling to porous media* course. We have one microscopic, local relationship between a forcing term, a response term and the local media properties. Here it is a Stokes equation coupled to incompressibility. We take volume average on the Representative Elementary Volume (REV), i.e. a volume whose porous structure and averaged physical quantity are uniform. With the appropriate gradient and divergence theorems, we obtain an average of the Stokes and continuity equations, with interfacial integrals which need to be estimated. To do that, we split the control and response variables as a sum of their average on the REV and their fluctuations with respect to this average. We can then obtain a second equation on the fluctuations. Hypotheses of homogeneity of the porous media and separation of the scales (pore, REV, macro) allow to simplify the equations. Then we use a closure relation linking linearly the fluctuations of a field to its average in order to close the system and obtain an equation relating only the means of the forcing and response terms. In the case of fluid flow, a Brinkman correction remains. Using the scale separation, we can neglect it and we get the Darcy's law.

0.25 pt 4. The porous media is homogeneous and isotropic.

0.25 pt 5. Kozeny's constant.

0.5 pt 6. Refs [11] and [12] of the article.

0.5 pt 7. The main limit is due to the Kozeny's coefficient which is not universal. Furthermore C can depend on ϕ.

0.5 pt 8. To cubic lattices (simple, body- and face-centered).

C Methods and sample geometry

C.1 Numerically generated samples

0.5 pt 1. Molecular dynamics approach.

1 pt 2. Polydispersivity is S in the article. If $S = 1$, the packing is made of monodisperse sphere. If $S = 0$, polydispersivity is maximal. S is defined as $S = \frac{\langle R \rangle \langle R \rangle^2}{\langle R \rangle^3}$ where R is the sphere radius. It corresponds to the ratio between the specific surface of a polydisperse system and the one of a monodisperse system of same porosity.

0.5 pt 3. Polydispersity : 0.1-0.99. Porosity : 0.25-0.9.

1 pt 4. Porosity is limiter by random close packing, the minimal porosity packing possible without spheres overlapping. When polydispersivity increases (S decreases), is possible to insert small spheres between large ones, and fill holes. It reduces the porosity, that explains the decrease of accessible porosity at low S in Figure 2(f).

0.75 pt 5. See lecture (exercise 2, chapter 1).

C.2 Numerical simulations

0.25 pt 1. Air.

0.5 pt 2. Klinkenberg effect. Knudsen number.

1 pt 3. The plateaus presented in Figure 3 are the average velocity after multiple iterations and numerical scheme convergence. We observe on both plots that the average velocity decreases with porosity. When polydispersivity increases (S decreases), at a given ϕ, $\langle u \rangle$ increases.

0.25 pt 4. $10^{-8} - 10^{-5}$.

D Results and model analysis

1 pt 1. Figure 5 represents permeability k vs. porosity ϕ for different polydispersivity. When ϕ increases, for a given S, k increases. For a fixed ϕ, k increases when polydispersivity increases.

1.5 pt 2. The permeability decrease when porosity decreases is expected as pore size reduces that limits fluid ability to cross the porous media. That represents a decrease of k. k increases when polydispersivity increases probably due to presence of preferential paths in the porous media.

1.75 pt 3. We have $k_s = \dfrac{2\delta^2}{9(1-\phi)}$. δ is defined as $\delta = \langle R \rangle S$. Kozeny-Carman stands for a monodisperse packing so $S = 1$ and $\langle R \rangle = R$. The normalization of the Kozeny-Carman relation for k by k_s gives the result.

1 pt 4. They want to normalize to get results independent of the average radius of the spheres, in order to get an universal scaling of $k(\phi, S)$.

1.25 pt 5. In Figure 6 we can see that $\bar{k} = f(\phi)$ increases. Data for different S and given ϕ have collapsed. Different models are plotted, including the normalized Kozeny-Carman one. There is a good agreement between data and this model and the data up to $\phi \approx 0.4$. Then there is an increasing discrepancy. So the Kozeny-Carman relation is not a good model to take into account polydispersity in permeability, except for low porosity.

E Discussion and Conclusion

0.5 pt 1. Kozeny-Carman model : $\phi_{rcp} < \phi < 0.38$; cubic lattice packing : $\phi > 0.38$. Thre is a cross-over range $0.35 < \phi < 0.55$.

0.5 pt 2. The percolation model is not a good model to take into account polydispersivity, it's better for overlapping spheres.